Two Types of Protein Salt Bridges Studied by Quantum Calculation

by

Sing Liao

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Abstract

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Two types of protein salt bridges in an aqueous environment, the arginine-acid salt bridge and the lysine-acid salt bridge, are studied here. The former is modeled by propionic acid and ethylguanidine, the latter by propionic acid and propyl amine. Both have been investigated by quantum calculations for the purpose of obtaining improved salt bridge potentials in an aqueous environment with constraints on the distances between the two functional groups, which are defined as the bridge lengths in this report, designed for applications to molecular dynamics simulations of ion channels. For the arginine-acid salt bridge, we perform optimization calculations on 13 molecular clusters corresponding to the salt bridge with 0 to 12 water molecules. For the lysine-acid salt bridge, we perform optimization calculations on 2 molecular clusters for the salt bridge with 0 or 1 water molecule. To each of the model systems, after obtaining its optimized geometry, we slowly vary the bridge lengths and bridge angles in three dimensions, and subsequently we perform COSMO, frequency and NBO calculations on the contracted and expanded model systems. COSMO calculations give the dielectric constant dependence, and the frequency provides the thermodynamic properties of the system while the NBO provides the electronic distributions and bonding information. We found: (1) there is a fill-in mechanism for water molecules to enter into the salt bridge systems; such a fill-in order may have periodicity in energy, as a function of number of water molecules. (2) we show

that the salt bridge systems have both hydrophilic and hydrophobic properties; (3) we look into the proton ionization process from several new aspects in terms of comparison between potentials in two different salt bridge systems and the rates of Wiberg bond order change; (4) we have an in-depth look at effects that can cause large variations to system potentials, and we take note of effects that resulted from environments of limited amounts of local waters and that may have been missed by classical treatments; (5) we look into a new aspect in the applications of Wiberg bond order that are closely associated with the electron density in predicting the formation and disruption of bonding in the systems; (6) in regard to applications to simulations of ion channels, we discuss a possible method to formulate system potentials in specific environments.

Dedication

I would like to dedicate this dissertation to Haiying Chen, my beloved friend, and Siu Ling Liao, my wonderful mom.

Acknowledgments

I would like to say many thanks to my mentor Professor Michael E. Green, who taught me, half of the knowledge for chemists should be chemistry, and the other half may not be chemistry; to Professor John R. Lombardi, who taught me to make physical sense from theoretical calculations; to Professor Marco Ceruso, who taught me to ask questions a step further; to Professor Nicholas D. K. Petraco, who taught me to understand what tools and methods are in use for research; to Professor Ronald L. Birke, who taught me to relate theoretical results with experimental data. And I would like to extend my thinks to Professor Gerald W. Koeppl, our former Executive Officer, who taught us to fight for life professionally; finally, and to all my friends, who taught me not only chemistry but also life.

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Chapter 1

Introduction

Proteins have in most cases a well-determined structure, held in place by several forms of linkages between different segments[1-5]. There are sometimes covalent interactions (as with cysteine-cysteine cross links), but also several forms of non-covalent interactions[6-10], including hydrogen bonds and salt bridges, which are interactions between basic and acidic amino acids. These latter are found in most, perhaps all, proteins, as charged amino acids exist in essentially all proteins and charge-charge interactions are then hard to avoid[11-15]. The positive charges (basic amino acids) are arginine and lysine, with arginine having a high enough pK that it is reasonable to assume it is always charged. Another possible positively charged amino acid is histidine, but its pK is low enough (in solution, about 6) that it is easily switched from charged to uncharged. Lysine has a solution pK near 9. The negatively charged amino acids, aspartate and glutamate, behave essentially as standard carboxylic acids. Our interest has been particularly in one class of protein, ion channels[16-22], which are membrane proteins that control entry and exit of potassium and sodium to cells. To study these, simulations are useful, but the potentials for some of the key non-bonded interactions need to be improved; the standard potentials do not include the interactions with neighbors that affect the electron density in the salt bridges. Currently, for salt bridge systems in aqueous environments, most of the molecular mechanics (MM) potentials have been parameterized in bulk[23-31], rather inadequate when being adapted to situations with a limited amount of water, which includes situations in which there are effects that are usually missed by classical treatments, such as in cases of ion channels.

In this work, two types of salt bridges are studied, with differing amounts of water, which is normally present in limited quantities in those regions of proteins where the charges are found[32-36]. Both types of protein salt bridge are modeled by compounds that do not include the backbone atoms of the amino acids. (1) The arginine-acid salt bridge: propionic acid is appropriate as the model for a carboxylic acid, as it is one. The side chain of arginine is a guanidinium, so ethylguanidine is an excellent model for that. (2) The lysine-acid salt bridge: propionic acid is again used for a carboxylic acid, but for the side chain of lysine, a propyl amine model is considered to be appropriate.

1.1 Protein Salt Bridges

The concept of salt bridge, or ion pairs, or salt bond, has been important and fundamental in understanding the structures, dynamics and functions of proteins. The theory and experimental evidence for opposite charged particle interactions can go far back to Faraday's work[37-38] in the early history of chemistry; molecular calculations have been pioneered in the early half of the last century by Schrödinger, Heisenberg, Born, et al[39-42]. However, massive parallel supercomputing of macromolecular structures, especially with certain specific targeted applications by quantum calculations in protein chemistry, has mainly developed in recent decades[43-49].

Perutz et al[50-54] interpreted the two-state model of the allosteric mechanism of hemoglobin in terms of an equilibrium between two alternative structures, a tense one (T) with low oxygen affinity, constrained by salt-bridges between the C-termini of the four subunits, and a relaxed one (R) lacking these bridges. In their study[55] of the symptoms of Huntington's disease in transgenic mice, Perutz et al reported that several beta-strands

and Alzheimer's amyloid beta-peptide are linked together by a network of salt bridges. Honig, et al[56-57] reported employing a model system with a salt bridge in their research on visual pigments and bacteriorhodopsin by photochemistry. Brown, et al[58] reported that evidence for a salt bridge interaction between the N-terminus and the C-terminus in the basic pancreatic trypsin inhibitor was obtained from the pH titration curves of the terminal amino acid residues determined by ^{1}H and ^{13}C NMR.

Barlow and Thornton[59, 1, 13] proposed a "working definition" for an ion pair based on analysis of the distance distributions for like- and oppositely charged groups of 38 proteins. Ion pairs defined according to this criterion (≤4 Å between charged groups) were analyzed for (1) the frequencies of different pair types, (2) residue separations and secondary structural locations of the residues involved, (3) flexibility of the side chains involved, (4) conformation, (5) environment (accessibility to solvent and proximity to active site or ligand binding regions), and (6) conservation in related proteins. They concluded that on the average, 1/3 of the charged residues in a protein are involved in ion pairs, and 76% of these are concerned with stabilizing the tertiary (rather than the secondary) structure. Only 17% of ion pairs are buried, and conservation of the interactions is generally low unless the residues involved have more specific functions to perform.

Musafia, et al[60] selected 94 proteins from the Protein Data Bank; they defined the term "simple salt bridging" as both non-bonded and hydrogen-bonded paired electrostatic interactions between acidic carboxyl groups and basic amino groups in single or adjacent protein chains, while "complex salt bridges" as those joining more than two charged residues, including Asp, Glu, Lys and Arg, and excluding His. They concluded: (1) the

abundance of complex salt bridges is high; one-third of all residues participating in salt-bridge formation were part of complex salt bridges; (2) the geometry of the interaction between acidic and basic residues is very similar in simple and complex salt bridges. Adding one residue to a simple interaction represents a minor change in the geometry but provides the molecules with a more complex interaction, a phenomenon that may explain the cooperative effect of salt bridges in proteins. Such moderate changes in salt-bridge networks can be generated stepwise and reversibly without trapping the protein in a local energetic minimum; (3) one important role of complex salt bridges is connecting protein subunits or joining two secondary structures to form quaternary structures, where they can connect as many as five secondary structure units; (4) arginine serves as a key connector and/or a branching unit because its geometry allows three possible directions of interactions. Madern, et al[61] in their study of the folding intermediates of a mutant of the LDH-like MalDH (L-lactate dehydrogenases (LDH) and MalDH belong to the same family of NAD-dependent enzymes), by using crystallographic analysis, suggested that it consisted of a tetramer made up of two dimers interacting mainly via complex salt bridge clusters. Gvritishvili, et al[62] reported their work on the cooperativity of the complex salt bridges.

Probing the salt bridge in the dihydrofolate reductase-methotrexate complex by using the coordinate-coupled free-energy perturbation method, Singh[63] suggested that the ion-pair contribution to the binding energy is insignificant, as the enzyme surroundings do not stabilize the salt bridge to the extent of the desolvation of the charged groups. Dao-Pin, et al[64] studied the structural and thermodynamic consequences of burying a charged residue within the hydrophobic core of T4 lysozyme, and they found that the stabilizing and

destabilizing effects are pH dependent. Phelan, et al[65] reported that the interhelical salt bridges destabilize a leucine zipper that was designed for maximizing ion pairing between helices, which they previously thought to have stabilizing effect. Rezac, et al[66], using both methods of DFT/COSMO with the CCSD(T) complete basis set and Amber empirical potential function with the generalized Born model, have calculated the Glu-Lys salt bridge in protein and in water environment, and found that the environment affects the stabilization energy of the salt bridge dramatically: the protein reduces the energy to less than one half of the original value, whereas water sometimes changes stabilization to destabilization. In the study of the Amino-terminal domain interactions of λ integrase on “arm-type” DNA, Lee[67] reported that the homomeric interaction between neighboring amino-terminal domains of integrase protein is contributed by R30-D71 salt-bridge in a non-equivalent manner on Holliday-junction intermediates, and both the R30 and D71 residues were investigated in regard to the cooperative binding of integrase protein to "arm-type" DNA and the attenuating function of "arm-type" DNA, from which the results suggest the electrostatic interaction between residues 30 and 71 is dependent on "arm-type" DNA and contributes the "selective" inhibition of catalytic activity of λ integrase. Horavitz, et al[68] proposed that many of the interactions that stabilize proteins are co-operative and cannot be reduced to a sum of pairwise interactions; such interactions may be analyzed by protein engineering methods using multiple thermodynamic cycles comprising wild-type protein and all combinations of mutants in the interacting residues. They suggested that the coupling of salt bridges could be of general importance to the stability and function of proteins.

Kumar and Nussinov[69] reported the results of continuum electrostatic calculations on a data set of 222 non-equivalent salt bridges derived from 36 non-homologous high resolution monomeric protein crystal structures. To ensure the selection of salt bridges with “good" geometries in their database, the salt bridge formation is inferred for a pair of oppositely charged residues (Asp or Glu with Arg, Lys or His) that meets the following criteria: (i) The centroids of the side-chain charged groups in oppositely charged residues lie within 4.0 A of each other; and (ii) at least one pair of Asp or Glu side-chain carboxyl oxygen atoms and side-chain nitrogen atoms of Arg, Lys or His are within a 4.0 A distance. They concluded that most of the salt bridges in their dataset are stabilizing, regardless of whether they are buried or exposed, isolated or networked, hydrogen bonded or non-hydrogen bonded. They suggested that a major finding of their work is that salt bridge geometry is a critical factor in determining salt bridge stability. In their other study[70] on the relationship between ion pair geometries and electrostatic strengths in proteins, they suggested that the electrostatic free energy contribution of an ion pair in a protein depends on two factors, geometrical orientation of the side-chain charged groups with respect to each other and the structural context of the ion pair in the protein. Kumar and Nussinov[71-74] have also reported their studies on salt bridges in various testing conditions, such as long range effects, short range effects, cold and heat effects, and individual and network effects. Waldburger, et al[75] reported their protein stability study between buried salt bridges and hydrophobic interactions, and similar studies have also been reported by Sindelar, et al[71].

In the review by Bosshard, et al[77-79, 5], they suggested that the net electrostatic free energy of a salt bridge can be partitioned into three components: (1) charge-charge interactions;

(2) interactions of charges with permanent dipoles; (3) desolvation of charges. Energetically favorable Coulombic charge-charge interaction is opposed by often unfavorable desolvation of interacting charges. As a consequence, salt bridges may destabilize the structure of the folded protein. They further pointed out that there are two ways to estimate the free energy contribution of salt bridges by experiment: the pKa approach and the mutation approach. In the pKa approach, the contribution of charges to the free energy of unfolding of a protein is obtained from the change of pKa of ionizable groups caused by altered electrostatic interactions upon folding of the protein. The pKa approach provides the relative free energy gained or lost when ionizable groups are being charged. In the mutation approach, the coupling free energy between interacting charges is obtained from a double mutant cycle. The coupling free energy is an indirect and approximate measure of the free energy of charge-charge interaction. Neither the pKa approach nor the mutation approach can provide the net free energy of a salt bridge. Bosshard, et al concluded that currently, this is obtained only by computational methods which, however, are often prone to large uncertainties due to simplifying assumptions and insufficient structural information on which calculations are based.

1.2 Thermostability of salt bridge structures

Among other important aspects of charge-charge interactions, probably the ionic character or non-covalent interactions of salt bridge systems may create thermostability; that is, the existence of salt bridge systems usually can improve protein stability at high temperature. Ge, et al[80], have studied the effect of temperature on the salt bridges in a hyperthermophilic protein, and they gave further support to the theoretical prediction that

salt bridges are resistant to temperature increase and thus are specially suited to improving protein stability at high temperature. Folch, et al[81] have studied the thermostability of salt bridges versus hydrophobic interactions in proteins, and they found, in general, a preference for more-compact salt bridges was noticeable in heat-resistant proteins.

1.3 Functioning of salt bridges

Salt bridges are ubiquitous in biological systems, responsible for various structural formations and multifarious chemical and dynamical activities. The concept of interactions of ion pairs is not only one of the basic but also rather complex tools used in daily biological research. Recent research involving salt bridge systems is extremely active as can be seen by a large body of published literature.

Fang, et al[82] studied the role of residue K97 at the C-terminal end of archaeal [P62A]Ssh10b (Ssh10b, a member of Sac10b superfamily, is a dimeric protein isolated from hyperthermophilic archaea sulfolobus shibatae; Ssh10b is a homodimeric protein having two conformations due to the cis–trans isomerization of the L61-P62 peptide bond in solution, while a P62A-mutant Ssh10b ([P62A]Ssh10b) has only a trans-form conformation.) in the hyperthermostability of the protein by using three K97-mutant variants: K97E-, K97A-, and ΔK97-mutant [P62A]Ssh10b, and they found that the K97E mutation leads to a stronger destabilization effect than the K97A mutation by disturbing the electrostatic interaction of the salt-bridge D63-K97 and drawing an unfavorable charge-charge repulsive interaction into the structure. Imai, et al[83], in their research on the functioning of α4 integrin, have demonstrated that the membrane-proximal salt bridge

plays a critical role in supporting proper α4 integrin adhesive dynamics. Mahalingam, et al[84], in their research on the activation of the G protein-coupled receptor (GPCR) rhodopsin, have demonstrated that the process is initiated by light-induced isomerization of the retinal ligand, in which one of the key steps is the disruption of an interhelical salt bridge by internal proton transfer. Dey, et al[85] have studied the dimerization interfaces on PKR and GCN2, and they suggested that a key feature of the PKR dimerization interface is a salt bridge interaction between Arg262 from one protomer and Asp266 from the second protomer. Barouch-Bentov, et al[86] have studied the functions of Src family and Abl protein tyrosine kinases, and they pointed out the physiological importance of the conserved G loop salt bridge. Roy and Case[87] reported the optimal positioning of salt-bridging interactions in a parallel α-helical homotrimeric coiled coil in a metal ion-assembled polypeptide trimer of 60 residues, and Fratev, et al[88] reported that a unique salt bridge network formed mainly by the catalytic residues was identified in the unbounded B-RAFs. Mamonova, et al[89] has studied the molecular structure and dynamics of the glutamate receptor ligand binding domain (GluR2 S1S2) in facilitating its conformational transition, and they found that the presence of the E705-K730 salt bridge seems to correlate strongly with the cleft opening transition. Aktas, et al[90], in their study of the role of residues in the adenosine binding site of NAD of the Ascaris suum malic enzyme, suggested that the salt bridge between D361 and R370 is important for maintaining the productive conformation of the NAD binding site. He, et al[91] reported that the conservation of salt bridge between the N- and C-terminal heptad repeat regions of the human immunodeficiency virus type 1 gp41 core structure is critical for virus entry and inhibition. Kawamura, et al[92] has studied the crystal structures of P. horikoshii MPGP

(PhoMPGP) in the holo-form and in the apo-form by the multiple-wavelength anomalous diffraction (MAD) method using SeMet-substituted PhoMPGP, and they reported that a salt bridge from the general acid/base Asp-10 to Arg-170 was observed in the holo-form PhoMPGP which was not present in the open form. Rajabi, et al[93] demonstrated that the conserved salt bridge in human α-defensin 5 is required for its precursor processing and proteolytic stability. Reyes-Lopez, et al[94] reported that the conserved salt bridge linking two C-terminal β/α units in homodimeric triosephosphate isomerase determines the folding rate of the monomer. Rodius, et al[95] showed that the talin rod IBS2 α-helix interacts with the β3 integrin cytoplasmic tail membrane-proximal helix by establishing charge complementary salt bridges.

Salt bridge systems are parts of biological components. It is almost impossible to define what specific roles that salt bridge systems may play in biological systems. Probably, functioning of salt bridges, includes charge-charge interactions between salt bridges and between salt bridges and other charged particles, formations and disruptions of salt bridges, conservation of salt bridges, loop formations and loop disruptions of salt bridge networks. Quantum mechanical aspects of salt bridge systems are even more complex, which we attempt to explore in this report.

1.4 Discovery of salt bridge structures

Evidence for salt bridge systems existing in various chemical and biological environments is discovered routinely; their importance continues to increase as they are found to have functional significance. In addition, their presence is noted by a range of evidence, in an increasing number of systems.

Using NMR, Tomlinson, et al[96] have studied the structure of the B1 domain in protein G, they found, of six lysine residues, three consistently form surface-exposed salt bridges in the crystal structure. Robinson, et al[97], in a study on the mechanism of transport by mitochondrial carriers by symmetry analysis, suggested that system residues in three [FY][DE]XX[RK] motifs are on the cytoplasmic side of the cavity and form a salt bridge network when the substrate-binding site is accessible from the mitochondrial matrix. From the new NMR structure of the Pdx-CYP101 complex, Zhang, et al[98] found new evidence to support the formation of a salt bridge between Asp38 of Pdx and Arg112 of CYP101. Wong, et al[99] reported the hot-spot residues at the E9/Im9 interface help binding via different mechanisms, and they also noted that Im9 Ser50 restricts Glu41 in a conformation appropriate for salt-bridge formation across the interface. Essen, et al[100] reported, in their structural study of a complete phytochrome sensory module in the Pr ground state, that a unique feature of the phytochrome structure is a long, tongue-like protrusion from the PHY domain that seals the chromophore pocket and stabilizes the photoactivated far-red-absorbing state (Pfr); the tongue carries a conserved PRxSF motif, from which an arginine finger points into the chromophore pocket close to ring D forming a salt bridge with a conserved aspartate residue.

1.5 Salt bridges of ion channels

For our own interest, we have paid particular attentions to salt bridge systems in one type of proteins, ion channels. In our previous work, Green, et al[101-107] in their study of KcsA channel gating, have analyzed the structure near and at the center of the pore when it gates. They pointed out that the KcsA channel, where the structure is clearer than the

K_v1.2 channel at the relevant residues, has several hydrogen bonding residues there: the most important are a glutamate, a glutamine, and an arginine, as these point toward each other. Other nearby residues include one glutamate and two arginines, but the latter point away from the center of the pore; perhaps they are salt bridges. In a review article, Green[44] also suggested that water can play a role in certain complexes, such as those between phosphate and arginine, as well as in modifying salt bridges in proteins.

Jiang, et al[108], in their structural study of the RCK domain from the E. coli K^+ channel, reported that the RCK domain (In MthK, a K+ channel from Methanobacterium thermoautotrophicum, the structure contains a C-terminal cytosolic ligand-binding domain homologous to eukaryotic NAD binding domains, but named RCK for their role in Regulation of Conductance for K^+) has a Rossmann-fold topology with unique positions (The Rossmann fold is a protein structural motif found in proteins that bind nucleotides, especially the cofactor NAD. The structure is composed of three or more parallel beta strands linked by two alpha helices in the topological order beta-alpha-beta-alpha-beta[109].), not commonly conserved among Rossmann-fold proteins, comprising a well-conserved salt bridge and a hydrophobic dimer interface. Using structure-based amino acid sequence alignments and mutational analysis, they further demonstrated that an RCK domain is also present and is an important component of the gating machinery in eukaryotic large-conductance Ca^{2+}-activated K^+ channels.

Treptow, et al[110], in their Molecular Dynamics (MD) study on the initial response of the potassium channel voltage sensor to a transmembrane potential, suggested that the gating charge (-2e) associated with the fast transition results mainly from salt bridge

rearrangements involving negative charges in segments S2 and S3 and all but the two top residues (R294 and R297) of S4.

Perozo, et al[111], in their study of Shaker K channels, reported that the S4 sequence of Shaker K channels comprises at least part of the voltage sensor to explain the effects of the mutation R368Q; R368 was hypothesized to be part of a salt bridge that is broken early in activation, and then subsequently, the S4 segment undergoes a conformational change. After a final, relatively voltage-independent step, the channel opens.

Based on Brownian dynamics and Poisson-Nernst-Plank electrodiffusion theories, Noskov, et al[112] have calculated the ion permeation through the α-hemolysin channel; they noted that the major determinant of the asymmetry is unbalanced charge in the triad of polar residues D127, D128, and K131, and the weak anionic selectivity of the channel results from the presence of the salt bridge between E111 and K147 in the constriction zone.

Hong, et al[113] in their study of the gating of OmpA ion channel noted that the gate of the OmpA channel is formed by the central Glu52-Arg138 salt bridge, which can open to form alternate ion pairs with Lys82 and Glu128. Craven, et al[114], in a study of the C-terminal movement during gating in cyclic nucleotide-modulated channels, hypothesized the primary intersubunit interface of these C termini includes two salt bridges per subunit. They concluded the existence of the salt bridges is largely responsible for the gating mechanisms of HCN2 and CNGA1 channels. Venkatachalan, et al[115] reported that a conserved salt bridge formed βE153 and βK196 is critical for GABAA receptor function and loop C dynamics. Wang, et al[116], in their study on the gating of γ-Aminobutyric acid type A (GABAA) receptors, have identified an ion pair interaction between two

conserved charged residues, Glu92 in loop 2 and Arg258 in the pre-M1 region. They found that several other charged residues at the gating interface are not critical to receptor function and they concluded that it is the global charge pattern of the gating interface that controls receptor function in the Cys-loop super family.

In a review article on theoretical and computational models of biological ion channels, Roux, et al[117] stated, "But even then, the basic elements discussed in sections 2–5 will continue to provide a fundamental conceptual framework to rigorously 'translate' the properties of the atomic level into the language of simple phenomenological permeation models (In Roux's article, Section 2: Dynamics of many-body systems; Section 3: Solvation free energy and electrostatics; Section 4: Statistical mechanical equilibrium theory; Section 5: From MD to I–V: a practical guide)." Roux's remark, as a whole, should be a fair observation to the current development in computational modeling of ion channels that will in the near future, in a way as yet not conceived of, bring profound practical values into exploring such complex biological structures.

1.6 Previous work on the salt bridges of guanidinium group and carboxyl group

We have examined other previous studies that are closely related to the two salt bridge models in this report. Sapse and Russell[118], using methods at the relatively low levels of HF/6-31G and HF/STO-4G, have calculated the interaction in gas phase between guanidinium and methylguanidinium ion with the carboxylate group of formate, and they reported binding energies and optimum geometries. Barril, et al[119], using HF/ 6-31G(d) for optimization calculation and MP2/6-31+G(d) for single point calculation, have calculated the stability of a salt bridge formed by acetate and methylguanidinium ions in

the gas phase, in solutions (water and chloroform), and in the interior of proteins, in which their study has been mainly focused on the interaction between acetate and methylguanidinium ions. They found that the high anisotropy of proteins and the local microenvironment in the interior of proteins make a decisive contribution in modulating the energetics of the salt bridge. Feng, et al[120] by a relatively high level methods of B3LYP/6-311G(d,p)//PM3 have calculated the salt bridge structure of arginine-carboxylate in gas phase and in an α-cyclodextrin cavity. They reported that the neutral forms are more stable than the zwitterionic counterparts in gas phase, while the zwitterionic forms become more stable than the corresponding neutral ones when in a α-cyclodextrin cavity. Zheng, et al[121] , at the method levels of RHF/6-31G*, RHF/6-311+G**, MP2/6-31G*, and MP2/6-311+G** further investigated the salt-bridge modeled by formate and guanidinium ions in gas phase, in water, in chloroform, and in DMSO, with the main focus on comparing the stability between the zwitterionic forms and neutral forms. Similar studies have been reported by Fournier, et al[122], and the three dimensional network of ion pairs of methylguanidinium formate, have also been studied by Bray, et al[123]. With guanidinium group and carboxyl residues in protein structures, semi-empirical calculation methods had been employed in earlier work, for example, Singh, et al[124]calculated the geometries of the interacting arginine-carboxyls in 37 high resolution protein structures.

With more than 700 research papers containing the concept of protein salt bridges in our literature search, it is unrealistic for us to list them all in this report, but only to include as many as possible of the most recent ones, especially the ones we consider can bring in valuable ideas relevant to our own interest.

As can be seen, salt bridge systems have very complex structural, functional and dynamic aspects, subject to their specific environments. Although a few general concepts for salt bridge systems have been developed, such as interactions of ion pairs, thermostability of salt bridge systems, stabilizing and destabilizing effects, networking and cooperativity effects, it seems, however, case to case study should be warranted to justify the specific individual system. Currently, most of the MM potentials used in Molecular Dynamics (MD) simulation or Monte Carlo (MC) methods have been calibrated in bulk, quite often, having rather poor accuracy when being adapted into certain specific environments, such as in simulations of ion channels.

1.7 Our approach to obtaining the salt bridge potentials

Subject to computational limitations, quantum calculations are only possible with a relatively small number of atoms that can be done by DFT (Density Functional Theory) or other high level quantum methods. MD and MC, or other semi-empirical molecular mechanic methods are capable of handling systems with larger numbers of molecules, but their accuracy is limited by the current MM potentials used and show uncertain effects that may be missed by classical treatments. The motivation for this work is that we can investigate a relatively small system in several targeted conditions by quantum calculations to learn about certain effects that may be missed by classical treatments in a specific environment and to get the improved potentials for use with further work in MD simulations.

We investigate two types of salt bridge models in aqueous environments, one formed by propionic acid and ethylguanidine and the other by propionic acid and propyl amine. The

former model is the focus in this report and its study is relatively thorough; the latter is mainly for reference and comparison.

We start by performing optimization calculations on the salt bridge models to obtain the geometries that can reasonably represent the geometries of a real system. With targeted applications to ion channels, we expand the salt bridge systems in three dimensional spaces on certain constraint conditions, in which we can have an in-depth study on the structures and effects that are directly related to the system potentials. Also, we do COSMO, frequency and NBO calculations[125-130] to learn about solvation effects, thermodynamic data, charge distributions and bonding information in the salt bridge systems.

Chapter 2
Optimized Geometry

Methods

There are 13 molecular clusters to be optimized[131-137]. Gaussian 03, on a local computer, is used for the salt bridges with 0 up to 4 water molecules, while the remote supercomputer, using NWChem, is for the salt bridges with 5 to 12 water molecules. Spherical coordinates are used in both Gaussian 03 and NWChem. Results run by both Gaussian 03 and NWChem at the level of B3LYP/6-311++G** are compared. In most of our cases, the results from NWChem are consistently lower than those from Gaussian03, and the discrepancies are within 0.5 k_BT; the largest discrepancy in our testing cases is 0.7 k_BT, and the average is within 0.5 k_BT. From here on, when energy is given in units of k_BT, T = 298 K is intended in all cases. This corresponds to 0.000944 au.

All of the 13 molecular clusters are initially optimized at a low level method, HF/3-21G*, and subsequently, are further optimized at the level of B3LYP/6-311++G**.

We perform optimization calculations on all possible initial structures that conceivably are appropriate for leading to the geometry of the lowest energy, but we do not prove that the lowest minimum we find is the true global minimum, although we have no reason to doubt that it is. We also perform frequency calculations on each of the 13 molecular clusters, and we notice that there is no imaginary frequency in any case, so that we are not at a saddle point.

Results and Discussion

From Figure-2-1 to Figure-2-13, the 13 optimized geometries calculated by B3LYP/6-311++G** are displayed.

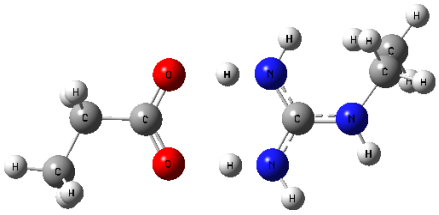


Figure-2-1: Salt bridge formed by a propionic acid and an ethylguanidine with zero water molecules; optimized by B3LYP/6-311++G**, C = carbon atom; H = hydrogen atom; O = oxygen atom; N = nitrogen atom; same notations are used in this report.

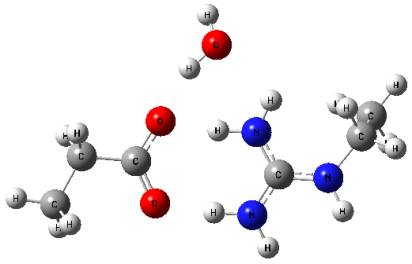


Figure-2-2: Optimized geometry of the salt bridge with one water molecule

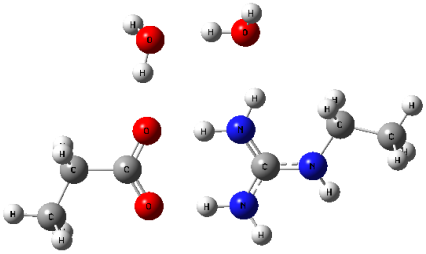


Figure-2-3: Optimized geometry of the salt bridge with two water molecules.

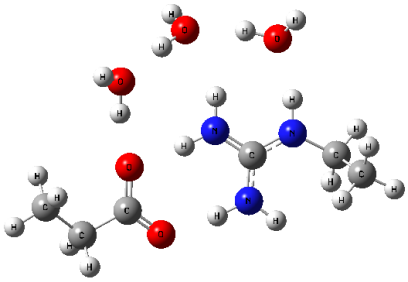


Figure-2-4: Optimized geometry of the salt bridge with three water molecules.

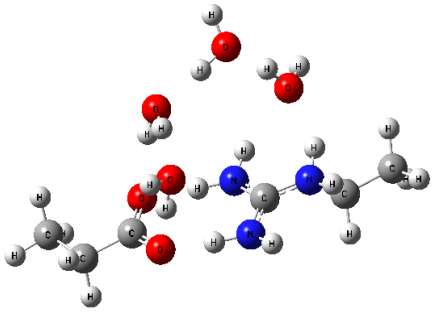


Figure-2-5: Optimized geometry of the salt bridge with four water molecules.

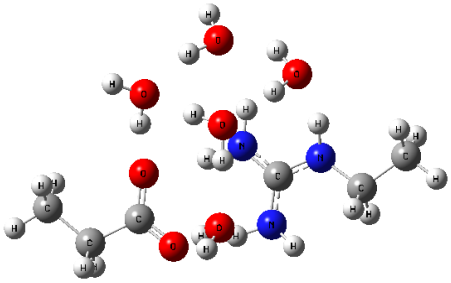


Figure-2-6: Optimized geometry of the salt bridge with five water molecules.

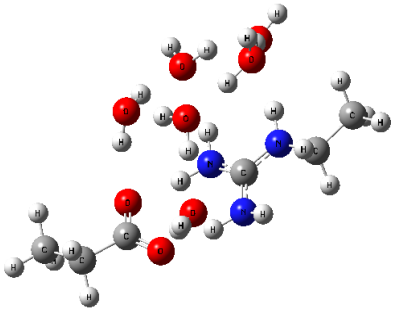


Figure-2-7: Optimized geometry of the salt bridge with six water molecules.

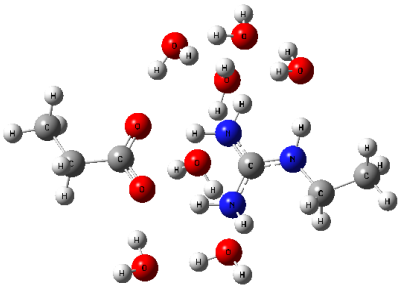


Figure-2-8: Optimized geometry of the salt bridge with seven water molecules.

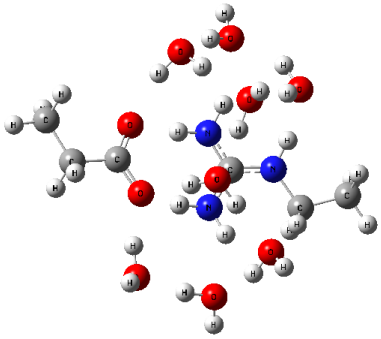


Figure-2-9: Optimized geometry of the salt bridge with eight water molecules.

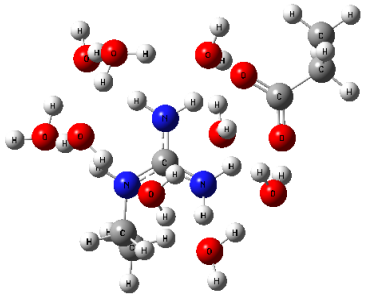


Figure-2-10: Optimized geometry of the salt bridge with nine water molecules.

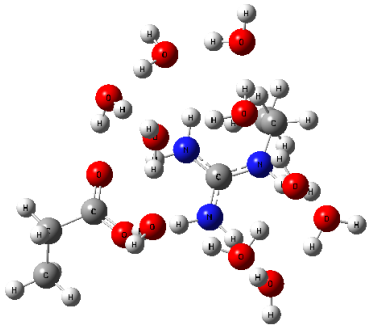


Figure-2-11: Optimized geometry of the salt bridge with ten water molecules.

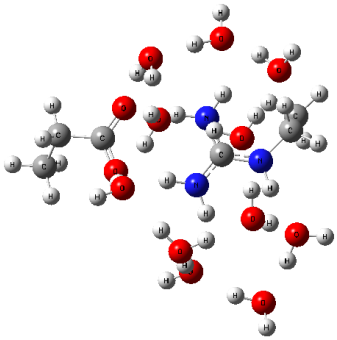


Figure-2-12: Optimized geometry of the salt bridge with eleven water molecules.

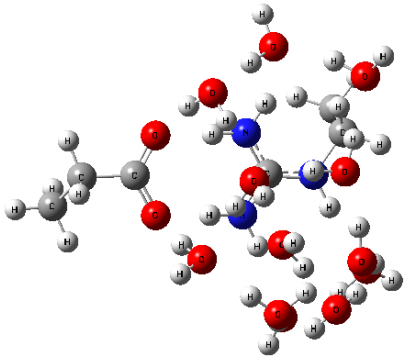


Figure-2-13: Optimized geometry of the salt bridge with twelve water molecules.

There are several structural features in these optimized geometries.

(A)Ring-like Patterns

In all the geometries, there are rings formed by the connections between the alternating O-H bond and hydrogen bond. Rings, as we define them here, are formed by either 4 oxygen members or 5 oxygen members. We use salt-bridge-with-7-water-molecules as an example to explain this feature of ring-like patterns. All the atoms in Figure-2-8 are labeled with numbers and displaced in a different angle of view, as shown in Figure-2-14.

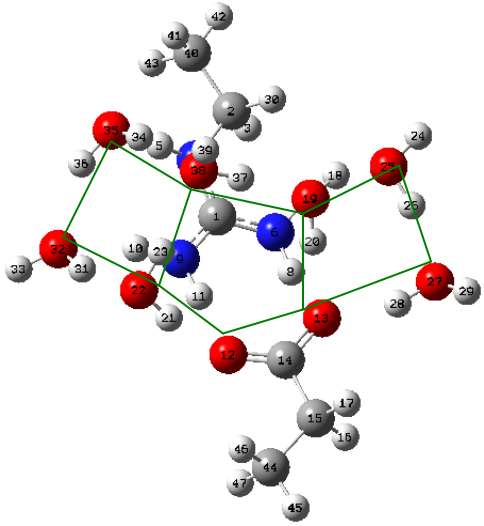


Figure-2-14: The salt bridge with seven waters; a different angle of view of Figure-2-8; one five-oxygen-member ring and two four-oxygen member rings connected by green line.

In Figure-2-14, the oxygen atoms numbered 22, 32, 35 and 38 form a ring; the oxygen atoms12, 13, 19, 38, 22 and the oxygen atoms13, 19, 25, 27 also form rings.

Another point is interesting, that a particular form of ring pattern can have lower energy than the other forms of ring pattern. Estimating from the Boltzmann factor between structures with ring and without ring, we found that the structure with a particular form of ring pattern can be about a million times more stable than the other minimum geometry without such a ring pattern. As an example, we compare the three optimized geometries shown in Figure-2-15. In Figure-2-15-a, oxygen-22-32-35-38, oxygen-22-38-19-13-12, and oxygen-13-19-41-25-27 form three rings. In Figure-2-15-b, oxygen-20-28-35-32-26, oxygen-20-26-22-13-12, and oxygen-26-32-41-37-22 also form three rings.

Both Figure-2-15-a and Figure-2-15-b have three rings but with different ring structural patterns. Figure-2-15-c has only one ring, formed by oxygen-20-25-32-29; notice that the oxygen numbered 49 is not part of any ring and only either 4 or 5 oxygen atoms here are counted as forming rings.

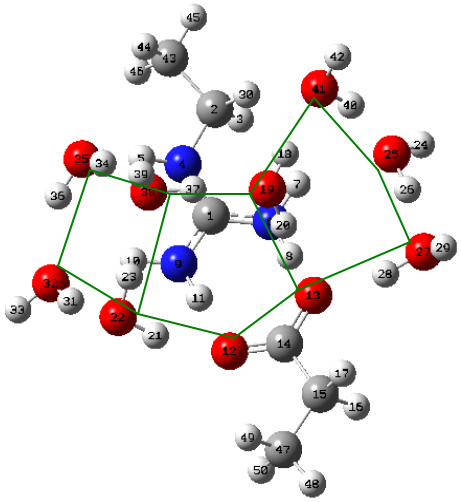


Figure-2-15-a

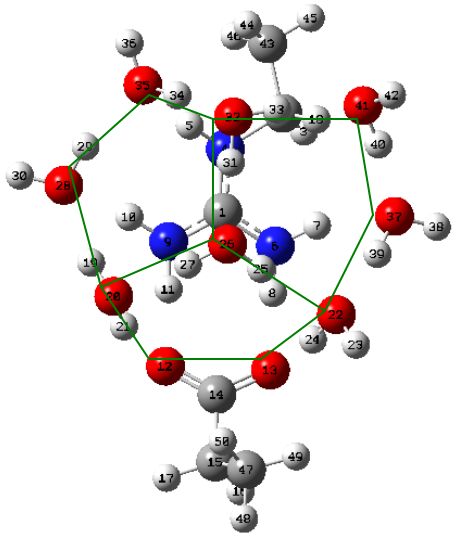


Figure-2-15-b

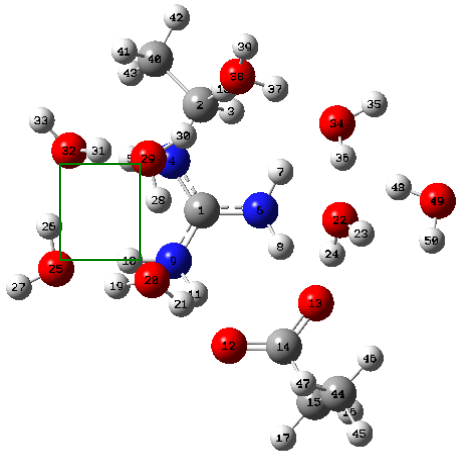


Figure-2-15-c

Figure-2-15: Including Figure-2-15-a, Figure-2-15-b, and Figure-2-15-c; the salt bridge with eight water molecules; optimized at B3LYP/6-311++G**. Figure-2-15-a has one four-oxygen-member ring and two five-oxygen-member rings; Figure-2-15-b has three five-oxygen-member rings; Figure-2-15-c has only one four-oxygen-member ring.

In Table-2-1, we tabulate the total energy values of the three optimized geometries. Using Boltzmann factor, we can find out the relative probabilities of the three optimized structures in Fingure-2-15.

Table-2-1: Three minimum geometries of salt-bridge-8-water calculated by B3LYP/6-311++G**

	Total Energy(au)	Total Energy difference in k_BT, at 298K
Picture-15-a	-1164.42327	0
Picture-15-b	-1164.41725	6.4
Picture-15-c	-1164.39886	25.9

$$N_i = N_O \, e^{-Ei/kBT}$$

where k_B is Boltzmann's constant, *Ei* is the energy of state *i*, and N_i/N_O is the probability ratio for the two configurations.

The Boltzmann distribution predicts the distribution function for the fractional number of particles N*i*/N occupying a set of states *i* which each respectively possess energy E*i*:

$$Ni/N = g_i \, e^{-Ei/k_BT} / Z(T) \qquad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

gi is the degeneracy, or number of states having energy *Ei*, *N* is the total number of particles:

$$N = \Sigma \, Ni \qquad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Z(T) is called the partition function, which is equal to,

$$Z(T) = \Sigma \, g_i \, e^{-Ei/k_BT} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

If the degeneracy g_i in the three cases is approximated about the same, then from equations (1) and (3), we have,

Probability of the structure of Figure-2-15-b/ Probability of the structure of Figure-2-15-a $\approx \text{Exp}(-6.4k_BT/\ k_BT) \approx 1.7*10^{-3}$

Probability of the structure of Figure-2-15-c/ Probability of the structure of Figure-2-15-b $\approx \text{Exp}(-25.9\ k_BT\ /\ k_BT)\ /\ \text{Exp}(-6.4\ k_BT\ /\ k_BT) \approx 3.4*10^{-9}$

Probability of the structure of Figure-2-15-c/ Probability of the structure of Figure-2-15-a $\approx \text{Exp}(-25.9\ k_BT\ /\ k_BT) \approx 5.6*10^{-12}$

We can interpret these results in terms of average lifetimes, or occupancies, of these states, showing that the form in Figure-2-15c is much less probable than those in Figure-2-15b, which in turn is much less probable than the structure in Figure-2-15a.

B) One-sided Patterns

In all the optimized geometries of lowest energy, we found that all the water molecules are gathered on only one side of the plane of the salt-bridge. In Figure-2-16, we redisplay Figure-2-11, Figure-2-12, and Figure-2-13 at a different angle of view, to give us a better view showing that all the water molecules are only on the top side while the bottom side is empty of water.

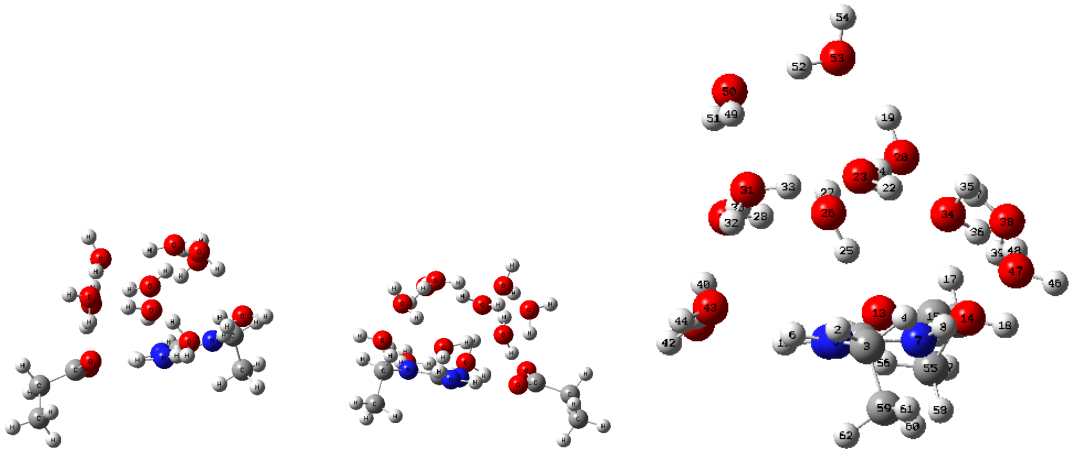


Figure-2-16-a Figure-2-16-b Figure-2-16-c

Figure-2-16: Salt bridge systems with (a)ten, (b)eleven and (c)twelve water molecules respectively; calculated by B3LYP/6-311++G**; Figure-2-16-a is a different angle of view of Figure-2-11; Figure-2-16-b a different angle of view of Figure-2-12; Figure-2-16-c a different angle of view of Figure-2-13.

Also, in Figure-2-16c, the oxygen atoms numbered 50 and 53 start forming the second layer of water shell, but still, there is no water on the other side of the salt-bridge plane. Since the water molecules start to form the second shell at the number of 10 water molecules, we only report results from the salt-bridge-0-water to the salt-bridge-12-water. While the reasons for the one-sidedness are not perfectly obvious, it appears that the salt bridge components may be acting as surfactants, placing themselves with their polar

surface facing a water drop, while the non-polar surface faces vacuum. In support of this interpretation, we note that the ethyl groups of the ethyguanidine and of the proprionic acid face away from the water, while the polar groups face the water. From this point of view, we are not surprised at the observation.

C) Possibility of a "build-up-rule" for Optimized Geometries with the Lowest Energy

The optimized total energy of one water molecule is -76.45853 atomic unit calculated by Gaussian03/B3LYP/6-311++G**. It is interesting to know how much the total energy difference caused by addition of one water molecule into a salt bridge system is. For example, for the total energy difference between salt-bridge-0-water and salt-bridge-1-water, it is the total energy of salt-bridge-1-water subtracted from the total energy of salt-bridge-0-water; for difference between salt-bridge-2-water and salt-bridge-3-water, it is salt-bridge-3-water minus salt-bridge-2-water, and so on. In Table-2-2, the optimized total energy values for salt bridge with 1 to 12 water molecules are listed in column 2, while salt bridge with 0 to 11 water molecules are in column 3. The results of subtractions between column 2 and column 3 are in column 4, which are the total energy values difference between the two corresponding salt bridge systems. Data in Table-2-2 are plotted in Figure-2-17.

Table-2-2: Difference in energy from subtraction of a water molecule from the salt bridge system

Number between subtraction	Total Energy from 1 water to 12 water (au)	Total Energy from 0 water to 11 water (au)	Difference between Total Energy from subtraction(au)
1-(w1-w0)	-629.07604	-552.60147	-76.47456
2-(w2-w1)	-705.55929	-629.07604	-76.48325
3-(w3-w2)	-782.03721	-705.55929	-76.47791
4-(w4-w3)	-858.51486	-782.03721	-76.47765
5-(w5-w4)	-934.99148	-858.51486	-76.47663
6-(w6-w5)	-1011.4642	-934.99148	-76.47275
7-(w7-w6)	-1087.9478	-1011.4642	-76.48359
8-(w8-w7)	-1164.4233	-1087.9478	-76.47545
9-(w9-w8)	-1240.8989	-1164.4233	-76.47565
10-(w10-w9)	-1317.3735	-1240.8989	-76.47461
11-(w11-w10)	-1393.8468	-1317.3735	-76.47325
12-(w12-w11)	-1470.3251	-1393.8468	-76.47828

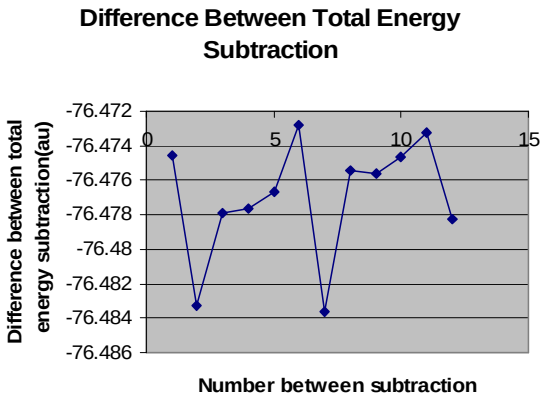


Figure-2-17: The number between subtractions versus the energy differences

As expected, all the values in column 4 of Table-2-2 are lower than the total energy of one water molecule since the salt bridge systems in this report have hydrophilic properties. In Figure-2-17 three observations are worthy of note. (1) The diagram has a periodic appearance, starting from 1 to 6, and then, from 6 to 11. (2) The difference between the maximum and the minimum is 0.0108 au, about 11 k_BT. (3) The number of water molecules to complete the first whole layer of water molecules is 10. (A more detailed calculation of energy discrepancies is given in Chapter 5).

We do not yet have a full understanding of the mechanisms presented in Figure-2-17. We notice, however, the two minima in the figure; one is at the second position, that is, the difference between salt-bridge-2-water and salt-bridge-1-water (please refer to Figure-2-3 and Figure-2-4), and the other is at the sixth position, that is, the difference between salt-bridge-7-water and salt-bridge-6-water (please refer to Figure-2-7 and Figure-2-8), Both minima are caused by the completion of an extra ring in the system. Also, at the two maximum positions, one between salt-bridge-6-water and salt-bridge-5-water (please refer to Figure-2-6 and Figure-2-7), and the other between salt-bridge-11-water and salt-bridge-10-water (please refer to Figure-2-11 and Figure-2-1, no extra ring is formed, but in both cases, the ring size changed from a 4-member-oxygen ring to 5-member-oxygen ring, which indicates the 5-oxygen ring size is slightly more favorable than the 4-oxygen ring size.

It suggests that there may be a periodical fill-in order for water molecules to enter into a salt bridge system. It starts forming 4-oxygen-member rings, then becoming 5-oxygen-member rings, and then the salt bridge systems expand in a cell unit of 5-oxygen-member ring into three dimensional spaces.

Chapter 3

Salt Bridge Length versus Total Energy

Methods

Gaussian 03 is used for the salt bridge plus 0 to 5 water molecules, while NWChem at the remote supercomputer of the Environmental Molecular Science Laboratory is for the cases with more water.

Starting with the optimized geometries in Chapter 2, we define the bridge length as the distance between the two closest carbon atoms: one from the propionic acid and the other from the ethylguanidine. The bridge length is defined, as shown in Figure-3-1, as the distance between the carbon-16C and carbon-1C for the salt-bridge-0-water. The bridge length is expanded 0.1 Å at each step, applying constraints[138-141] to the bridge length; the system is optimized using HF/3-21G*, and then subsequently, further optimized using B3LYP/6-311++G**.

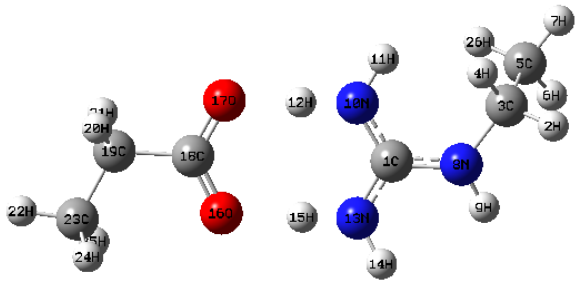


Figure-3-1: Salt bridge formed by a propionic acid and an ethylguanidine with zero water molecule; optimized at B3LYP/6-311++G**; showing the salt bridge length between carbon-16 and carbon-1C, C = carbon atom; H = hydrogen atom; O = oxygen atom; N = nitrogen atom.

Results and Discussion

Plots of bridge length in Å versus energy in units of k_BT at 298K, all calculated by B3LYP/6-311++G**, are shown in figures from Figure-3-2 to Figure-3-14. Data are tabulated in tables from Table-3-1 to table-3-13 in Appendix A.

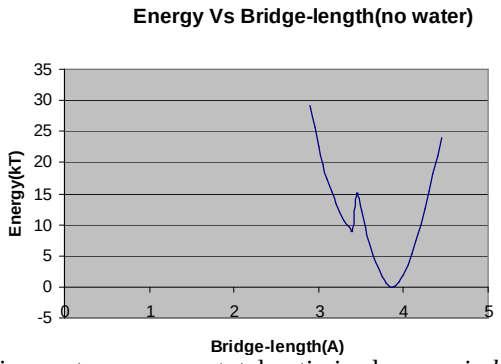


Figure-3-2: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-0-water.

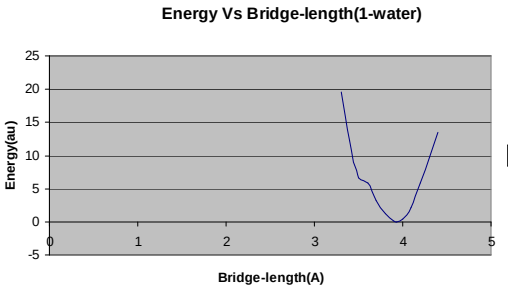


Figure-3-3: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-1-water.

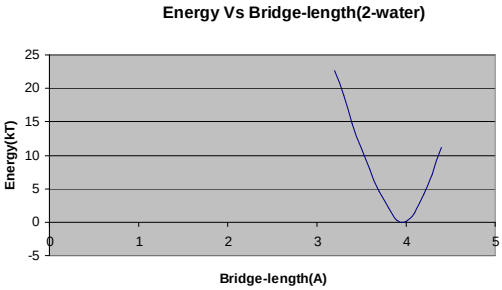


Figure-3-4: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-2-water.

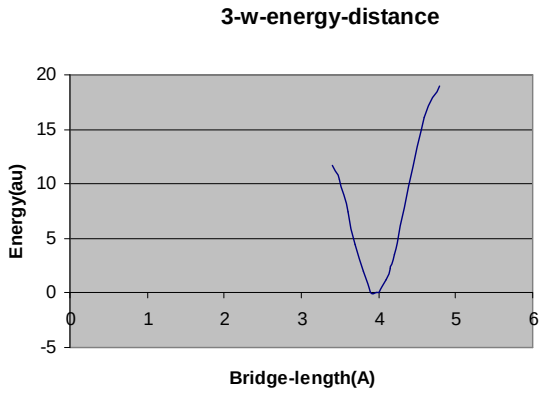


Figure-3-5 Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-3-water.

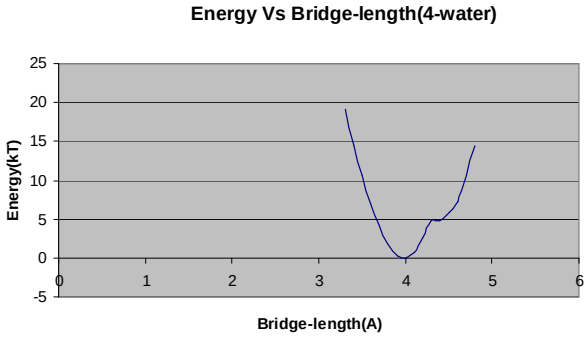


Figure-3-6: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-4-water.

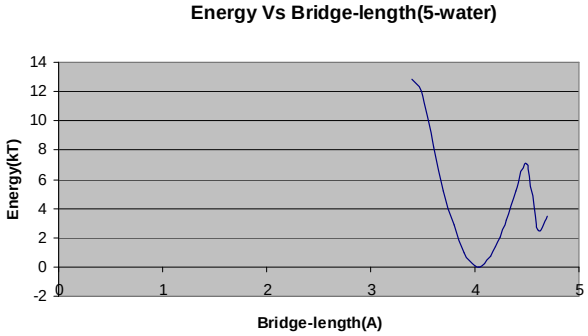


Figure-3-7: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-5-water.

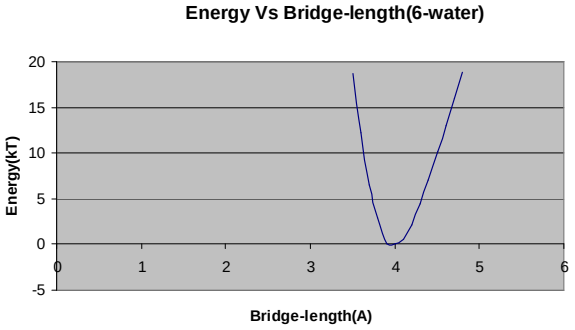


Figure-3-8: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-6-water.

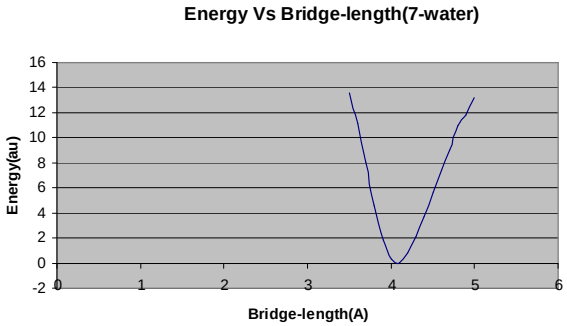


Figure-3-9: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-7-water.

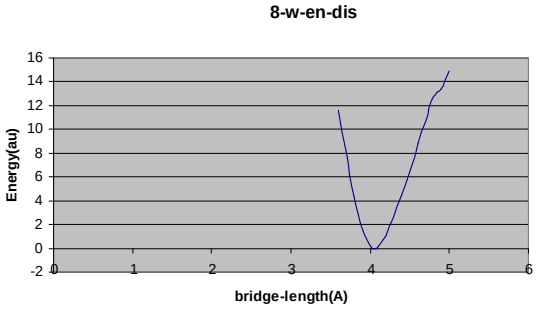


Figure-3-10: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-8-water.

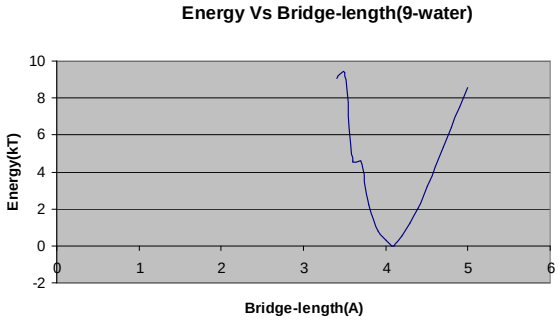


Figure-3-11: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-9-water.

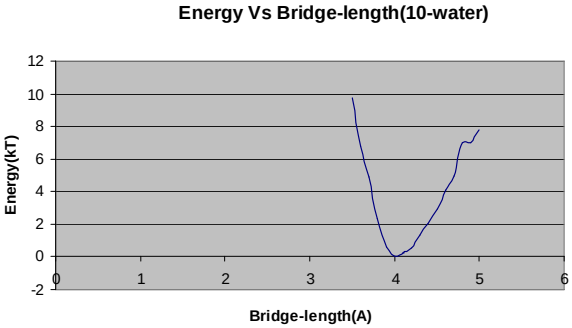


Figure-3-12: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-10-water.

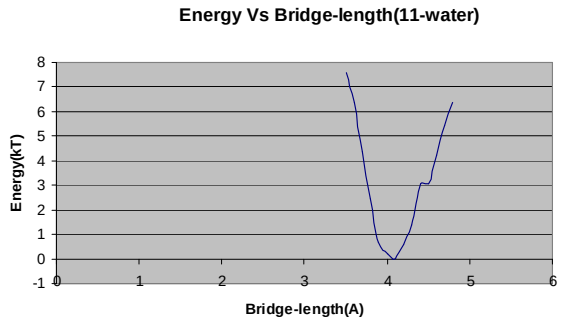


Figure-3-13: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-11-water.

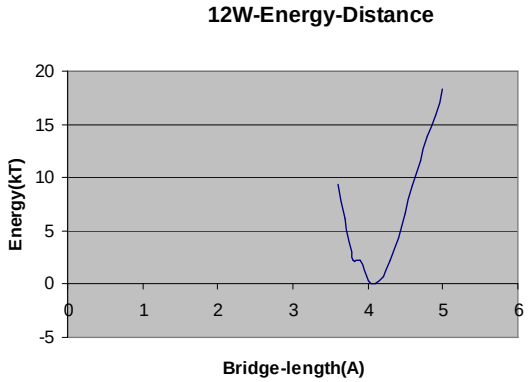


Figure-3-14: Bridge length in angstroms versus total optimized energy in k_BT for salt-bridge-12-water.

In Figure-3-2, we notice there is a deep local minimum at the bridge length of 3.4 angstroms for the salt bridge with no water. This local minimum indicates the system energy decreases when the proton transfers from propionic acid to ethylguanidine during the ionization process (more detailed data associated with the distance ratio O-H/N-H can be found in the Chapter 9, NBO Calculations). As water molecules are added into the salt bridge, the local minimum disappears, which, in part, is because of the redistribution of electron density in the salt bridge system (more detailed discussions in Chapter 9, NBO Calculations).

The bridge lengths slightly increase as there are more water molecules in the system, but the bridge lengths largely depend on the arrangement of the surrounding water. For the salt bridge with 5 waters in Figure-3-7, after 4.20 angstroms, the total energy decreases as the bridge length increases. We do not have a full explanation as to the

cause of this, but we observed the salt bridge with 5 waters has a high bridge binding energy (Table-6-1 in Chapter 6) at optimized bridge length.

Chapter 4

Angle Study

Methods

The software packages used in Chapter 3 are Gaussian 03 and GaussView3.0, and the calculations are performed by B3LYP/6-311++G**. We use the optimized geometries of the salt bridges from Chapter 2 as the starting geometries.

Part-1: Method for the Dihedral-angle-[1]C-[2]O-[3]H-[4]C versus Total Energy

As shown in Figure-4-1, the dihedral angle ᴅ is defined by the angle between the plane Atom-[4]C-Atom-[3]H-Atom-[2]O, with respect to the plane of Atom-[1]C, Atom-[2]O and Atom-[3]H. The system is set up in z-matrix format by GaussView03, followed by allowing the plane formed by Atom-[1]C, Atom-[2]O and Atom-[3]H to be fixed, and then systematically, varying the orientation of the plane Atom-[4]C-Atom-[3]H-Atom-[2]O, thus altering the dihedral angle ᴅ. At each dihedral angle, a single point energy calculation is performed using B3LYP/6-311++G**. We can gain a physical sense from Figure-4-1 to Figure-4-4 on how the dihedral angle turns in the process.

For the dihedral angle ᴅ, we only perform calculations on salt bridge with no water.

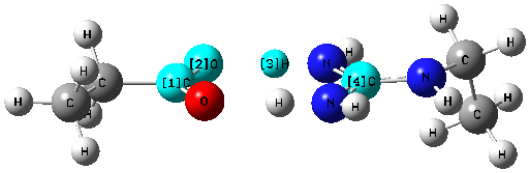


Figure-4-1: Optimized at B3LYP/6-311++G**, the geometry of salt-bridge-0-water with the dihedral angle, ᴅ = 0.56°.

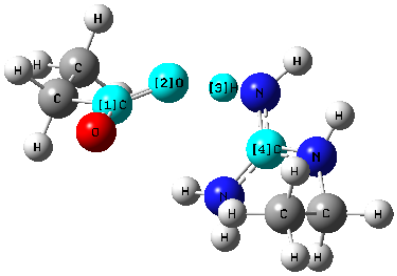


Figure-4-2: The geometry of salt-bridge-0-water with the dihedral angle, ᴅ = 45.42°.

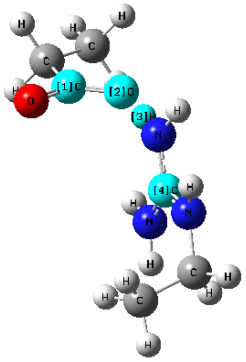


Figure-4-3: The geometry of salt-bridge-0-water with the dihedral angle, ᴅ = 90.28°.

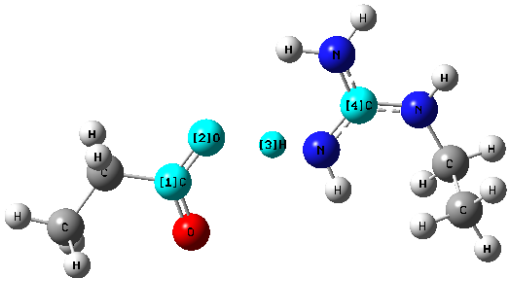


Figure-4-4: The geometry of salt-bridge-0-water with the dihedral angle, ᴅ = 180.00°.

Part-2: Method for the Angle-[1]N-[2]C-[3]C versus Total Energy

As seen in Figure-4-5, using the z-matrix format of GaussView03, let the distance between [3]C and [2]C remain constant, and let the coordinates of [2]C and [1]N be fixed; then systematically, we vary Atom-[3]C to obtain a set of values of angle-[3]C-[2]C-[1]N, which is defined as angle α, and at each angle we do single point energy calculation using B3LYP/6-311++G**. We can gain a physical sense from Figure-4-5 to Figure-4-7 how the angle turns in the process.

For salt bridge with water molecules, the coordinates of water molecules are assumed to be unmoved and the distance between Atom[3[C and Atom[2] to be frozen, when angle α changes, and the procedure used is the same as the one with no water.

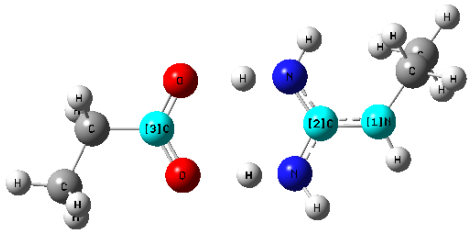


Figure-4-5: Optimized geometry of salt-bridge-0-water; calculated at B3LYP/6-311++G**; at angle α = 176.7 degrees.

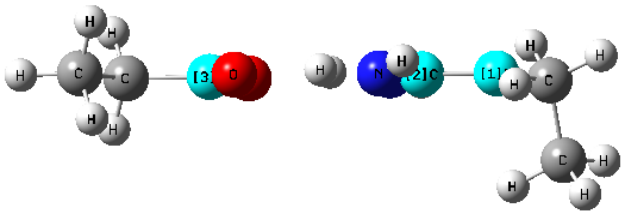


Figure-4-6: The geometry of salt-bridge-0-water; at angle α = 180.0 degrees.

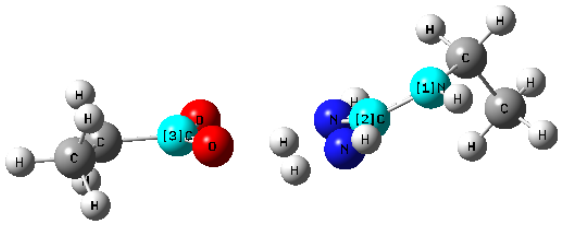


Figure-4-7: The geometry of salt-bridge-0-water; at angle α = 156.0 degrees.

Results and Discussion

Plots for dihedral angle ᴅ and angle α versus total energy, calculated by B3LYP/6-311++G**, are shown in figures from Figure-4-8 to Figure-4-21. Data are tabulated in tables from Table-4-1 to table-4-14 in Appendix B.

As to be expected, when both the dihedral angle ᴅ and angle α move away from the respective optimized angles, the total energy increases. The turning of the dihedral angle ᴅ represents a direct disruption of the salt bridge bonding. When comparing

both the dihedral angle D and angle α diagrams for total energy increase per degree, it shows that the total energy increases faster in diagram for the dihedral angle D.

For salt-bridge-0-water, when the changes of angle α are within the range from 173 and 180 degrees, an interval of about 7 degrees, the differences between the total energy values are within 1 k_BT. For salt bridges with waters, the total energy increases faster as the angles increase. Our results indicate that the surrounding water molecules make a salt bridge more "rigid" in terms of resistance to total energy change. The rigidity depends on the spatial arrangement of the water molecules.

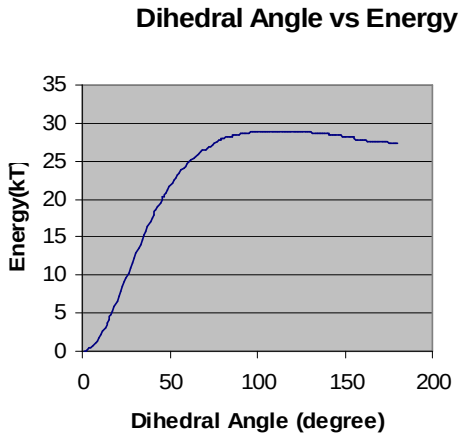


Figure-4-8: Dihedral angle D in degrees versus total energy in k_BT for salt-bridge-0-water.

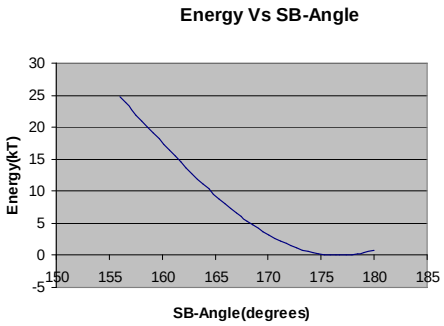


Figure-4-9: Angle α in degrees versus total energy in k_BT for salt-bridge-0-water.

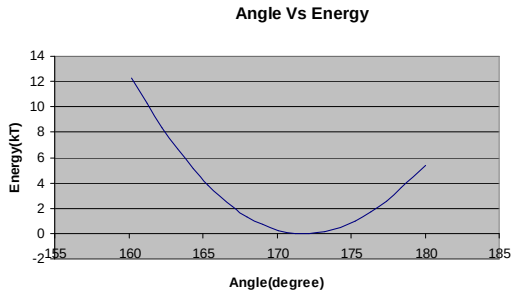


Figure-4-10: Angle α in degrees versus total energy in k_BT for salt-bridge-1-water.

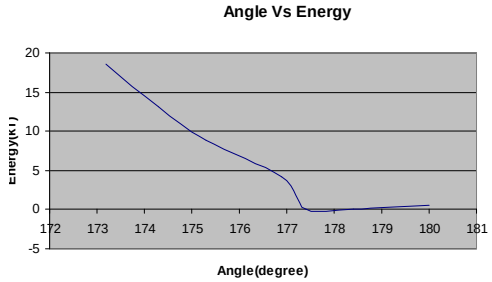


Figure-4-11: Angle α in degrees versus total energy in k_BT for salt-bridge-2-water.

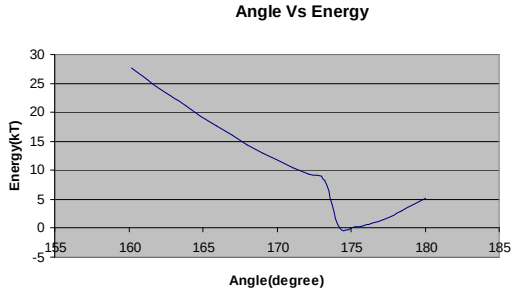


Figure-4-12: Angle α in degrees versus total energy in k_BT for salt-bridge-3-water.

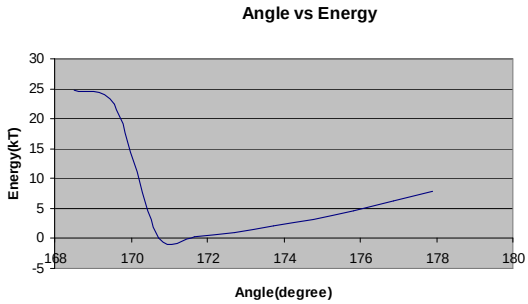


Figure-4-13: Angle α in degrees versus total energy in k_BT for salt-bridge-4-water.

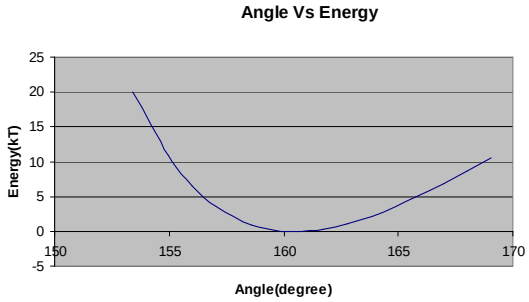


Figure-4-14: Angle α in degrees versus total energy in k_BT for salt-bridge-5-water.

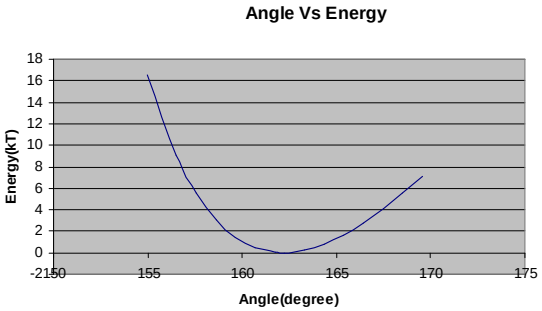


Figure-4-15: Angle α in degrees versus total energy in k_BT for salt-bridge-6-water.

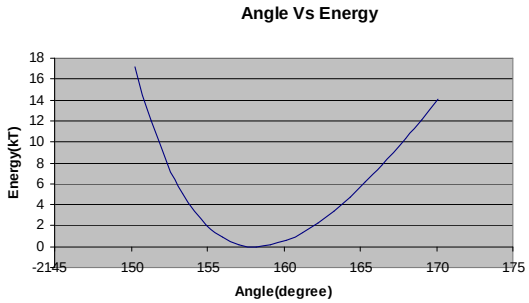


Figure-4-16: Angle α in degrees versus total energy in k_BT for salt-bridge-7-water.

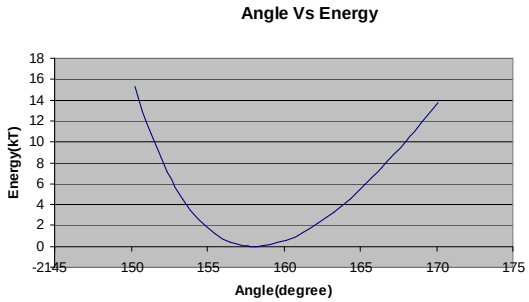


Figure-4-17: Angle α in degrees versus total energy in k_BT for salt-bridge-8-water.

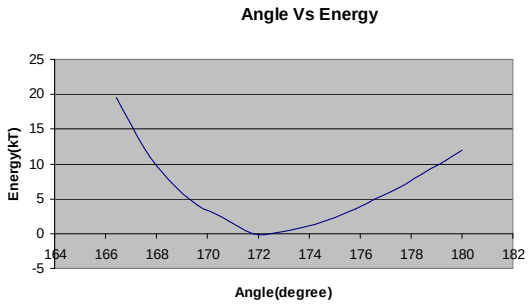


Figure-4-18: Angle α in degrees versus total energy in k_BT for salt-bridge-9-water.

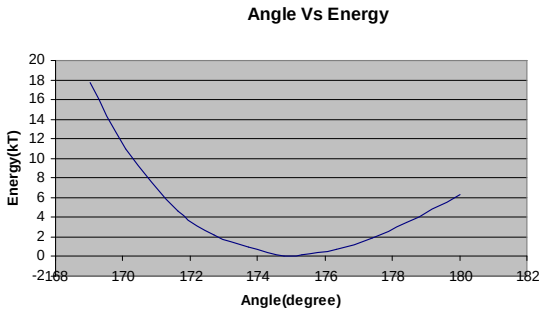


Figure-4-19: Angle α in degrees versus total energy in k_BT for salt-bridge-10-water.

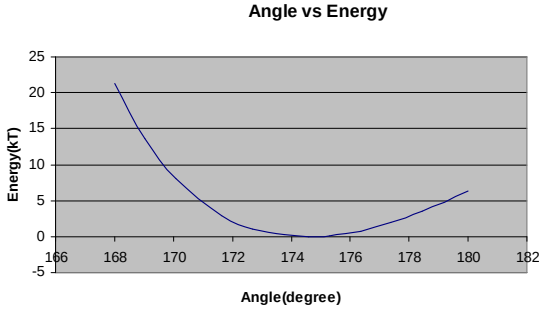


Figure-4-20: Angle α in degrees versus total energy in k_BT for salt-bridge-11-water.

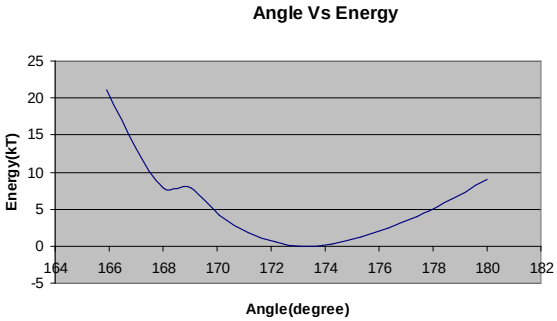


Figure-4-21: Angle α in degrees versus total energy in k_BT for salt-bridge-12-water.

Chapter 5

Best Fit Potential Functions in First Water Shell

Methods

Mathematica 6.0 is used to find the best fit potential functions in this section. Data for the best fit potential functions against bridge lengths are from Chapter 3, the optimized energies at different bridge lengths for the 13 salt-bridges. With each addition of one water molecule into the salt bridge system, we calculate the total energy difference resulting from such an addition. We also compare ΔE, which is defined as the difference between the individual values and their average, for the different amounts of water molecules. The calculated data are tabulated in Table-5-1 to Table-5-12.

For the best fit potential functions against angles, results from Chapter 4 are used in calculations. The same method is used as with the bridge lengths.

Results and Discussion

Examining the data from Table-5-1 to Table-5-12, we notice that the ΔE in Table-5-10 and Table-5-11 are less than $0.5k_BT$. It shows that for the salt bridge system with ten water molecules, the total energy changes have the minimum affect by either the subtraction or the addition of an extra water molecule. It suggests that the number of water molecules in the first shell is ten. We also notice that the ΔE in Table-5-3 is within 0.5 k_BT because when the systems have less than 4 water molecules only one

oxygen atom of the carboxyl group is involved in hydrogen bonding. In all the other tables, the ΔE values are larger than 0.5 k_BT.

Using the data for ten water molecules in Table-3A-11, the potential function against bridge length in first water shell is,

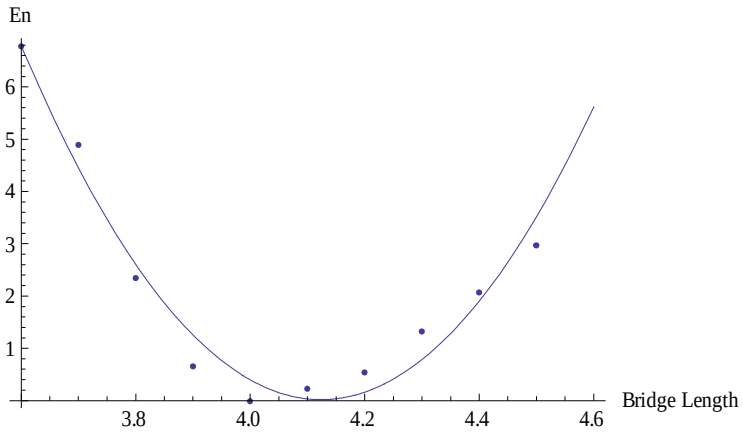


Figure-5-1, Comparing data with the best fit function against bridge lengths; calculated by Mathematica 6.0.

$$En = 419.765 - 203.574X + 24.6831X^2 \quad (3.6 < x < 4.5)$$

where En is the total energy in k_BT, and x is the bridge length in angstroms.

Similarly, when examining the angle data in Table-5-13, Table-5-14 and Table-5-15, we notice that the ΔE of the system with ten water molecules in Table-5-14 are less than 0.5 k_BT, which gives further supports to that the number of water molecules is ten in the first shell.

Using the data of salt-bridge-10-water in Table-4B-12, we have the potential function against angles in first water shell as,

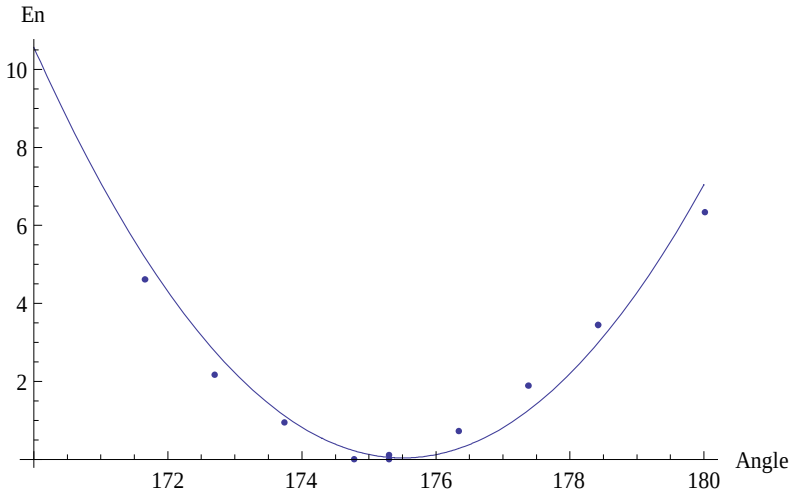


Figure-5-2, Comparing data with the best fit function against bridge angles; calculated by Mathematica 6.0.

$$\mathrm{En}(\alpha) = 10695.5 - 121.881\,\alpha + 0.347229\,\alpha^2$$

$$(170^{o} < \alpha < 180^{o};\ \text{at bridge length of 4.0 angstroms})$$

where $\mathrm{En}(\alpha)$ is the total energy in k_BT, and α is the angle-[1]N-[2]C-[3]C defined in Chapter 4.

It is no surprise that the number of water molecules to complete the first shell is ten. When reexamining Figure-2-16-c, it can be noticed that the two water molecules (with oxygen-50 and oxygen-53) on top started forming the second water shell. Also, the periodicity in Figure-2-17 shows that ten is the integer number to complete the cycle.

Table-5-1: ΔE between salt-bridge-0-water and salt-bridge-1-water.

Bridge Length (A)	w-0 Total energy(au)	w-1 Total energy(au)	Difference between w-0 and w-1(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-552.59485	-629.07045	76.4756	-0.0002	-0
3.7	-552.59855	-629.07298	76.47443	-0.0014	-1
3.8	-552.60097	-629.07494	76.47397	-0.0018	-2
3.9	-552.60135	-629.07598	76.47463	-0.0012	-1
4	-552.59969	-629.07565	76.47596	0.00016	0.2
4.1	-552.59647	-629.07405	76.47758	0.00178	1.9
4.2	-552.59214	-629.07055	76.47841	0.00261	2.8
Average (au): 76.4758					

Table-5-2: ΔE between salt-bridge-1-water and salt-bridge-2-water

Bridge Length (A)	w-1 Total energy(au)	w-2 Total energy(au)	Difference between w-1 and w-2(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-629.07045	-705.55186	76.48141	-0.0016	-1.7
3.7	-629.07298	-705.55498	76.482	-0.001	-1.1
3.8	-629.07494	-705.5573	76.48236	-0.0006	-0.7
3.9	-629.07598	-705.55897	76.48299	0	-0
4	-629.07565	-705.55916	76.48351	0.0005	0.5
4.1	-629.07405	-705.55802	76.48397	0.00096	1
4.2	-629.07055	-705.55537	76.48482	0.00181	1.9
Average (au): 76.48301					

Table-5-3: ΔE between salt-bridge-2-water and salt-bridge-3-water

Bridge Length (A)	w-2 Total energy(au)	w-3 Total energy(au)	Difference between w-2 and w-3(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-705.55186	-782.03018	76.47832	0.000209	0.2
3.7	-705.55498	-782.03298	76.478	-0.00011	-0.1
3.8	-705.5573	-782.03533	76.47803	-8.14E-05	-0.1
3.9	-705.55897	-782.03687	76.4779	-0.00021	-0.2
4	-705.55916	-782.03714	76.47798	-0.00013	-0.1
4.1	-705.55802	-782.03606	76.47804	-7.14E-05	-0.1
4.2	-705.55537	-782.03388	76.47851	0.000399	0.4
Average (au): 76.47811					

Table-5-4: ΔE between salt-bridge-3-water and salt-bridge-4-water

Bridge Length (A)	w-3 Total energy(au)	w-4 Total energy(au)	Difference between w-3 and w-4(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-782.03018	-858.50823	76.47805	5.57E-05	0.1
3.7	-782.03298	-858.51101	76.47803	3.57E-05	0
3.8	-782.03533	-858.51319	76.47786	-0.00013	-0.1
3.9	-782.03687	-858.51455	76.47768	-0.00031	-0.3
4	-782.03714	-858.51486	76.47772	-0.00027	-0.3
4.1	-782.03606	-858.51409	76.47803	3.57E-05	0
4.2	-782.03388	-858.51247	76.47859	0.000596	0.6
Average (au): 76.47799					

Table-5-5: ΔE between salt-bridge-4-water and salt-bridge-5-water

Bridge Length (A)	w-4 Total energy(au)	w-5 Total energy(au)	Difference between w-4 and w-5(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-858.50823	-934.98379	76.47556	-0.00075	-0.8
3.7	-858.51101	-934.98655	76.47554	-0.00077	-0.8
3.8	-858.51319	-934.98876	76.47557	-0.00074	-0.8
3.9	-858.51455	-934.99056	76.47601	-0.0003	-0.3
4	-858.51486	-934.99144	76.47658	0.000274	0.3
4.1	-858.51409	-934.99129	76.4772	0.000894	0.9
4.2	-858.51247	-934.99015	76.47768	0.001374	1.5
Average (au): 76.47631					

Table-5-6: ΔE between salt-bridge-5-water and salt-bridge-6-water

Bridge Length (A)	w-5 Total energy(au)	w-6 Total energy(au)	Difference between w-5 and w-6(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-934.98379	-1011.4528	76.469	-0.00293	-3.1
3.7	-934.98655	-1011.4581	76.47151	-0.00042	-0.4
3.8	-934.98876	-1011.4615	76.47278	0.00085	0.9
3.9	-934.99056	-1011.4635	76.47292	0.00099	1.1
4	-934.99144	-1011.4642	76.47279	0.00086	0.9
4.1	-934.99129	-1011.4637	76.47237	0.00044	0.5
4.2	-934.99015	-1011.4623	76.47213	0.0002	0.2
Average (au): 76.47193					

Table-5-7: ΔE between salt-bridge-6-water and salt-bridge-7-water

Bridge Length (A)	w-6 Total energy(au)	w-7 Total energy(au)	Difference between w-6 and w-7(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-1011.45279	-1087.93738	76.48459	0.001217	1.3
3.7	-1011.45806	-1087.94023	76.48217	-0.0012	-1.3
3.8	-1011.46154	-1087.94351	76.48197	-0.0014	-1.5
3.9	-1011.46348	-1087.94612	76.48264	-0.00073	-0.8
4	-1011.46423	-1087.94755	76.48332	-5.29E-05	-0.1
4.1	-1011.46366	-1087.94779	76.48413	0.000757	0.8
4.2	-1011.46228	-1087.94707	76.48479	0.001417	1.5
Average (au): 76.48337					

Table-5-8: ΔE between salt-bridge-7-water and salt-bridge-8-water

Bridge Length (A)	w-7 Total energy(au)	w-8 Total energy(au)	Difference between w-7 and w-8(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-1087.93738	-1164.41235	76.47497	-0.00045	-0.5
3.7	-1087.94023	-1164.41566	76.47543	1.3E-05	0
3.8	-1087.94351	-1164.41921	76.4757	0.000281	0.3
3.9	-1087.94612	-1164.42182	76.4757	0.000284	0.3
4	-1087.94755	-1164.4231	76.47555	0.000137	0.2
4.1	-1087.94779	-1164.42314	76.47535	-6.8E-05	-0.1
4.2	-1087.94707	-1164.42229	76.47522	-0.0002	-0.2
Average (au):76.47542					

Table-5-9: ΔE between salt-bridge-8-water and salt-bridge-9-water

Bridge Length (A)	w-8 Total energy(au)	w-9 Total energy(au)	Difference between w-8 and w-9(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-1164.41235	-1240.89281	76.48046	0.003206	3.4
3.7	-1164.41566	-1240.8946	76.47894	0.001686	1.8
3.8	-1164.41921	-1240.89682	76.47761	0.000356	0.4
3.9	-1164.42182	-1240.89815	76.47633	-0.00092	-1
4	-1164.4231	-1240.89866	76.47556	-0.00169	-1.8
4.1	-1164.42314	-1240.89892	76.47578	-0.00147	-1.6
4.2	-1164.42229	-1240.89839	76.4761	-0.00115	-1.2
Average (au): 76.47725					

Table-5-10: ΔE between salt-bridge-9-water and salt-bridge-10-water

Bridge Length (A)	w-9 Total energy(au)	w-10 Total energy(au)	Difference between w-9 and w-10(au)	Difference - Ave(au)	Difference - Ave(k_BT) $\Delta E<0.5\ k_BT$
3.6	-1240.89281	-1317.36717	76.47436	-0.00019	-0.2
3.7	-1240.8946	-1317.36893	76.47433	-0.00022	-0.2
3.8	-1240.89682	-1317.37132	76.4745	-4.71E-05	-0
3.9	-1240.89815	-1317.37292	76.47477	0.000223	0.2
4	-1240.89866	-1317.37353	76.47487	0.000323	0.3
4.1	-1240.89892	-1317.3733	76.47438	-0.00017	-0.2
4.2	-1240.89839	-1317.37301	76.47462	7.29E-05	0.1
Average (au): 76.47455					

Table-5-11: ΔE between salt-birdge-10-water and salt-bridge-11-water

Bridge Length (A)	w-10 Total energy(au)	w-11 Total energy(au)	Difference between w-10 and w-11(au)	Difference - Ave(au)	Difference -Ave(k_BT) ΔE<0.5 k_BT
3.6	-1317.36717	-1393.84078	76.47361	0.00026	0.3
3.7	-1317.36893	-1393.84269	76.47376	0.00041	0.4
3.8	-1317.37132	-1393.84447	76.47315	-0.0002	-0.2
3.9	-1317.37292	-1393.84613	76.47321	-0.00014	-0.1
4	-1317.37353	-1393.84655	76.47302	-0.00033	-0.3
4.1	-1317.3733	-1393.84674	76.47344	9.43E-05	0.1
4.2	-1317.37301	-1393.84624	76.47323	-0.00012	-0.1
Average (au): 76.47335					

Table-5-12: ΔE between salt-bridge-11-water and salt-bridge-12-water

Bridge Length (A)	w-11 Total energy(au)	w-12 Total energy(au)	Difference between w-11 and w-12(au)	Difference - Ave(au)	Difference - Ave(k_BT)
3.6	-1393.84078	-1470.31619	76.47541	-0.00153	-1.6
3.7	-1393.84269	-1470.31927	76.47658	-0.00036	-0.4
3.8	-1393.84447	-1470.31968	76.47521	-0.00173	-1.8
3.9	-1393.84613	-1470.32292	76.47679	-0.00015	-0.2
4	-1393.84655	-1470.32473	76.47818	0.001244	1.3
4.1	-1393.84674	-1470.32502	76.47828	0.001344	1.4
4.2	-1393.84624	-1470.32434	76.4781	0.001164	1.2
Average (au): 76.47694					

Table-5-13: ΔE between salt-bridge-9-water and salt-bridge-10-water in bridge angle α

Bridge Angle α in degrees	w-9 Total Energy(au)	w-10 Total Energy(au)	Difference between w-9 and w-10(au)	Difference - Ave(au)	Difference - Ave(k_BT)
172.7	-1240.89871	-1317.37123	76.47251	-0.00375	-4
173.7	-1240.89802	-1317.37241	76.47439	-0.00187	-2
175.3	-1240.89623	-1317.37319	76.47696	0.000699	0.7
176.4	-1240.89468	-1317.3726	76.47792	0.001654	1.8
177.4	-1240.89287	-1317.3715	76.47863	0.002371	2.5
178.4	-1240.89087	-1317.37005	76.47918	0.002916	3.1
180	-1240.8876	-1317.36731	76.47971	0.003442	3.6
Average: 76.47704					

Table-5-14: ΔE between salt-bridge-10-water and salt-bridge-11-water in bridge angle α

Bridge Angle α in degrees	w-10 Total Energy(au)	w-11 Total Energy(au)	Difference between w-10 and w-11(au)	Difference - Ave(au)	Difference - Ave(k_BT) ΔE<0.5 k_BT
173.7	-1317.37241	-1393.84656	76.47415	0.000505	0.5
174.8	-1317.3733	-1393.84677	76.47347	-0.00017	-0.2
175.3	-1317.37319	-1393.84661	76.47342	-0.00023	-0.2
176.4	-1317.3726	-1393.846	76.4734	-0.00024	-0.3
177.4	-1317.3715	-1393.8449	76.47339	-0.00025	-0.3
178.4	-1317.37005	-1393.84345	76.4734	-0.00024	-0.3
180	-1317.36731	-1393.84074	76.47343	-0.00021	-0.2
Average: 76.47365					

Table-5-15: ΔE between salt-bridge-11-water and salt-bridge-12-water in bridge angle α

Bridge Angle α in degrees	w-11 Total Energy(au)	w-12 Total Energy(au)	Difference between w-11 and w-12(au)	Difference - Ave(au)	Difference - Ave(k_BT)
172.7	-1393.84572	-1470.32475	76.47904	0.001583	1.7
173.7	-1393.84656	-1470.32489	76.47833	0.000873	0.9
175.3	-1393.84661	-1470.324	76.47733	-0.00013	-0.1
176.4	-1393.846	-1470.323	76.47673	-0.00072	-0.8
177.4	-1393.8449	-1470.321	76.47638	-0.00108	-1.1
178.4	-1393.84345	-1470.32	76.47608	-0.00137	-1.5
180	-1393.84074	-1470.317	76.47582	-0.00163	-1.7
Average: 76.4771					

Chapter 6

Salt Bridge Binding Energy

Method

The software packages used in Chapter 6 are Gaussian 03 and GaussView03. The calculations of binding energy[142-146] are done by B3LYP/6-311++G** with the dielectric constant equal to 1. We use the 13 optimized geometries from Chapter 2.

Step 1

(i) In the case of a salt bridge with no water, we calculate the total energy of the salt-bridge optimized geometry obtained from Chapter 2, which we call T.

(ii) In cases of salt bridge with water molecules, we start with the optimized geometry obtained from Chapter 2, removing all the water molecules by GaussView03, and then we calculate the total energy of the salt-bridge, which we also called T.

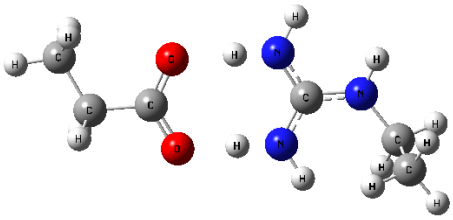
Step-2

We separately calculate the total energy of the propionic acid, which we call A; also the total energy of the ethylguanidine, and we call B.

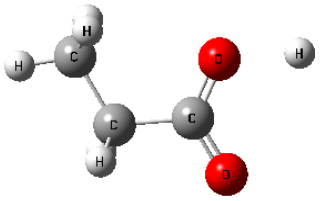
Step-3

We calculate the binding energy; that is, Binding Energy = T-(A + B).

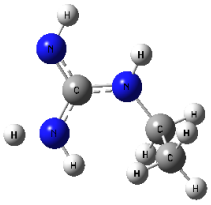
We illustrate the above steps for the calculation of salt-bridge-0-water in Figure-6-1 and for the calculation of salt-bridge-6-water in Figure-6-2.



The geometry of the Total Energy of the salt-bridge, T:

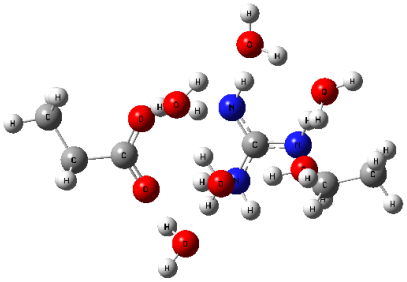


Geometry of the propionic acid, A.

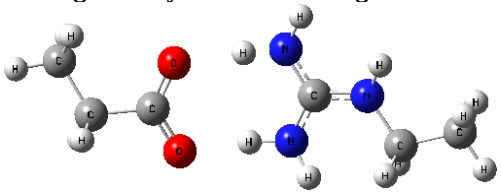


Geometry of the ethylguanidine, B.

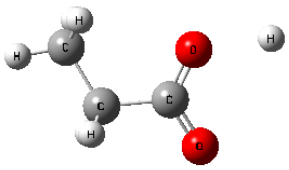
Figure-6-1: The illustration of the process of calculating the salt-bridge-bonding-energy, Binding Energy = T-(A+B), for the case of salt-bridge-0-water.



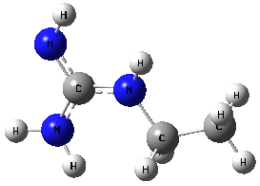
The geometry of the salt-bridge-6-water



The geometry of the salt-bridge after removal of the six water molecules, T.



Geometry of the propionic acid, A.



Geometry of the ethylguanidine, B.

Figure-6-2: The illustration of the process of calculating the salt-bridge-bonding-energy, Binding Energy = T-(A+B), for the case of salt-bridge-6-water.

Results and Discussion

The results of salt bridge binding energy for the 13 molecular clusters are tabulated in Table-6-1; showing that the lowest value is for the salt-bridge-0-water, which gives

further support to our previous suggestions (please refer to Discussion Section on “One-sided Patterns” in Chapter 2) that the salt bridge formed by propionic acid and ethylguanidine has hydrophilic properties.

Table-6-1: Bridge Bonding Energy calculated by B3LYP/6-311++G with dielectric constant 1**

	A (au)	B (au)	T (au)	Binding Energy (au)	Binding Energy (k_BT) at 298K
SB-0-water	-268.38836	-284.07371	-552.60126	-0.13919	-148.1
SB-1-water	-268.36742	-284.07031	-552.59517	-0.15743	-167.5
SB-2-water	-268.34934	-284.06972	-552.59957	-0.1805	-192
SB-3-water	-268.3333	-284.07197	-552.59247	-0.1872	-199.1
SB-4-water	-268.37591	-284.07399	-552.59741	-0.14751	-156.9
SB-5-water	-268.31825	-284.07118	-552.58827	-0.19885	-211.5
SB-6-water	-268.34263	-284.07214	-552.59398	-0.17921	-190.7
SB-7-water	-268.30331	-284.06946	-552.58419	-0.21141	-224.9
SB-8-water	-268.3124	-284.07134	-552.58562	-0.20188	-214.8
SB-9-water	-268.32977	-284.06992	-552.58966	-0.18997	-202.1
SB-10-water	-268.32817	-284.07115	-552.58998	-0.19066	-202.8
SB-11-water	-268.32978	-284.07069	-552.58991	-0.18944	-201.5
SB-12-water	-268.33016	-284.07098	-552.59145	-0.19031	-202.5

Chapter 7

COSMO Calculations

Methods

The software package used in Chapter 6 is NWChem. We use the 13 optimized geometries for the salt-bridge with 0 to 12 water molecules from Chapter 3, and we performed COSMO calculations[147-152] using B3LYP/6-311++G**on each of the 13 optimized geometries with the dielectric constants at 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75 and 80. The calculations did not converge on the salt bridge with nine waters.

Results and Discussion

The total energy values calculated with the dielectric constants at 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75 and 80 for the 13 molecular clusters are tabulated into tables from Table-7-1 to Table-7-13, and data are plotted as Figure-7-1 to Figure-7-13. It shows in the diagrams, that in the dielectric constants within 20, the total energy decreases sharply as the dielectric constants increase; in the range from 30 to 60, the total energy decreases slowly; over 60, the total energy decreases only slightly.

Table-7-1: Salt bridge with no water in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-552.6288
10	-552.63272
15	-552.63405
20	-552.63472
25	-552.63513
30	-552.6354
35	-552.63559
40	-552.63574
45	-552.63585
50	-552.63594
55	-552.63602
60	-552.63608
65	-552.63613
70	-552.63618
75	-552.63622
80	-552.63625

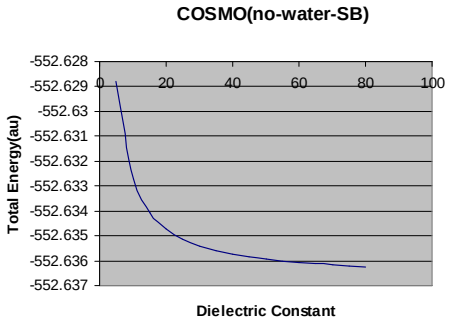


Figure-7-1: Total energy versus dielectric constant for salt-bridge-0-water.

Table-7-2: Salt bridge with one water molecule in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-629.09948
10	-629.1034
15	-629.10474
20	-629.10541
25	-629.10582
30	-629.10609
35	-629.10628
40	-629.10643
45	-629.10654
50	-629.10663
55	-629.10671
60	-629.10677
65	-629.10682
70	-629.10687
75	-629.10691
80	-629.10694

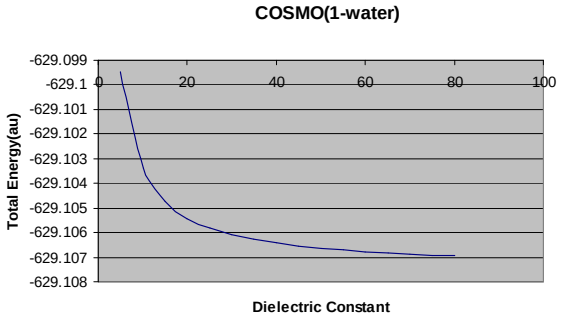


Figure-7-2: Total energy versus dielectric constant for salt-bridge-1-water.

Table-7-3: Salt bridge with two water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-705.58788
10	-705.59193
15	-705.59331
20	-705.59401
25	-705.59442
30	-705.5947
35	-705.5949
40	-705.59505
45	-705.59517
50	-705.59527
55	-705.59534
60	-705.5954
65	-705.59546
70	-705.59551
75	-705.59555
80	-705.59558

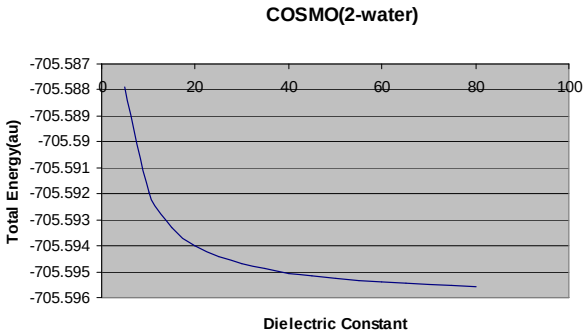


Figure-7-3: Total energy versus dielectric constant for salt-bridge-2-water.

Table-7-4: Salt bridge with three water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-782.06234
10	-782.06673
15	-782.06822
20	-782.06896
25	-782.06941
30	-782.06972
35	-782.06993
40	-782.07009
45	-782.07022
50	-782.07032
55	-782.0704
60	-782.07047
65	-782.07053
70	-782.07058
75	-782.07062
80	-782.07066

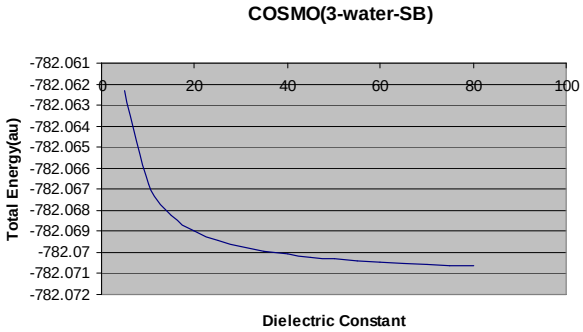


Figure-7-4: Total energy versus dielectric constant for salt-bridge-3-water.

Table-7-5: Salt bridge with four water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-858.54315
10	-858.54746
15	-858.54891
20	-858.54965
25	-858.55009
30	-858.55038
35	-858.55059
40	-858.55075
45	-858.55087
50	-858.55097
55	-858.55105
60	-858.55112
65	-858.55118
70	-858.55122
75	-858.55127
80	-858.5513

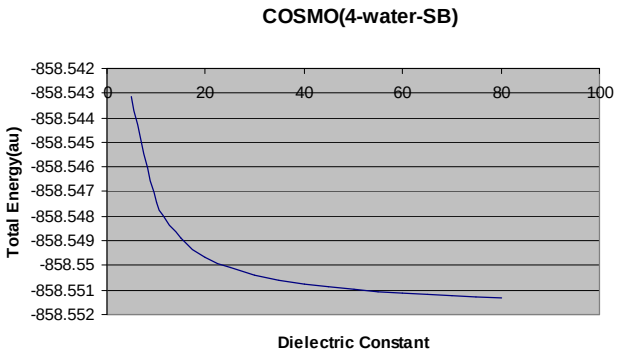


Figure-7-5: Total energy versus dielectric constant for salt-bridge-4-water.

Table-7-6: Salt bridge with five water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-935.0265
10	-935.03131
15	-935.03293
20	-935.03375
25	-935.03424
30	-935.03457
35	-935.03481
40	-935.03498
45	-935.03512
50	-935.03523
55	-935.03532
60	-935.0354
65	-935.03546
70	-935.03551
75	-935.03556
80	-935.0356

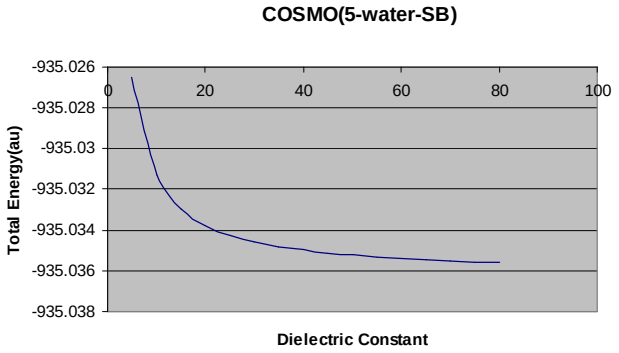


Figure-7-6: Total energy versus dielectric constant for salt-bridge-5-water.

Table-7-7: Salt bridge with six water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-1011.50177
10	-1011.5069
15	-1011.50863
20	-1011.50951
25	-1011.51003
30	-1011.51038
35	-1011.51063
40	-1011.51082
45	-1011.51097
50	-1011.51109
55	-1011.51118
60	-1011.51126
65	-1011.51133
70	-1011.51139
75	-1011.51144
80	-1011.51148

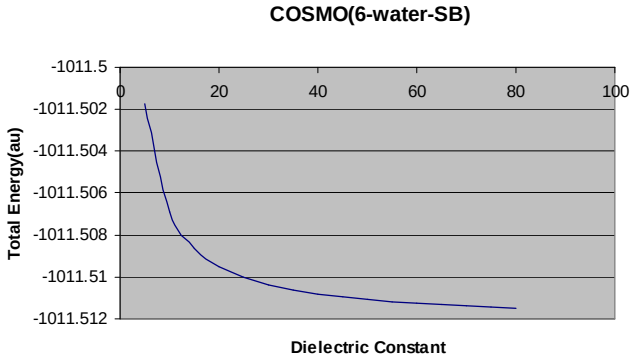


Figure-7-7: Total energy versus dielectric constant for salt-bridge-6-water.

Table-7-8: Salt bridge with seven water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-1087.98459
10	-1087.98961
15	-1087.99131
20	-1087.99216
25	-1087.99268
30	-1087.99302
35	-1087.99327
40	-1087.99345
45	-1087.99359
50	-1087.99371
55	-1087.9938
60	-1087.99388
65	-1087.99395
70	-1087.994
75	-1087.99405
80	-1087.9941

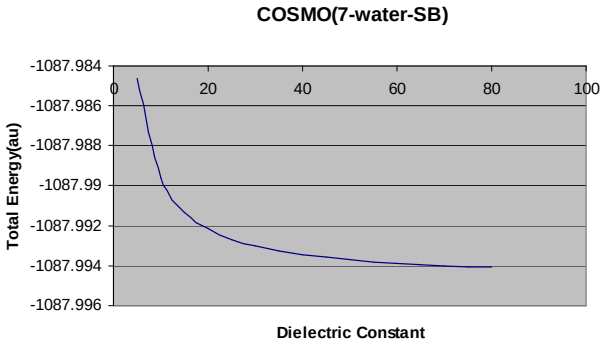


Figure-7-8: Total energy versus dielectric constant for salt-bridge-7-water.

Table-7-9: Salt bridge with eight water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-1164.459
10	-1164.46387
15	-1164.46552
20	-1164.46635
25	-1164.46685
30	-1164.46718
35	-1164.46742
40	-1164.4676
45	-1164.46774
50	-1164.46785
55	-1164.46794
60	-1164.46802
65	-1164.46808
70	-1164.46813
75	-1164.46818
80	-1164.46822

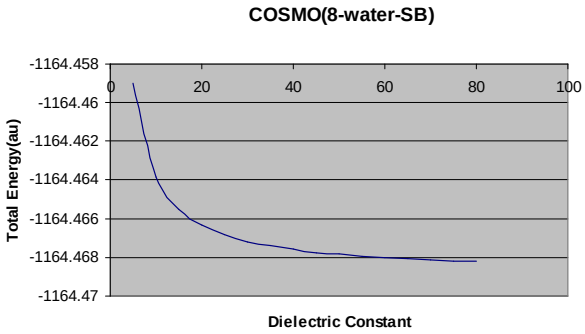


Figure-7-9: Total energy versus dielectric constant for salt-bridge-8-water.

Table-7-10: Salt bridge with ten water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-1317.42027
10	-1317.42669
15	-1317.42886
20	-1317.42996
25	-1317.43062
30	-1317.43106
35	-1317.43137
40	-1317.43161
45	-1317.43179
50	-1317.43194
55	-1317.43206
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70	-1317.43231
75	-1317.43238
80	-1317.43243

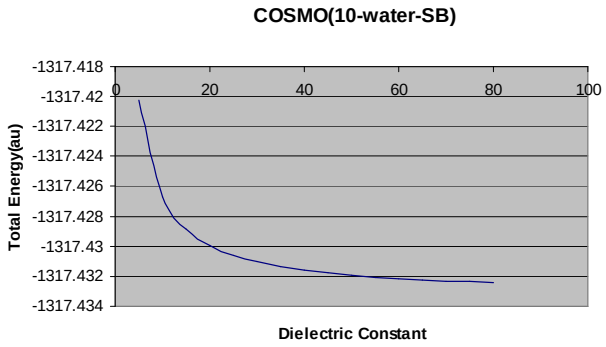

Figure-7-10: Total energy versus dielectric constant for salt-bridge-10-water.

Table-7-11: Salt bridge with eleven water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-1393.8944
10	-1393.90091
15	-1393.90311
20	-1393.90421
25	-1393.90488
30	-1393.90532
35	-1393.90564
40	-1393.90588
45	-1393.90606
50	-1393.90621
55	-1393.90633
60	-1393.90644
65	-1393.90652
70	-1393.90659
75	-1393.90666
80	-1393.90671

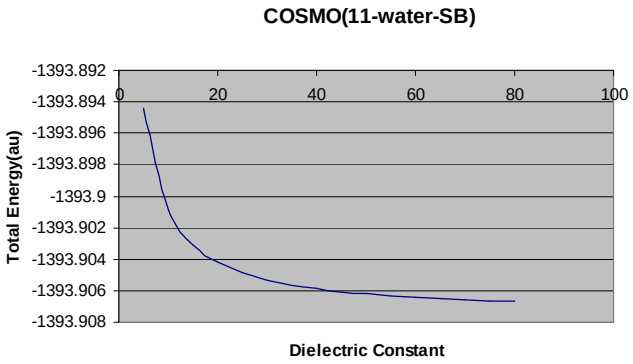

Figure-7-11: Total energy versus dielectric constant for salt-bridge-11-water.

Table-7-12: Salt bridge with twelve water molecules in different dielectric constants

Dielectric constant	Total Energy in atomic unit
5	-1470.37252
10	-1470.37895
15	-1470.38113
20	-1470.38222
25	-1470.38287
30	-1470.38331
35	-1470.38363
40	-1470.38386
45	-1470.38404
50	-1470.38419
55	-1470.38431
60	-1470.38441
65	-1470.3845
70	-1470.38457
75	-1470.38463
80	-1470.38469

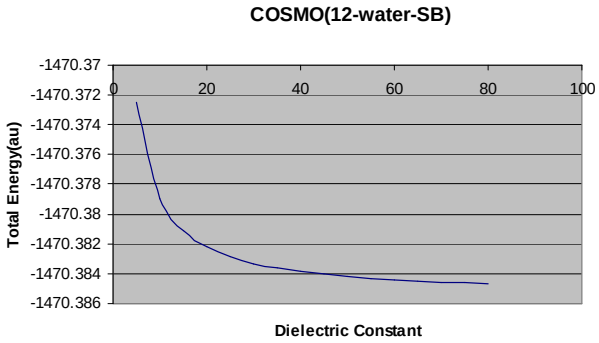

Figure-7-12: Total energy versus dielectric constant for salt-bridge-12-water.

Chapter 8

Frequency Calculations

Methods

The software packages used in Chapter 8 are Gaussian03 and GaussView03. We use the optimized geometries constrained by bridge length for the salt-bridge with zero to twelve water molecules from Chapter 3, and we perform a frequency calculation[153-157] on each of the optimized geometries using B3LYP/6-311++G** at 298K and 1 atmosphere.

Results and Discussion

Frequency calculations in this chapter are mostly concerned with thermodynamic data. These data are given from Table-8-1 to Table-8-15, and show that, at 298K, thermal correction energy values over individual bridge lengths are in the range of about 3 to 5 k_BT. Using a single set of thermodynamic data for Molecular Dynamics simulations can cause errors as high as 5 k_BT. Each water molecule adds about 0.02 atomic units (au) to the Gibbs free energy correction, so these are probably mostly the internal degrees of freedom of the water.

Table-8-1: Thermodynamic data of salt bridge with no water
(Temperature 298 Kelvin; Pressure 1 Atmosphere, same conditions for data in this chapter)

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy(au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy(au)	Thermal correction to Gibbs Free Energy(au)
3.3	0.22211	0.23622	0.19441	0.23716	0.1792
3.4	0.22204	0.23695	0.20891	0.2379	0.17561
3.5	0.22199	0.23671	0.19898	0.23765	0.17833
3.6	0.22185	0.23643	0.19678	0.23737	0.17871
3.7	0.22165	0.23613	0.19565	0.23707	0.17874
3.8	0.22139	0.23581	0.19585	0.23675	0.17836
3.9	0.22102	0.23548	0.20025	0.23643	0.17672
4.0	0.22109	0.23551	0.20314	0.23645	0.17589
4.1	0.22118	0.23456	0.18808	0.2355	0.17942
4.2	0.22132	0.2346	0.18792	0.23554	0.17951
4.3	0.2234	0.23783	0.19834	0.23878	0.17964
4.4	0.22346	0.23781	0.19653	0.23875	0.18016

Table-8-2: Thermodynamic data of salt bridge with one water molecule

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy(au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy(au)	Thermal correction to Gibbs Free Energy(au)
3.5	0.24697	0.26411	0.21809	0.26505	0.20003
3.6	0.24689	0.26515	0.2327	0.2661	0.19672
3.7	0.24668	0.26404	0.22131	0.26499	0.199
3.8	0.24714	0.26492	0.22745	0.26586	0.19805
3.9	0.2471	0.26479	0.22675	0.26573	0.19813
4.0	0.24727	0.26482	0.22478	0.26576	0.19875
4.1	0.24772	0.26508	0.22291	0.26602	0.19956
4.2	0.24811	0.26532	0.22182	0.26627	0.20013
4.3	0.24921	0.26627	0.21719	0.26722	0.20246
4.4	0.24864	0.26579	0.22248	0.26674	0.2004

Table-8-3: Thermodynamic data of salt bridge with two waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy(au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy(au)	Thermal correction to Gibbs Free Energy(au)
3.4	0.27354	0.29348	0.24414	0.29443	0.22164
3.5	0.2734	0.29339	0.24393	0.29434	0.22161
3.6	0.27318	0.29327	0.24541	0.29422	0.22105
3.7	0.27323	0.29335	0.24504	0.29429	0.22123
3.8	0.27327	0.29338	0.24302	0.29433	0.22187
3.9	0.27329	0.29343	0.2428	0.29438	0.22199
4.0	0.27327	0.29348	0.24363	0.29443	0.22179
4.1	0.27324	0.2935	0.24453	0.29444	0.22153
4.2	0.26952	0.28819	0.2282	0.28913	0.22109
4.3	0.27317	0.29249	0.23491	0.29344	0.2234
4.4	0.27297	0.29232	0.23666	0.29327	0.2227

Table-8-4: Thermodynamic data of salt bridge with three waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy(au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy(au)	Thermal correction to Gibbs Free Energy(au)
3.4	0.29979	0.32208	0.25992	0.32303	0.24553
3.5	0.29943	0.32189	0.25941	0.32283	0.24549
3.6	0.2993	0.32172	0.26067	0.32267	0.24495
3.7	0.29897	0.32154	0.26272	0.32249	0.24416
3.8	0.29875	0.32142	0.26324	0.32237	0.24388
3.9	0.29868	0.32143	0.26379	0.32237	0.24372
4.0	0.29865	0.32145	0.26267	0.3224	0.24408
4.1	0.29859	0.32148	0.26345	0.32242	0.24387
4.2	0.29852	0.3215	0.26532	0.32244	0.24333
4.6	0.29877	0.32053	0.25257	0.32148	0.24617
4.8	0.29819	0.31996	0.25414	0.3209	0.24513

Table-8-5: Thermodynamic data of salt bridge with four waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy(au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy(au)
3.5	0.32566	0.35045	0.28155	0.35139	0.26745
3.6	0.32578	0.3505	0.27819	0.35145	0.26851
3.7	0.32578	0.3505	0.27688	0.35144	0.26889
3.8	0.32564	0.35043	0.27781	0.35138	0.26855
3.9	0.32536	0.35029	0.27915	0.35123	0.268
4.0	0.32519	0.35021	0.27919	0.35115	0.26791
4.1	0.32517	0.35025	0.27952	0.35119	0.26785
4.2	0.32515	0.35028	0.28039	0.35123	0.26763
4.3	0.32514	0.35035	0.28366	0.3513	0.26672
4.4	0.32586	0.35061	0.27605	0.35156	0.26925
4.5	0.3257	0.35047	0.27603	0.35142	0.26912
4.6	0.32533	0.35024	0.28358	0.35119	0.26664
4.8	0.3249	0.35006	0.28473	0.351	0.26611

Table-8-6: Thermodynamic data of salt bridge with five waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy (au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy(au)	Thermal correction to Gibbs Free Energy(au)
3.4	0.35217	0.37918	0.29602	0.38012	0.29187
3.5	0.35189	0.37903	0.29338	0.37997	0.2925
3.6	0.35189	0.37903	0.29143	0.37997	0.29308
3.7	0.35205	0.37915	0.29093	0.38009	0.29335
3.8	0.35188	0.37908	0.29335	0.38002	0.29256
3.9	0.35203	0.37917	0.29093	0.38012	0.29337
4.0	0.35197	0.37912	0.28998	0.38006	0.2936
4.1	0.35189	0.37905	0.28927	0.37999	0.29375
4.2	0.35174	0.37896	0.29047	0.37991	0.2933
4.3	0.35155	0.37887	0.29404	0.37981	0.29215
4.4	0.35139	0.37786	0.28538	0.3788	0.29371
4.5	0.35151	0.3778	0.28316	0.37874	0.29432
4.6	0.35168	0.3787	0.29096	0.37965	0.2929
4.7	0.35168	0.37864	0.29042	0.37959	0.293

Table-8-7: Thermodynamic data of salt bridge with six waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy(au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy(au)	Thermal correction to Gibbs Free Energy(au)
3.5	0.37611	0.40266	0.28486	0.40361	0.31868
3.6	0.37625	0.40275	0.2829	0.4037	0.31935
3.7	0.37642	0.40459	0.30464	0.40553	0.3147
3.8	0.37642	0.40459	0.30464	0.40553	0.3147
3.9	0.37675	0.40655	0.31563	0.40749	0.31339
4.0	0.3766	0.40553	0.304	0.40647	0.31584
4.1	0.3765	0.40546	0.30369	0.4064	0.31586
4.2	0.37653	0.40646	0.3173	0.4074	0.3128
4.3	0.37644	0.40556	0.30735	0.4065	0.31487
4.4	0.37623	0.40551	0.31342	0.40645	0.313
4.5	0.37606	0.40357	0.29295	0.40452	0.31717
4.6	0.37601	0.40433	0.3044	0.40528	0.31452
4.7	0.37629	0.40355	0.29098	0.40449	0.31774
4.8	0.37628	0.40442	0.30294	0.40537	0.31505

Table-8-8: Thermodynamic data of salt bridge with seven waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy (au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)
3.5	0.40288	0.43337	0.31452	0.43431	0.34054
3.6	0.40349	0.43372	0.30974	0.43466	0.34231
3.7	0.40323	0.43458	0.32133	0.43553	0.33972
3.8	0.40361	0.43474	0.31561	0.43568	0.34159
3.9	0.40378	0.43576	0.32746	0.4367	0.33907
4.0	0.40373	0.43568	0.32394	0.43662	0.34004
4.1	0.40348	0.43551	0.3243	0.43646	0.33977
4.2	0.40319	0.43537	0.32668	0.43632	0.33892
4.3	0.40312	0.43532	0.32698	0.43627	0.33878
4.4	0.40303	0.43532	0.33233	0.43627	0.33718
4.5	0.4028	0.4343	0.32709	0.43525	0.33773
4.6	0.40287	0.43331	0.31321	0.43426	0.34088
4.7	0.403	0.43322	0.31029	0.43416	0.34165
4.8	0.40284	0.43314	0.31159	0.43409	0.34119
4.9	0.40244	0.43297	0.31847	0.43391	0.33896
5.0	0.40229	0.43285	0.32004	0.4338	0.33838

Table-8-9: Thermodynamic data of salt bridge with eight waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy (au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)
3.6	0.42866	0.46148	0.32838	0.46243	0.36452
3.7	0.42792	0.46134	0.33578	0.46228	0.36217
3.8	0.42833	0.46226	0.33771	0.4632	0.36251
3.9	0.42823	0.4623	0.34028	0.46324	0.36179
4.0	0.42819	0.46317	0.35125	0.46411	0.35938
4.1	0.42799	0.46304	0.351	0.46398	0.35933
4.2	0.4277	0.46284	0.35228	0.46379	0.35876
4.3	0.4276	0.46288	0.35416	0.46382	0.35823
4.4	0.42745	0.46188	0.34853	0.46282	0.35891
4.5	0.42716	0.45989	0.33107	0.46083	0.36213
4.6	0.427	0.45981	0.3329	0.46076	0.3615
4.7	0.42703	0.45975	0.33372	0.4607	0.3612
4.8	0.42691	0.45967	0.33638	0.46061	0.36032
4.9	0.42692	0.45862	0.32207	0.45957	0.36354
5.0	0.42685	0.45952	0.33628	0.46047	0.36021

Table-8-10: Thermodynamic data of salt bridge with nine waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy (au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)
3.5	0.45438	0.48971	0.35066	0.49066	0.38611
3.6	0.45489	0.49143	0.36061	0.49237	0.38486
3.7	0.45365	0.48893	0.35283	0.48987	0.38468
3.8	0.45515	0.49006	0.34272	0.491	0.38882
3.9	0.45513	0.49003	0.34177	0.49098	0.38908
4.0	0.45519	0.49183	0.36227	0.49277	0.38476
4.1	0.455	0.49164	0.36051	0.49259	0.3851
4.2	0.45481	0.49158	0.3626	0.49252	0.38441
4.3	0.4546	0.49151	0.36545	0.49246	0.3835
4.4	0.4544	0.49132	0.36664	0.49226	0.38295
4.5	0.45407	0.49017	0.35973	0.49111	0.38386
4.6	0.45383	0.48908	0.35104	0.49003	0.38536
4.7	0.45365	0.48893	0.35283	0.48987	0.38468
4.8	0.45368	0.48893	0.35339	0.48988	0.38451
4.9	0.4536	0.48881	0.35236	0.48975	0.3847
5.0	0.45355	0.48867	0.35181	0.48962	0.38473

Table-8-11: Thermodynamic data of salt bridge with ten waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy (au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)
3.5	0.48027	0.51959	0.3857	0.52053	0.40554
3.6	0.48031	0.51962	0.38513	0.52056	0.40573
3.7	0.48021	0.51949	0.38422	0.52043	0.40588
3.8	0.47951	0.51743	0.37258	0.51838	0.40729
3.9	0.47985	0.51768	0.36623	0.51863	0.40943
4.0	0.4799	0.51855	0.37433	0.5195	0.40789
4.1	0.47978	0.51936	0.38623	0.52031	0.40515
4.2	0.4796	0.51924	0.38649	0.52018	0.40495
4.3	0.47938	0.51907	0.38767	0.52002	0.40443
4.4	0.47913	0.51905	0.39832	0.52	0.40124
4.5	0.47892	0.51798	0.38585	0.51893	0.40388
4.6	0.47868	0.51591	0.3646	0.51686	0.40815
4.7	0.47869	0.5168	0.37791	0.51775	0.40507
4.8	0.47848	0.51578	0.36843	0.51673	0.40688
4.9	0.4786	0.51483	0.35559	0.51577	0.40975
5.0	0.47857	0.5157	0.37032	0.51664	0.40623

Table-8-12: Thermodynamic data of salt bridge with eleven waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy (au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)
3.5	0.5053	0.54734	0.40612	0.54829	0.4272
3.6	0.50496	0.54722	0.41261	0.54816	0.42514
3.7	0.50519	0.54737	0.40938	0.54832	0.42626
3.8	0.50472	0.54548	0.39255	0.54642	0.42938
3.9	0.5049	0.54552	0.38859	0.54646	0.4306
4.0	0.50495	0.5474	0.41163	0.54835	0.42562
4.1	0.50478	0.54729	0.41027	0.54823	0.42591
4.2	0.50446	0.54711	0.41504	0.54805	0.42431
4.3	0.50427	0.54694	0.41148	0.54788	0.4252
4.4	0.50406	0.54679	0.41528	0.54774	0.42392
4.5	0.50382	0.54562	0.40515	0.54657	0.42577
4.6	0.50365	0.54458	0.3962	0.54552	0.4274
4.7	0.50354	0.54449	0.3972	0.54543	0.42701
4.8	0.50358	0.54443	0.39652	0.54537	0.42715
4.9	0.5035	0.54435	0.3969	0.54529	0.42695
5.0	0.50343	0.54427	0.39726	0.54522	0.42677

Table-8-13: Thermodynamic data of salt bridge with twelve waters

Bridge-length(A)	Zero-point correction (au)	Thermal correction to Energy (au)	Thermal correction to Entropy ($1x10^{-3}$au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)
3.5	0.5307	0.57378	0.41371	0.57472	0.45137
3.6	0.5304	0.57353	0.41576	0.57448	0.45052
3.7	0.53094	0.57476	0.42038	0.5757	0.45037
3.8	0.53115	0.57415	0.4083	0.5751	0.45336
3.9	0.53089	0.57395	0.4088	0.5749	0.45301
4.0	0.53047	0.57375	0.41547	0.57469	0.45082
4.1	0.53047	0.57463	0.42312	0.57558	0.44942
4.2	0.5306	0.57559	0.43535	0.57654	0.44674
4.3	0.53074	0.57568	0.42954	0.57663	0.44856
4.4	0.53056	0.57464	0.4234	0.57558	0.44934
4.5	0.53042	0.57442	0.42268	0.57536	0.44934
4.6	0.53016	0.57333	0.41482	0.57427	0.4506
4.7	0.52999	0.57151	0.39622	0.57245	0.45432
4.8	0.52987	0.57132	0.39618	0.57226	0.45414
4.9	0.52999	0.57134	0.39625	0.57228	0.45414
5.0	0.52953	0.57104	0.39809	0.57199	0.4533

Chapter 9

NBO Calculations

Methods

The software packages used in Chapter 9 are Gaussian03 and GaussView3.0. We use the optimized geometries constrained by bridge length for the salt-bridge with zero to twelve water molecules from Chapter 3, and we perform NBO calculations[158-160] on each of the optimized geometries using B3LYP/6-311++G**. Detailed Wiberg bond order tables are given in appendix C.

Results and Discussion

Part 1: The NBO results show us that the local minimum at 3.46 angstroms in the potential diagram of Figure-3-2 is due to the transfer of the proton from propionic acid to ethylguanidine. The NBO calculation also may lead to an experimental check on the work (see discussion at the end of Chapter 11).

In Figure-3-1, the transfer of the Hydrogen-12 or the Hydrogen-15 from acid to base is defined as salt bridge ionization. The Wiberg indices of these two hydrogen atoms change rapidly at the bridge length of 3.46 angstroms, as shown in Figure-9-1, indicating the proton ionization of propionic acid.

Table-9-1: Wiberg indices of the two ionizabe hydrogen atoms for salt bridge with no water

Bridge length (A)	Total Energy (au)	Wiberg Index				
		12H-10N	12H-17O	15H-13N	15H-16O	Sum of the bond order
3.10	-552.58512	0.1874	0.5496	0.8341	0.0002	1.5713
3.20	-552.5887	0.1728	0.5609	0.8353	0.0002	1.5692
3.30	-552.59125	0.1585	0.5718	0.8364	0.0002	1.5669
3.40	-552.59307	0.1526	0.5761	0.8370	0.0002	1.5659
3.43	-552.59359	0.1485	0.5789	0.8367	0.0002	1.5643
3.46	-552.59394	0.1469	0.5800	0.8368	0.0002	1.5639
3.50	-552.58983	0.5504	0.2332	0.6466	0.1407	1.5709
3.60	-552.59468	0.5668	0.2157	0.6270	0.1588	1.5683
3.70	-552.59837	0.5747	0.2061	0.6219	0.1616	1.5643
3.80	-552.60076	0.5796	0.1984	0.6289	0.1513	1.5582
3.90	-552.60111	0.5985	0.1743	0.6409	0.1335	1.5472
4.00	-552.59967	0.6181	0.1493	0.6525	0.1167	1.5366
4.10	-552.59641	0.6356	0.1269	0.6666	0.0984	1.5275
4.20	-552.59197	0.6514	0.1070	0.6795	0.0821	1.52
4.30	-552.58708	0.6644	0.0907	0.6928	0.0668	1.5147
4.40	-552.58157	0.6784	0.0755	0.7051	0.0547	1.5137

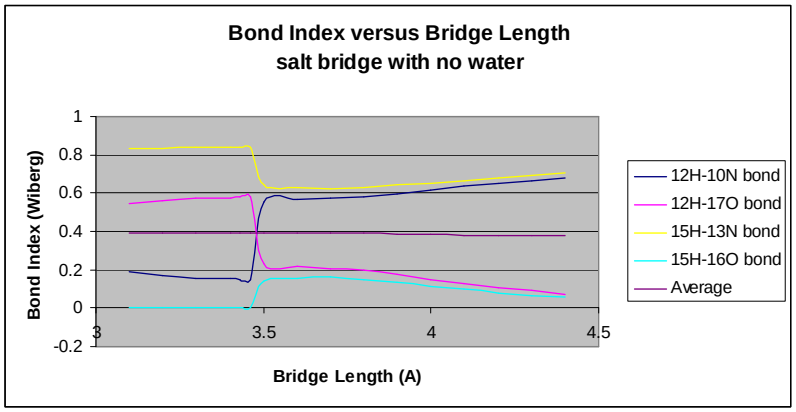

Figure-9-1: Bridge length (angstroms) versus Wiberg index of the four bonds of the two ionizable hydrogen atoms, showing rapid changes of indices at 3.46 angstroms.

Relations between bond lengths and Wiberg indices largely depend on bond types and the specific structural environments. In Table-9-2, we tabulate several data points of bond length versus Wiberg index for salt bridge with seven water molecules (refer to Figure-9-5 for the corresponding locations of hydrogen bonding). As shown in Figure-9-2, in general, for the same bonding types in similar structural environments, Wiberg indices decrease as bond lengths increase.

Table-9-2: Bond length versus Wiberg Index for salt bridge with seven waters (at bridge length of 4.0 Å)

Bond between Atoms	Bond Length (Å)	Wiberg Index
19O-37H	1.70540	0.0699
22O-31H	1.71566	0.0769
13O-28H	1.72324	0.0601
26O-27H	1.75043	0.0620
13O-20H	1.84121	0.0430
12O-21H	1.90435	0.0249
32O-36H	1.91817	0.0270
38O-23H	1.94092	0.0295
38O-34H	1.94735	0.0261
25O-18H	2.01758	0.0199

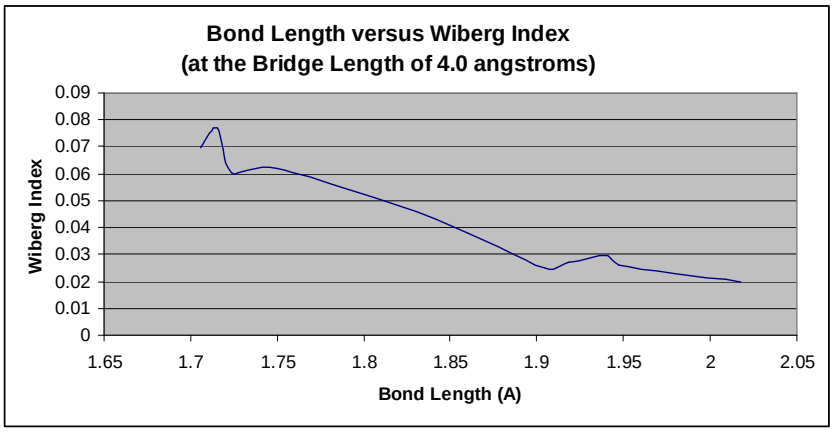

Figure-9-2: Bond length versus Wiberg Index for salt bridge with seven waters at bridge length of 4.0 Å.

Part 2: We can understand how the water molecules incorporate into the salt bridge system following the so-called “build-up rule” as we proposed in Chapter 2.

The figures displayed below are focused on the ring structures of the salt bridge system, indicating the labels and numbers of hydrogen bonding (For the overall geometries, please refer to Figure-2-6 to Figure-2-13 in Chapter 2).

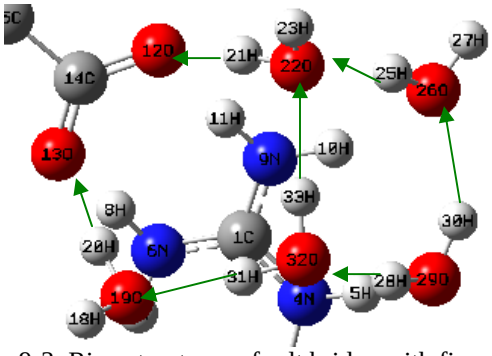

Figure-9-3: Ring structures of salt bridge with five waters.

Table-9-3: Wiberg indices of the ring structures for salt bridge with 5 waters

Bridge Length (Å)	Wiberg Index							
	5-oxygen-member-ring				4-oxygen-member-ring			
	12O-21H	22O-33H	19O-31H	13O-20H	32O-28H	22O-33H	22O-25H	26O-30H
3.80	0.0625	0.0203	0.0386	0.0577	0.0506	0.0203	0.0428	0.0142
4.00	0.0642	0.0199	0.0346	0.0519	0.0462	0.0199	0.0434	0.0150
4.20	0.0714	0.0210	0.0350	0.0571	0.0465	0.0210	0.0463	0.0149

Examining the data in Table-9-3, we notice the lowest bond order is the bond between 26O and 30H in the 4-oxygen-member ring, and we predict the next water molecule will come in at this 26O-30H bond and form a 5-oxygen-member ring while the other 5-oxygen-member (13O-12O-22O-32O-19O) remains intact. Comparing Figure-9-4 with Figure-9-3, we notice salt-bridge-6-water does have two five-oxygen-member rings while salt-bridge-5-water only has one five-oxygen-member ring and one 4-oxygen-member ring. It suggests that one of the five-oxygen-member rings of salt-bridge-6-water is formed by breaking the four-oxygen-member ring of salt-bridge-5-water. So, it seems our prediction is reasonable.

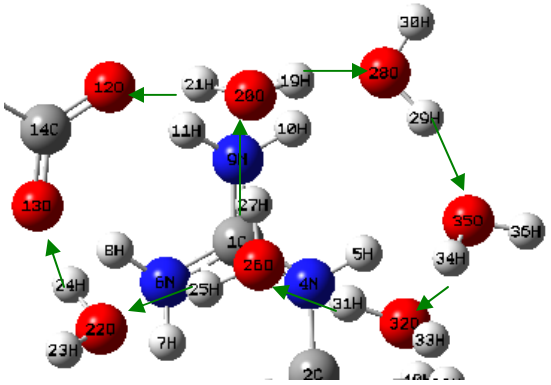

Figure-9-4: Ring structures of salt bridge with six waters.

Table-9-4: Wiberg indices of the ring structures for salt bridge with 6 waters

Bridge Length (Å)	Wiberg Index								
	Ring-12O-20O-26O-22O-13O				Ring-20O-26O-32O-35O-28O				
	12O-21H	20O-27H	22O-25H	13O-24H	20O-27H	26O-31H	32O-34H	35O-29H	28O-19H
3.80	0.0262	0.0547	0.0369	0.0467	0.0547	0.0943	0.0838	0.0480	0.0218
4.00	0.0294	0.0557	0.0406	0.0556	0.0557	0.0991	0.0840	0.0445	0.0192
4.20	0.0309	0.0561	0.0414	0.0600	0.0561	0.1006	0.0864	0.0443	0.0175

Next, looking at Table-9-4, we notice the lowest bond order is the bond between 28O and 19H, where the 28O-19H bond is in the 5-oxygen-member ring away from the two oxygen atoms of the carboxyl group, so we predict when the next water molecule will break this 28O-19H bond, while the other 5-oxygen-member ring of carboxyl group should remain intact. Comparing Figure-9-5 with Figure-9-4, we observe that this 28O-19H bond does break and two 4-oxygen-member rings are formed while the 5-oxygen-member ring of the carboxyl group remains intact.

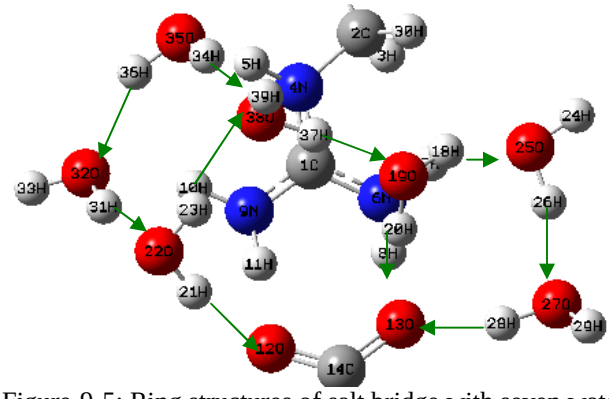

Figure-9-5: Ring structures of salt bridge with seven waters.

Table-9-5: Wiberg indices of the ring structures for salt bridge with 7 waters

Bridge Length (Å)	Wiberg Index				
	12O-21H	38O-23H	190-37H	13O-20H	5-oxygen-member-ring
3.80	0.0220	0.0299	0.0700	0.0411	
4.00	0.0249	0.0295	0.0699	0.0430	
4.20	0.0248	0.0288	0.0697	0.0410	
	13O-20H	25O-18H	26O-27H	13O-28H	4-oxygen-member-ring
3.80	0.0411	0.0193	0.0588	0.0564	
4.00	0.0430	0.0199	0.0620	0.0601	
4.20	0.0410	0.0198	0.0636	0.0642	
	38O-23H	38O-34H	32O-36H	22O-31H	4-oxygen-member-ring
3.80	0.0299	0.0256	0.0273	0.0747	
4.00	0.0295	0.0261	0.0270	0.0769	
4.20	0.0288	0.0263	0.0273	0.0786	

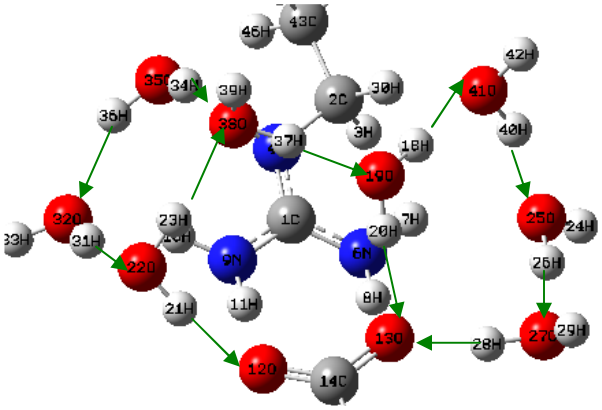

Figure-9-6: Ring structures of salt bridge with eight waters.

Table-9-6: Wiberg indices of the ring structures for salt bridge with 8 waters

Bridge Length (Å)	Wiberg Index				5-oxygen-member-ring
	12O-21H	38O-23H	190-37H	13O-20H	
3.80	0.0217	0.0333	0.0815	0.0368	
4.00	0.0232	0.0323	0.0793	0.0347	
4.20	0.0234	0.0317	0.0793	0.0331	
	13O-20H	41O-18H	25O-40H	27O-26H	13O-28H
3.80	0.0368	0.0377	0.0460	0.0732	0.0685
4.00	0.0347	0.0367	0.0465	0.0768	0.0754
4.20	0.0331	0.0359	0.0467	0.0786	0.0802
	38O-23H	38O-34H	32O-36H	22O-31H	
3.80	0.0333	0.0265	0.0255	0.0758	
4.00	0.0323	0.0266	0.0252	0.0781	4-oxygen-member-ring
4.20	0.0317	0.0267	0.0255	0.0800	

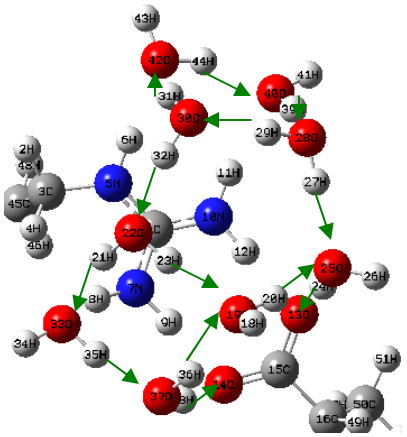

Figure-9-7: Ring structures of salt bridge with nine waters.

Table-9-7: Wiberg indices of the ring structures for salt bridge with 9 waters

Bridge Length (Å))	Wiberg Index				
	14O-38H	19O-36H	25O-20H	13O-24H	5-oxygen-member-ring
3.80	0.0311	0.0271	0.0517	0.0808	
4.00	0.0337	0.0263	0.0527	0.0851	
4.20	0.0355	0.0257	0.0540	0.0870	
	19O-23H	22O-32H	30O-29H	25O-27H	25O-20H
3.80	0.0271	0.0411	0.0603	0.0304	0.0517
4.00	0.0277	0.0414	0.0591	0.0308	0.0527
4.20	0.0282	0.0411	0.0576	0.0320	0.0540
	28O-39H	30O-29H	42O-31H	40O-44H	4-oxygen-member-ring
3.80	0.1074	0.0603	0.0180	0.0546	
4.00	0.1088	0.0591	0.0172	0.0555	
4.20	0.1102	0.0576	0.0165	0.0574	
	37O-35H	33O-21H	19O-23H	19O-36H	4-oxygen-member-ring
3.80	0.0807	0.0233	0.0271	0.0271	
4.00	0.0819	0.0236	0.0277	0.0263	
4.20	0.0830	0.0235	0.0282	0.0257	

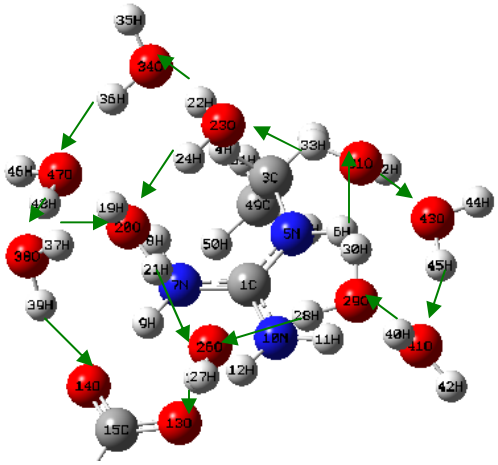

Figure-9-8: Ring structures of salt bridge with ten waters.

Table-9-8: Wiberg indices of the ring structures for salt bridge with 10 waters

Bridge Length (Å)	Wiberg Index				
	14O-39H	20O-37H	26O-21H	13O-25H	
3.80	0.0395	0.0419	0.0616	0.0982	5-oxygen-member-ring
4.00	0.0365	0.0283	0.0525	0.0852	
4.20	0.0386	0.0275	0.0527	0.0886	
	20O-37H	20O-24H	34O-22H	47O-36H	38O-48H
3.80	0.0419	0.0298	0.0438	0.0603	0.1060
4.00	0.0283	0.0272	0.0337	0.0494	0.0922
4.20	0.0275	0.0278	0.0336	0.0504	0.0946
	26O-21H	26O-28H	31O-30H	23O-33H	20O-24H
3.80	0.0616	0.0362	0.0723	0.0589	0.0298
4.00	0.0525	0.0297	0.0627	0.0443	0.0272
4.20	0.0527	0.0302	0.0617	0.0445	0.0278
	29O-40H	41O-45H	43O-32H	31O-30H	
3.80	0.1205	0.0596	0.0185	0.0723	
4.00	0.1083	0.0562	0.0177	0.0627	4-oxygen-member-ring
4.20	0.1107	0.0576	0.0171	0.0617	

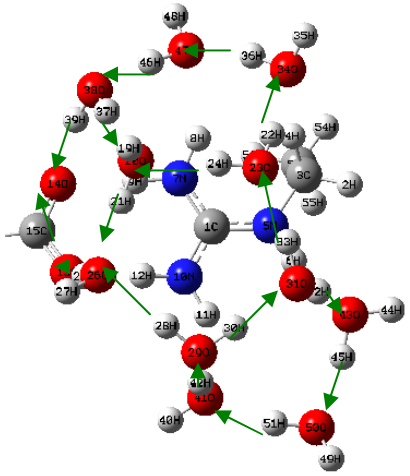

Figure-9-9: Ring structures of salt bridge with eleven waters.

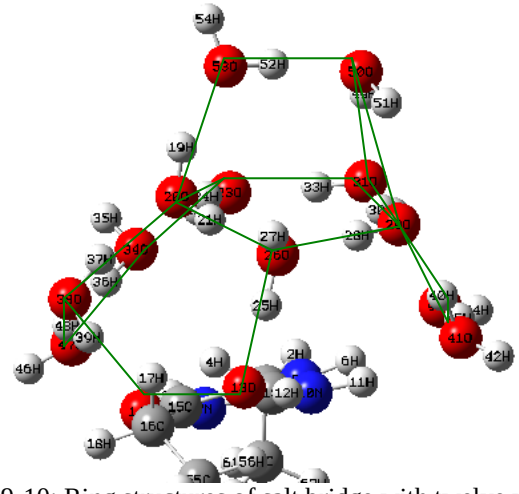

Figure-9-10: Ring structures of salt bridge with twelve waters.

Also, we notice in Table-9-5, the lowest bond order is the bond between 25O and 18H, which is in the 5-member-oxygen ring of carboxyl group, so the eighth water will attack this 25O-18H bond.

Following the above steps: first by looking for the lowest bond order in the tables, then predicting this bond with the lowest bond order will be broken by the next coming water molecule, we can formulate the “build-up rule” for the first water shell.

The general rules are, (1) the 5-oxygen-member that includes two oxygen atoms of the carboxyl group is the most stable ring, remaining intact in the building up process, (2) 5-oxygen-member-rings are more stable than 4-oxygen-member rings, (3) when there are two 4-oxygen-member rings, one away from the alpha hydrogen atom of ethylguanidine is expected to break as water molecules are added into the system.

After the eleventh and then the twelfth water enter into the system, and we believe, so on after, all the rings are 5-member-oxygen rings, and the rings are formed into three dimensional networks.

Chapter 10

Salt Bridge of Propionic Acid and Propyl Amine

Part-1: Finding Geometry of lowest minimum

Methods

Software packages used in Chapter 10 are Gaussian 03 and GaussView03.

We perform optimization calculations on a salt bridge formed by propionic acid and propyl amine with various initial arrangements that conceivably can lead to the geometry of the lowest minimum. We also do optimization calculations on the salt bridge with one water molecule.

Started with a low level method, HF/3-21G*, after the initial structure is optimized, then it is further optimized at the level of B3LYP/6-311++G**.

We do not prove that the lowest minimum we find is the true global minimum, although we have no reason to doubt that it is. We have not run frequency calculations on these two clusters.

Results and Discussion

The two optimized geometries are shown in Figure-10-1 and Figure-10-2. It shows, in Figure-10-1, that the hydrogen atom on propionic acid incorporates into the lone electron pairs of the nitrogen atom on propylamine. In Figure-10-2, it seems 22O-25H-26O-8H-7N-24H-23O forming a ring-like structure.

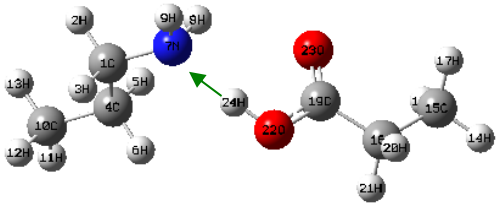

Figure-10-1: The optimized geometry of Propionic-propanylamine-0-water, calculated by Gaussian 03/B3LYP/6-311++G**; green arrow indicated hydrogen bonding.

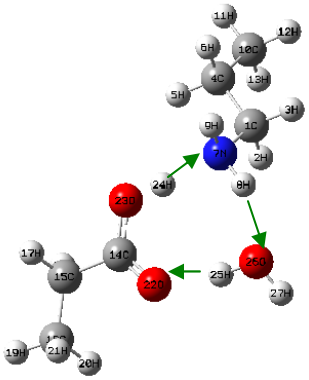

Figure-10-2: The optimized geometry of Propionic-propanylamine-1-water, calculated by Gaussian 03/B3LYP/6-311++G**; green arrows indicated a hydrogen bonding network.

Part-2: Bridge Length Versus Total Energy

Methods

Starting with the optimized geometries from Part-1, we define the bridge length as the distance between the two closest carbon atoms: one from the propionic acid and the other from the propylamine, as shown in figures from Figure-10-1. The bridge length for this propionic-propanylamine-0-water is the distance between the carbon-1C and carbon-19C. Systematically, the bridge length is expanded in 0.1 angstroms at each step. Applying constraints to the bridge length, the system is optimized at the level of HF/3-21G*, and then subsequently, is further optimized at the level of B3LYP/6-311++G**. The energy values are converted into k_BT units. The data are plotted into the diagrams in Figure-10-3 and Figure-10-4.

Results and Discussion

The data for the bridge lengths versus the energy values are tabulated in Table-10-1. In Figure-10-3, for this salt bridge with no water, we notice that there is a local minimum at the bridge length of 3.6A, which is similar to the other salt bridge formed by propionic acid and ethylguanidine in Chapter 3. It suggests that the cause for this local minimum is also due to the proton transfer from propionic acid to propylamine. With an addition of one water molecule into this salt bridge, as shown in Figure-9-4, the local minimum disappears, which is also similar to that salt bridge with one water in Chapter 3.

Table-10-1: Bridge length and total energy with no water

Bridge Length (Å)	Total Energy(au)	Difference from Opt in atomic unit	Difference from Opt in k_BT at 298K
3.0	-443.04163	0.01147	12.1
3.1	-443.04451	0.00859	9.1
3.2	-443.04691	0.00619	6.6
3.3	-443.04888	0.00421	4.5
3.4	-443.05045	0.00264	2.8
3.5	-443.05165	0.00145	1.5
3.6	-443.05248	0.00061	0.7
3.7	-443.04693	0.00617	6.5
3.8	-443.04882	0.00428	4.5
3.9	-443.0503	0.00279	3
4.0	-443.05139	0.00171	1.8
4.1	-443.05211	0.00098	1
4.2	-443.0526	0.0005	0.5
4.3	-443.05291	0.00018	0.2
4.4	-443.05305	4.08E-05	0
4.5	-443.05309	0	0
4.6	-443.05297	0.00012	0.1
4.7	-443.0527	0.0004	0.4
4.8	-443.05234	0.00076	0.8
4.9	-443.05182	0.00127	1.4
5.0	-443.05093	0.00217	2.3
5.1	-443.05003	0.00307	3.3
5.3	-443.04767	0.00543	5.8
5.5	-443.04551	0.00758	8

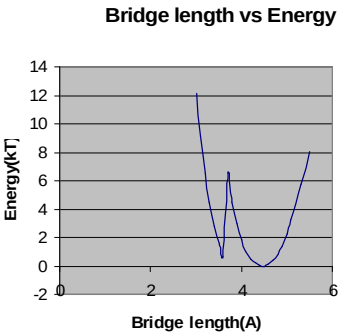

Figure-10-3: Bridge length in angstroms versus total energy in k_BT for propionic-propanylamine-0-water.

Table-10-2: Bridge length and total energy with one water molecule

Bridge Length (Å)	Total Energy(au)	Difference from Opt in atomic unit	Difference from Opt in k_BT at 298K
3.0	-519.48483	0.04387	46.5
3.1	-519.4881	0.04061	43
3.2	-519.47387	0.05484	58.1
3.3	-519.48359	0.04511	47.8
3.4	-519.49242	0.03629	38.4
3.5	-519.50024	0.02847	30.2
3.6	-519.50438	0.02432	25.8
3.7	-519.51237	0.01633	17.3
3.8	-519.51586	0.01284	13.6
3.9	-519.5201	0.0086	9.1
4.0	-519.52294	0.00576	6.1
4.1	-519.52543	0.00327	3.5
4.2	-519.52694	0.00177	1.9
4.3	-519.52817	0.00054	0.6
4.4	-519.52871	0	0
4.5	-519.5286	0.00011	0.1
4.6	-519.52806	0.00065	0.7
4.7	-519.52708	0.00162	1.7
4.8	-519.52582	0.00288	3.1
4.9	-519.52423	0.00448	4.8
5.0	-519.52286	0.00585	6.2
5.2	-519.51984	0.00887	9.4
5.4	-519.51714	0.01157	12.3
5.6	-519.51481	0.0139	14.7
6.0	-519.51176	0.01695	18

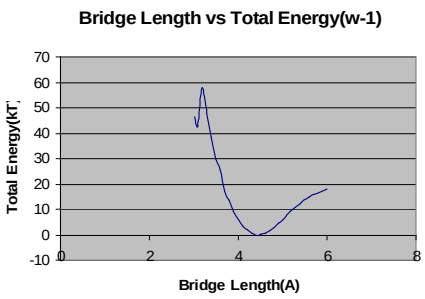

Figure-10-4: Bridge length in angstroms versus total energy in k_BT for propionic-propanylamine-1-water.

Chapter 11

Conclusion

As stated in the introduction, improvements for salt bridge potentials used in various structural and functional environments are the main focus of our project. Contributions made to this goal may be summarized from several points of view.

(A) *From the structural point of view:*

We have calculated the optimized geometries of 13 molecular clusters for salt bridge models formed by propionic acid and ethylguanidine in aqueous environments. Our results suggest that there is a fill-in mechanism for water molecules to form a structure that interacts with the salt bridge structure. When water molecules one by one are added to a salt bridge system, the total energy resulted from such an addition shows periodicity as the number of water molecules increases. As shown in Figure-2-17, although the full explanation of the periodicity has not yet been obtained, certain patterns have been observed: water molecules enter into the salt bridge system. At first, a 4-member-oxygen ring-like structure forms, and then it evolves into a 5-member-oxygen ring-like structure; next come multiples of the 4-member-oxygen rings, and then the 4-member-oxygen rings become 5-member-oxygen rings to the completion of the first water shell which takes a total of 10 molecules. Data from NBO calculations provide further evidence of such formation patterns, in which weak bonding can be identified in terms of Wiberg bond orders. After the completion of the first water shell, the ring structures turn into a complex three dimensional network, forming in cell unit of 5-member-oxygen rings and proliferating on the hydrophilic side of a salt bridge system. Water molecules always are

gathered on one side of the salt bridge systems. That is, the hydrophobic tails of ethyl guanidinium and proprionic acid are on the opposite side of the guanidinium plane from the hydrophilic moiety of the system. It suggests that the salt bridge model used in this work has both hydrophilic and hydrophobic sides. It further suggests that this may be of general interest because most salt bridges have similarly hydrophobic and hydrophilic moieties, and are hydrated on one side as a consequence. This work would be particularly relevant to those salt bridge systems with structures similar to our models, which should include most of the interesting cases. It has general applicability in its other features. Currently, potentials used in Molecular Dynamics (MD) and Monte Carlo (MC) methods have not taken into account such mechanisms of formation and interaction between ring networks. Understanding such a periodic fill-in mechanism for water molecules should be helpful in determining how the use of these potentials can be improved.

Potentials of salt bridge systems in environments where there are limited numbers of water molecules are especially important in cases such as simulations of ion channels. There, water molecules can form a water wire, in which the molecules are connected consecutively in a pore in such a way that they can transmit protons. It has been proposed that the water wire may be anchored by salt bridge connections. However, currently no molecular mechanics (MM) potential has been adequately parameterized for dealing with such environments. We have investigated the salt bridge systems in zero water environments and up to the completion of the first water shell. We have given, as examples, the potential functions for the first water shell, from which similar potential functions can also be so constructed for use with other limited water environments and other situations of research interest.

(B) *From the theoretical point of view:*

Most of the MM potentials are inadequate since they have been parameterized for bulk systems. Improved potentials for small size systems can be obtained by quantum calculations, which can be further parameterized for use with larger size systems in MD and MC methods.

The formation of ring networks for salt bridge systems in aqueous environments is partially due to quantum polarization effects. The mechanisms of such network formation are difficult to properly investigate by current MD and MC methods.

We can compare salt bridge systems in environments of limited water to environments of bulk water, and we notice that they are different structurally. 4-oxygen-member rings can only form in environments of limited water before the completion of the first water shell, while after the completion of first water shell that is formed by 10 water molecules, the ring structures begin to proliferate in three dimensions in the basic cell unit of 5-oxygen-member ring. It suggests that in bulk water the common basis cell unit is approached by the 5-oxygen-member ring, which may become equivalent to the familiar tetrahedral unit, and the probability of formation of the 4-oxygen-member ring is low. In particular, we note that the 5 member ring has 108^{o} bond angles, close to the tetrahedral 109^{o}. While five member planar rings are not found in bulk, they are clearly a step on the way towards a tetrahedral structure.

When the salt bridge has no water, the potential diagrams exhibit a local minimum that is due to the proton transfer from propionic acid to ethylguanidine; when the salt bridge is in an environment of extremely limited water, such as one or two water molecules, the electron density of such a proton transfer can be treated more quantitatively by

identifying the electron density change in hydrogen bonding of a system (please refer to Figure-9-4 and Figure-9-6); but when the salt bridge is in environments of just three or four water molecules, the electron density of proton transfer and the electron density of hydrogen bonding cannot be treated separately (please refer to Figure-9-8 and Figure-9-10); better quantitative results can only be obtained by treating the system in its entirety and by quantum investigations.

We have also studied another salt bridge model formed by propionic acid and propyl amine, which is a model for lysine. For this salt bridge system with no water, as with the salt bridge system formed by propionic acid and ethylguanidine, a local minimum near the lowest minimum in the potential diagram (Figure-10-1) has also been observed. Similarly, when a water molecule is added into the system, the local minimum (i.e, the proton transfers, and the system goes from two neutral molecules to the zwitterion) in the potential diagram disappears (Figure-10-2). It suggests, in terms of proton transfer, the two salt bridge systems are similar, so both local minima in the absence of water are due to the ionization of propionic acid.

The total energy of a single water molecule is -76.45853 atomic units (Hartrees), but when a single water molecule is added into a salt bridge system, the change in total energy of the salt bridge is by no means just a simple addition but rather complex. The change in total energy by an addition of one water molecule to a salt bridge system can be dramatically different from one system to another. The difference between the total energy changes can be about $11.5k_BT$. Such effects in energy change also have shown a pattern of periodicity (please refer to Figure-2-17), which suggests that such energy

effects are at least partially related to structural formations in salt bridge systems. Current MD or MC methods generally miss such effects.

We have developed potential diagrams for salt bridge systems with zero up to 12 water molecules by quantum calculations, showing that they have dramatically different shapes. It has not been possible to fit a single parabola to represent data of these potential diagrams without huge errors. However, the results can be represented in specific individual cases. For angle stretches near the optimized angles, individual potential functions of bridge angles can also be formulated from our data. Stretches in distance have been found to have larger effects in total energy than angular deformations (that is, the relative change in bond distance required for a given energy change is smaller than the relative change required with angular deformation). Such information may be useful in understanding certain constricted stretches of ion channels.

Our data have explicitly shown that salt bridge systems may have hydrophilic and hydrophobic properties. Using small size models for quantum investigations that concentrate at or near the pore regions of ion channels may provide us much better tools than current MD or MC methods in understanding certain unknown structures and gating processes of ion channels.

We have calculated the bridge binding energy in an environment with dielectric constant equal to 1. Comparing to other current published reports, as expected, the bridge binding energy values at this dielectric constant are higher. We have determined how the total energy of the salt bridge systems can be affected in environments of different dielectric constants. Our results show that when in environments of high dielectric constants (greater than 60), the total energy of the salt bridge systems decreases slowly as the

dielectric constants increase; when in low dielectric constants (less than 30), the total energy drops sharply as the dielectric constants increase, The dielectric constants in protein environments may be uncertain, such as in cases of ion channels. However, if the structures of a complete system are well determined, a few conclusions can be drawn, such as that in the dielectric constant range from 1 to 30, the potentials would drop substantially as the dielectric constants increase, making the bridge binding energy drop substantially, as well. With this adjustment, our results essentially agree with most of the published experimental data.

The frequency calculations give thermodynamic data. We see that, for the same salt bridge system, distorted by 1 Å, the thermal corrections to energy can vary about 3 to 5 k_BT. Therefore, a single set of thermal data used for simulations as most of the current MD or MC methods do is not advisable if the targeted errors are less than 5 k_BT. Specific thermal corrections are needed to correct the corresponding bridge lengths when the salt bridge systems stretch in simulations.

From the NBO results, we observe that for a salt bridge system with no water, the rates of Wiberg bond order change rapidly at the bridge length of 3.46 angstroms, matching well with the local minimum in the potential diagram at the same bridge length, at the same point where the bridge stretch distance triggers the proton ionization process of propionic acid. Also, we notice that the particular bond with the lowest Wiberg bond order is where the bond breaks when the next water enters the salt bridge systems, in which it corresponds to the transition from 4-oxygen-member rings to 5-oxygen-member rings before the completion of the first water shell. The correlations between Wiberg bond orders and potentials in salt bridge systems have not yet been fully investigated and

understood. It seems, however, that it is possible by identifying the major bonding networks we can learn about effects on potentials in a salt bridge system.

(C) *From the practical point of view*

The incorporation of quantum tools into MD and MC methods is important in understanding the structures, dynamics and functions of proteins, such as ion channels. At the current stage, quantum investigations of large size systems are limited by computational capability, while MD and MC methods can handle much larger size systems. Once the details of quantum effects for a particular system are properly understood and properly parameterized into a MD or MC methods, the results from such MD or MC methods can be directly compared with experimental data in a real system. As we show, it is crucial, and possible, that by a stepwise procedure the mechanisms obtained from quantum investigations, such as the periodical fill-in order of ring formation in environments of insufficient water and effects that may be missed by classical treatments, can be incorporated into MD or MC methods. Also, from our quantum calculation data, potential functions used in specific environments can also be formulated and incorporated into MD or MC methods. Potentials of different dielectric constants and thermodynamic data can also be carefully calibrated in MD or MC methods. In our follow-up work, we would like to further improve potentials in salt bridge systems in some specific constricted environments, including those similar to the environments of ion channels.

Experimental tests: It is difficult to directly test these calculations experimentally, as it requires isolating parts of a protein. However some possibilities exist, if gas phase clusters of the appropriate form are produced. In principle, one could use IR

spectroscopy with frequency calculations, for example. However, the Wiberg bond indices should allow one possible rigorous test. These indices are proportional to the electron charge density in a bond, and soft X-ray spectroscopy of the oxygen K shell should be a good test of the accuracy of the density calculation[161].

The potentials derived from the calculations will in the end be the best test of the usefulness of the method; it should be possible to compare the output of simulations using these potentials (and those derived from extending this work) to experimental results. Therefore, in the end, the work will be testable experimentally.

Appendix A
Bridge Length versus Total Energy

Table-3A-1 Bridge length versus total energy for salt bridge with no water (All calculations in appendix A done by B3LYP/6-311++G)**

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
2.9	-552.57403	0.02744	29.2
2.95	-552.57739	0.02408	25.6
3	-552.58034	0.02113	22.5
3.05	-552.58292	0.01855	19.7
3.1	-552.58517	0.01631	17.3
3.15	-552.5871	0.01437	15.3
3.2	-552.58875	0.01272	13.5
3.25	-552.59014	0.01134	12.1
3.3	-552.5913	0.01018	10.8
3.35	-552.59229	0.00918	9.8
3.4	-552.59312	0.00836	8.9
3.45	-552.58725	0.01423	15.1
3.5	-552.59001	0.01146	12.2
3.55	-552.59256	0.00891	9.5
3.6	-552.59485	0.00662	7.1
3.65	-552.59686	0.00462	4.9
3.7	-552.59855	0.00292	3.1
3.75	-552.59993	0.00155	1.6
3.8	-552.60097	0.0005	0.5
3.83	-552.60132	0.00015	0.2
3.87(opt)	-552.60147	0	0
3.9	-552.60135	0.00012	0.1
3.95	-552.60075	0.00072	0.8
4	-552.59969	0.00178	1.9
4.05	-552.59825	0.00323	3.4
4.1	-552.59647	0.005	5.3
4.15	-552.59442	0.00706	7.5
4.2	-552.59214	0.00933	9.9
4.25	-552.58969	0.01178	12.5
4.3	-552.58711	0.01436	15.3
4.35	-552.58443	0.01704	18.1
4.4	-552.5817	0.01977	21
4.45	-552.57894	0.02254	24

Table-3A-2: Bridge length versus total energy for salt bridge with one water molecule

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.3	-629.05766	0.01838	19.5
3.4	-629.06457	0.01146	12.2
3.5	-629.06973	0.00631	6.7
3.6	-629.07045	0.00558	5.9
3.7	-629.07298	0.00306	3.3
3.8	-629.07494	0.00109	1.2
3.9	-629.07598	6.02E-05	0.1
3.93(opt)	-629.07604	0	0
4	-629.07565	0.00038	0.4
4.09	-629.07405	0.00198	2.1
4.2	-629.07055	0.00548	5.8
4.3	-629.0669	0.00914	9.7
4.4	-629.06328	0.01276	13.6

Table-3A-3: Bridge length versus total energy for salt bridge with two water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.2	-705.53796	0.02133	22.7
3.3	-705.54153	0.01776	18.9
3.4	-705.54537	0.01392	14.8
3.5	-705.54895	0.01034	11
3.59	-705.55186	0.00743	7.9
3.7	-705.55498	0.00431	4.6
3.8	-705.5573	0.00199	2.1
3.9	-705.55897	0.00032	0.4
3.96(opt)	-705.55929	0	0
4	-705.55916	0.00013	0.1
4.09	-705.55802	0.00127	1.4
4.2	-705.55537	0.00392	4.2
4.29	-705.55253	0.00676	7.2
4.4	-705.5488	0.01049	11.2

Table-3A-4: Bridge length versus total energy for salt bridge with three water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.4	-782.02615	0.01106	11.8
3.5	-782.02747	0.00974	10.4
3.6	-782.03018	0.00702	7.5
3.7	-782.03298	0.00423	4.5
3.8	-782.03533	0.00188	2
3.9	-782.03687	0.00033	0
3.97(opt)	-782.0372	0	0
4	-782.03714	6.71E-05	0.1
4.1	-782.03606	0.00114	1.2
4.15	-782.03509	0.00211	2.3
4.2	-782.03388	0.00333	3.5
4.6	-782.02201	0.0152	16.2
4.8	-782.01938	0.01783	19

Table-3A-5: Bridge length versus total energy for salt bridge with four water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.4	-858.50125	0.01361	14.5
3.5	-858.50496	0.0099	10.5
3.6	-858.50823	0.00662	7.1
3.7	-858.51101	0.00385	4.1
3.8	-858.51319	0.00167	1.8
3.9	-858.51455	0.0003	0.3
4(opt)	-858.51486	0	0
4.1	-858.51409	0.00077	0.8
4.2	-858.51247	0.00239	2.5
4.3	-858.5103	0.00455	4.8
4.4	-858.51036	0.0045	4.8
4.5	-858.50929	0.00557	5.9
4.6	-858.50797	0.00689	7.3
4.8	-858.50126	0.0136	14.5

Table-3A-6: Bridge length versus total energy for salt bridge with five water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.4	-934.97945	0.01203	12.8
3.49	-934.98022	0.01126	12
3.6	-934.98379	0.00769	8.2
3.7	-934.98655	0.00493	5.2
3.8	-934.98876	0.00272	2.9
3.9	-934.99056	0.00092	1
4	-934.99144	4.41E-05	0.1
4.05(opt)	-934.99146	2.41E-05	0
4.09	-934.99129	0.00019	0.2
4.2	-934.99015	0.00133	1.4
4.3	-934.98848	0.003	3.2
4.4	-934.98655	0.00493	5.3
4.5	-934.9849	0.00658	7
4.6	-934.98909	0.00239	2.5
4.7	-934.98823	0.00325	3.5

Table-3A-7: Bridge length versus total energy for salt bridge with six water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.5	-1011.4467	0.01754	18.7
3.6	-1011.45279	0.01145	12.2
3.7	-1011.45806	0.00618	6.6
3.8	-1011.46154	0.00269	2.9
3.9	-1011.46348	3.22E-06	0
4(opt)	-1011.46423	0	0
4.1	-1011.46366	0.00058	0.6
4.2	-1011.46228	0.00196	2.1
4.3	-1011.46007	0.00416	4.4
4.4	-1011.45755	0.00668	7.1
4.5	-1011.45475	0.00949	10.1
4.6	-1011.45198	0.01226	13
4.7	-1011.44916	0.01508	16
4.8	-1011.44651	0.01772	18.9

Table-3A-8: Bridge length versus total energy for salt bridge with seven water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.5	-1087.93509	0.01274	13.5
3.6	-1087.93738	0.01044	11.1
3.7	-1087.94023	0.00759	8.1
3.8	-1087.94351	0.00431	4.6
3.9	-1087.94612	0.0017	1.8
4	-1087.94755	0.00027	0.3
4.08(opt)	-1087.94782	0	0
4.1	-1087.94779	3.18E-05	0
4.2	-1087.94707	0.00075	0.8
4.3	-1087.94582	0.00201	2.1
4.4	-1087.94437	0.00345	3.7
4.5	-1087.94255	0.00527	5.6
4.6	-1087.94083	0.00699	7.4
4.7	-1087.93935	0.00847	9
4.8	-1087.93748	0.01034	11
4.9	-1087.93669	0.01114	11.8
5	-1087.9354	0.01242	13.2

Table-3A-9: Bridge length versus total energy for salt bridge with eight water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.6	-1164.41235	0.01092	11.6
3.7	-1164.41566	0.00761	8.1
3.8	-1164.41921	0.00406	4.3
3.9	-1164.42182	0.00145	1.5
4	-1164.4231	0.00016	0.2
4.05(opt)	-1164.42327	0	0
4.1	-1164.42314	0.00013	0.1
4.2	-1164.42229	0.00098	1
4.3	-1164.42076	0.0025	2.7
4.4	-1164.41913	0.00413	4.4
4.5	-1164.41708	0.00618	6.6
4.6	-1164.41496	0.00831	8.8
4.7	-1164.41318	0.01009	10.7
4.8	-1164.41131	0.01196	12.7
4.9	-1164.41064	0.01262	13.4
5	-1164.40927	0.01399	14.9

Table-3A-10: Bridge length versus total energy for salt bridge with nine water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.4	-1240.89042	0.0085	9
3.5	-1240.89012	0.0088	9.4
3.6	-1240.89281	0.0061	4.6
3.7	-1240.8946	0.00432	4.6
3.8	-1240.89682	0.0021	2.2
3.9	-1240.89815	0.00076	0.8
4	-1240.89866	0.00026	0.3
4.08	-1240.8989	1.31E-05	0
4.1(opt)	-1240.89892	0	0
4.2	-1240.89839	0.00053	0.6
4.3	-1240.89778	0.00114	1.2
4.4	-1240.89702	0.00189	2
4.5	-1240.89587	0.00305	3.2
4.6	-1240.89492	0.004	4.3
4.7	-1240.89388	0.00503	5.4
4.8	-1240.8929	0.00602	6.4
4.9	-1240.89183	0.00708	7.5
4.99	-1240.89089	0.00803	8.5

Table-3A-11: Bridge length versus total energy for salt bridge with ten water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.5	-1317.36439	0.00914	9.7
3.6	-1317.36717	0.00636	6.8
3.7	-1317.36893	0.0046	4.9
3.8	-1317.37132	0.0022	2.3
3.9	-1317.37292	0.0006	0.6
4(opt)	-1317.37353	0	0
4.1	-1317.3733	0.00023	0.2
4.2	-1317.37301	0.00052	0.6
4.3	-1317.37227	0.00125	1.3
4.4	-1317.37158	0.00195	2.1
4.5	-1317.37074	0.00278	3
4.6	-1317.36964	0.00388	4.1
4.7	-1317.36883	0.0047	5
4.8	-1317.36774	0.00657	7
4.9	-1317.36696	0.00657	7
5	-1317.36617	0.00736	7.8

Table-3A-12: Bridge length versus total energy for salt bridge with eleven water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.5	-1393.83964	0.00713	7.6
3.6	-1393.84078	0.00599	6.4
3.7	-1393.84269	0.00408	4.3
3.8	-1393.84447	0.0023	2.5
3.9	-1393.84613	0.00064	0.7
4	-1393.84655	0.00022	0.2
4.07(opt)	-1393.84677	0	0
4.1	-1393.84674	3.03E-05	0
4.2	-1393.84624	0.00053	0.6
4.3	-1393.84547	0.0013	1.4
4.4	-1393.84466	0.00286	3
4.5	-1393.84391	0.00286	3
4.6	-1393.84282	0.00395	4.2
4.7	-1393.84165	0.00512	5.4
4.8	-1393.84079	0.00598	6.4

Table-3A-13: Bridge length versus total energy for salt bridge with twelve water molecules

Bridge Length (angstroms)	Total Energy (au)	Total Energy - Opt-Energy(au)	Total Energy - Opt-Energy(k_BT) At 298K
3.6	-1470.31619	0.00885	9.4
3.7	-1470.31927	0.00577	6.1
3.8	-1470.31968	0.00212	2.2
3.9	-1470.32292	0.00212	2.3
4	-1470.32473	0.00032	0.3
4.05(opt)	-1470.32505	0	0
4.1	-1470.32502	2.81E-05	0
4.2	-1470.32434	0.00071	0.8
4.3	-1470.3229	0.00215	2.3
4.4	-1470.32097	0.00408	4.3
4.5	-1470.31878	0.00626	6.7
4.6	-1470.31641	0.00864	9.2
4.7	-1470.31413	0.01091	11.6
4.8	-1470.31199	0.01305	13.9
4.9	-1470.31016	0.01489	15.8
5	-1470.30781	0.01723	18.3

Appendix B

Data of Bridge Angle versus Total Energy

Table-4B-1: Dihedral angle versus total energy for salt bridge with no water (All calculations in appendix B done by B3LYP/6-311++G)**

Dihedral Angle-[1]C-[2]O-[3]H-[4]C, ᴅ (in degree)	Total Energy(au)	Total energy Difference from optimized geometry(au)	Total energy Difference from optimized geometry in k_BT at 298K
0.56(opt)	-552.60122	0	0
1.68	-552.60113	8.69E-05	0.1
2.8	-552.601	0.00022	0.2
3.93	-552.60081	0.00041	0.4
5.05	-552.60077	0.00044	0.5
6.17	-552.60052	0.0007	0.7
7.29	-552.60023	0.00099	1.1
8.41	-552.5999	0.00132	1.4
9.53	-552.59953	0.00169	1.8
10.65	-552.59914	0.00208	2.2
11.78	-552.5987	0.00251	2.7
12.9	-552.59825	0.00297	3.2
14.02	-552.59777	0.00345	3.7
15.14	-552.59726	0.00395	4.2
16.26	-552.59674	0.00448	4.8
17.38	-552.59618	0.00503	5.4
18.5	-552.59569	0.00552	5.9
19.63	-552.59511	0.00611	6.5
20.75	-552.59446	0.00676	7.2
21.87	-552.59383	0.00738	7.9
22.99	-552.59323	0.00799	8.5
24.11	-552.59263	0.00859	9.1
25.23	-552.59213	0.00909	9.7
26.36	-552.59152	0.0097	10.3
27.48	-552.59092	0.0103	11
28.6	-552.59032	0.0109	11.6
29.72	-552.58972	0.0115	12.2
30.84	-552.58913	0.01208	12.9
31.96	-552.58855	0.01267	13.5
33.08	-552.58798	0.01324	14.1
34.21	-552.58741	0.01381	14.7
35.33	-552.58686	0.01436	15.3
36.45	-552.58631	0.0149	15.9
37.57	-552.58578	0.01544	16.4
38.69	-552.58526	0.01595	17
39.81	-552.58476	0.01646	17.5
40.93	-552.58426	0.01695	18
42.06	-552.58378	0.01744	18.6
43.18	-552.58331	0.0179	19
44.3	-552.58286	0.01836	19.5
45.42	-552.58242	0.01922	20.4
46.54	-552.582	0.01922	20.4
47.66	-552.58159	0.01962	20.9

Table-4B-2: Angle α versus total energy for salt bridge with zero water

Angle-[3]C-[2]C-[1]N, α (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
180	-552.60044	0.000815	0.9
178.96	-552.60087	0.000388	0.4
178.43	-552.60103	0.00023	0.2
177.91	-552.60114	0.000115	0.1
177.39	-552.60122	3.96E-05	0
176.69(opt)	-552.60126	0	0
176.35	-552.60125	6.50E-06	0
175.83	-552.60121	4.87E-05	0.1
175.3	-552.60113	0.000132	0.1
174.78	-552.60101	0.000252	0.3
174.26	-552.60085	0.000411	0.4
173.74	-552.60065	0.000607	0.7
173.22	-552.60042	0.00084	0.9
172.7	-552.60015	0.001109	1.2
172.17	-552.59984	0.00142	1.5
171.65	-552.5995	0.001761	1.9
171.13	-552.59912	0.002135	2.3
170.61	-552.59871	0.002543	2.7
170.09	-552.59827	0.002983	3.2
169.57	-552.5978	0.003455	3.7
169.04	-552.59729	0.003968	4.2
168.52	-552.59676	0.004502	4.8
168	-552.59619	0.005066	5.4
167.48	-552.5956	0.005656	6
166.96	-552.59498	0.006273	6.7
166.43	-552.59433	0.006927	7.4
165.91	-552.59367	0.007592	8.1
165.39	-552.59298	0.008276	8.8
164.87	-552.59228	0.008979	9.6
164.35	-552.59155	0.009708	10.3
163.83	-552.59078	0.010477	11.1
163.3	-552.59007	0.011191	11.9
162.78	-552.58925	0.012009	12.8
162.26	-552.58842	0.012834	13.7
161.74	-552.5876	0.013658	14.5
161.22	-552.58677	0.01449	15.4
160.7	-552.58593	0.015332	16.3
160.17	-552.58506	0.016196	17.2
159.65	-552.58421	0.017052	18.1
159.13	-552.58334	0.017915	19.1
158.61	-552.58247	0.018786	20
158.09	-552.58159	0.019663	20.9
157.57	-552.58071	0.020547	21.9
157.04	-552.5798	0.021453	22.8
156.52	-552.57891	0.022345	23.8
156	-552.57802	0.023239	24.7

Table-4B-3: Angle α versus total energy for salt bridge with one water molecule

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.2	-629.06439	0.01162	12.3
161.2	-629.06631	0.00969	10.3
162.3	-629.06808	0.00793	8.4
163.3	-629.06968	0.00632	6.7
164.4	-629.07113	0.00488	5.2
165.4	-629.07239	0.00362	3.8
167.0	-629.07395	0.00206	2.2
168.0	-629.07474	0.00127	1.3
169.0	-629.07535	0.00066	0.7
170.1	-629.07575	0.00025	0.3
171.3	-629.07599	1.85E-05	0
172.2	-629.07601	0	0
173.2	-629.07586	0.00015	0.2
174.3	-629.07553	0.00047	0.5
175.3	-629.07504	0.00097	1
176.4	-629.07438	0.00163	1.7
177.4	-629.07357	0.00244	2.6
178.4	-629.07261	0.0034	3.6
180.0	-629.06439	0.00509	5.4

Table-4B-4: Angle α versus total energy for salt bridge with two waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.2	-705.33559	0.22363	236.9
161.2	-705.36122	0.19799	209.7
162.3	-705.38567	0.17355	183.8
163.3	-705.40888	0.15033	159.2
164.9	-705.44101	0.11821	125.2
165.9	-705.46006	0.09916	105
167.0	-705.47738	0.08184	86.7
168.0	-705.49258	0.06663	70.6
169.0	-705.50585	0.05336	56.5
170.1	-705.51735	0.04186	44.4
171.1	-705.52699	0.03223	34.1
172.2	-705.53501	0.0242	25.6
173.2	-705.54163	0.01759	18.6
174.3	-705.54685	0.01237	13.1
175.3	-705.55091	0.00831	8.8
176.9	-705.55521	0.00401	4.2
177.4	-705.55922	0	0
178.4	-705.55913	8.21E-05	0.1
180.0	-705.55871	0.0005	0.5

Table-4B-5: Angle α versus total energy for salt bridge with three waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.17	-782.01117	0.02607	27.6
161.22	-782.013	0.02424	25.7
162.78	-782.01565	0.02159	22.9
163.87	-782.01738	0.01986	21
164.87	-782.01904	0.01821	19.3
165.91	-782.02063	0.01661	17.6
166.96	-782.02217	0.01507	16
168	-782.02363	0.01361	14.4
169.04	-782.02498	0.01226	13
170.09	-782.02627	0.01097	11.6
171.13	-782.02743	0.00981	10.4
172.17	-782.02848	0.00876	9.3
173.22	-782.02942	0.00782	8.3
174.22	-782.03724	0	0
175.3	-782.03708	0.00016	0.2
175.83	-782.03683	0.00041	0.4
176.35	-782.03649	0.00075	0.8
177.39	-782.0356	0.00164	1.7
178.43	-782.03447	0.00277	2.9
180.00	-782.03238	0.00486	5.2

Table-4B-6: Angle α versus total energy for salt bridge with four waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.17	-858.46874	0.04588	48.6
161.22	-858.47184	0.04278	45.3
162.26	-858.47489	0.03973	42.1
163.3	-858.47788	0.03673	38.9
164.35	-858.48083	0.03378	35.8
165.39	-858.48365	0.03097	32.8
166.43	-858.48634	0.02828	30
167.48	-858.48891	0.02571	27.2
168.52	-858.49128	0.02333	24.7
169.57	-858.4935	0.02112	22.4
170.733	-858.51462	0	0
171.65	-858.51432	0.00029	0.3
172.7	-858.51366	0.00096	1
173.74	-858.51274	0.00188	2
174.78	-858.51159	0.00302	3.2
175.83	-858.51025	0.00436	4.6
176.87	-858.50878	0.00583	6.2
177.91	-858.50717	0.00744	7.9
180	-858.50364	0.01098	11.6

Table-4B-7: Angle α versus total energy for salt bridge with five waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
150.26	-934.9415	0.04985	52.8
151.83	-934.95972	0.03163	33.5
152.35	-934.9645	0.02685	28.4
153.39	-934.97248	0.01887	20
154.96	-934.98115	0.0102	10.8
156	-934.98516	0.00619	6.6
157.04	-934.98797	0.00338	3.6
158.61	-934.99045	0.0009	1
159.65	-934.99118	0.00017	0.2
160.5	-934.99135	0	0
161.74	-934.99103	0.00032	0.3
162.78	-934.99034	0.00101	1.1
163.83	-934.98931	0.00204	2.2
164.87	-934.98805	0.0033	3.5
165.91	-934.98659	0.00476	5
166.96	-934.98496	0.00639	6.8
168	-934.98321	0.00814	8.6
169.04	-934.98137	0.00998	10.6

Table-4B-8: Angle α versus total energy for salt bridge with six waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
150.26	-1011.40258	0.06165	65.3
151.3	-1011.41697	0.04725	50.1
152.35	-1011.42874	0.03549	37.6
153.39	-1011.43804	0.02619	27.7
154.96	-1011.44858	0.01565	16.6
156.52	-1011.45565	0.00858	9.1
157.57	-1011.45895	0.00528	5.6
158.61	-1011.46129	0.00294	3.1
159.65	-1011.46286	0.00137	1.5
160.7	-1011.4638	0.00043	0.5
161.74	-1011.46419	3.37E-05	0
162.26	-1011.46423	0	0
163.3	-1011.46401	0.00022	0.2
164.35	-1011.46348	0.00075	0.8
165.39	-1011.46266	0.00157	1.7
166.43	-1011.46162	0.00261	2.8
167.48	-1011.46038	0.00385	4.1
168.52	-1011.45901	0.00522	5.5
169.57	-1011.45749	0.00674	7.1
170.61	-1011.45587	0.00835	8.9

Table-4B-9: Angle α versus total energy for salt bridge with seven waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
150.26	-1087.93166	0.01617	17.1
151.3	-1087.936519	0.01131	12
152.35	-1087.940295	0.00753	8
153.39	-1087.9431	0.00473	5
154.96	-1087.945913	0.00191	2
156	-1087.94702	0.00081	0.9
157.04	-1087.947633	0.00019	0.2
158.21	-1087.947827	0	0
159.13	-1087.947675	0.00015	0.2
160.17	-1087.947245	0.00058	0.6
161.22	-1087.946554	0.00127	1.4
162.26	-1087.945658	0.00217	2.3
163.3	-1087.944585	0.00324	3.4
164.35	-1087.943347	0.00448	4.8
165.39	-1087.941988	0.00584	6.2
166.43	-1087.940513	0.00731	7.8
168	-1087.938089	0.00974	10.3
169.04	-1087.936377	0.01145	12.1
170.09	-1087.934549	0.01328	14.1

Table-4B-10: Angle α versus total energy for salt bridge with eight waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
150.26	-1164.40885	0.01442	15.3
151.3	-1164.41315	0.01012	10.7
152.35	-1164.4165	0.00677	7.2
153.39	-1164.419	0.00427	4.5
154.43	-1164.42083	0.00244	2.6
155.48	-1164.42211	0.00116	1.2
156.52	-1164.42288	0.00039	0.4
157.57	-1164.42323	4.01E-05	0
158.03	-1164.42327	0	0
159.13	-1164.42312	0.00015	0.2
160.17	-1164.4227	0.00057	0.6
161.22	-1164.42204	0.00123	1.3
162.26	-1164.42118	0.00209	2.2
163.3	-1164.42015	0.00312	3.3
164.35	-1164.41895	0.00432	4.6
165.39	-1164.41762	0.00565	6
166.43	-1164.41617	0.0071	7.5
168	-1164.41378	0.00949	10.1
169.04	-1164.41207	0.0112	11.9
170.09	-1164.41025	0.01302	13.8

Table-4B-11: Angle α versus total energy for salt bridge with nine waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.17	-1240.75504	0.14386	152.4
161.22	-1240.79218	0.10672	113.1
162.26	-1240.82052	0.07838	83
163.3	-1240.84229	0.05661	60
164.35	-1240.85896	0.03995	42.3
165.39	-1240.87132	0.02758	29.2
166.43	-1240.88049	0.01842	19.5
167.48	-1240.88716	0.01174	12.4
168.52	-1240.89179	0.00711	7.5
169.57	-1240.89493	0.00397	4.2
170.61	-1240.89679	0.00211	2.2
171.8	-1240.8989	0	0
172.7	-1240.89871	0.00019	0.2
173.74	-1240.89802	0.00088	0.9
174.78	-1240.89696	0.00194	2.1
175.83	-1240.8955	0.0034	3.6
176.35	-1240.89468	0.00422	4.5
177.39	-1240.89287	0.00603	6.4
178.43	-1240.89087	0.00803	8.5
180	-1240.8876	0.0113	12

Table-4B-12: Angle α versus total energy for salt bridge with ten waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.17	-1317.07892	0.29438	311.8
161.22	-1317.15205	0.22125	234.4
162.26	-1317.20813	0.16517	175
163.3	-1317.25123	0.12207	129.3
164.35	-1317.28439	0.08891	94.2
165.91	-1317.31931	0.05399	57.2
166.96	-1317.33568	0.03762	39.9
168	-1317.34771	0.02559	27.1
169.04	-1317.35654	0.01676	17.8
170.09	-1317.36295	0.01035	11
171.65	-1317.36894	0.00436	4.6
172.7	-1317.37123	0.00207	2.2
173.74	-1317.37241	0.00089	0.9
174.77	-1317.3733	0	0
175.3	-1317.37319	0.0001	0.1
176.35	-1317.3726	0.0007	0.7
177.39	-1317.3715	0.00179	1.9
178.43	-1317.37005	0.00325	3.4
180	-1317.36731	0.00599	6.3

Table-4B-13: Angle α versus total energy for salt bridge with eleven waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.17	-1393.63068	0.2161	228.9
161.22	-1393.68042	0.16636	176.2
162.26	-1393.72017	0.1266	134.1
163.3	-1393.75179	0.09498	100.6
164.35	-1393.77683	0.06994	74.1
165.91	-1393.80402	0.04275	45.3
166.96	-1393.81703	0.02974	31.5
168	-1393.82673	0.02005	21.2
169.04	-1393.83391	0.01287	13.6
170.09	-1393.8391	0.00767	8.1
171.65	-1393.84394	0.00283	3
172.7	-1393.84572	0.00106	1.1
173.74	-1393.84656	0.00021	0.2
174.57	-1393.84677	0	0
175.3	-1393.84661	0.00016	0.2
176.35	-1393.846	0.00077	0.8
177.39	-1393.8449	0.00187	2
178.43	-1393.84345	0.00332	3.5
180	-1393.84074	0.00603	6.4

Table-4B-14: Angle α versus total energy for salt bridge with twelve waters

Angle-[3]C-[2]C-[1]N (in degree)	Total Energy(au)	Energy Difference from Opt-structure(au)	Total energy Difference from optimized geometry in k_BT at 298K
160.17	-1470.19089	0.13416	142.1
161.22	-1470.22638	0.09867	104.5
162.26	-1470.25318	0.07187	76.1
163.3	-1470.27357	0.05148	54.5
164.35	-1470.2891	0.03595	38.1
165.91	-1470.30517	0.01988	21.1
166.96	-1470.31244	0.01261	13.4
168	-1470.31758	0.00747	7.9
169.04	-1470.31758	0.00747	7.9
170.09	-1470.32108	0.00397	4.2
171.13	-1470.32327	0.00178	1.9
172.17	-1470.32445	0.00059	0.6
173.11	-1470.32505	0	0
174.26	-1470.32473	0.00032	0.3
175.3	-1470.32394	0.00111	1.2
176.35	-1470.32273	0.00232	2.5
177.39	-1470.32127	0.00377	4
178.43	-1470.31953	0.00552	5.8
180	-1470.31656	0.00849	9

Appendix C

Data of Wiberg Index

Table-9C-1-1: Wiberg index for salt bridge with no water (bridge length=3.1angstroms) (All calculations in appendix C done by B3LYP/6-311++G)**

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0058	0.0110	0.0018	0.0056	0.0001	0.0005	1.1765	0.0027
2. H	0.0058	0.0000	0.9288	0.0013	0.0025	0.0016	0.0009	0.0046	0.0027
3. C	0.0110	0.9288	0.0000	0.9241	1.0237	0.0024	0.0031	0.9653	0.0038
4. H	0.0018	0.0013	0.9241	0.0000	0.0023	0.0123	0.0008	0.0079	0.0057
5. C	0.0056	0.0025	1.0237	0.0023	0.0000	0.9431	0.9423	0.0202	0.0012
6. H	0.0001	0.0016	0.0024	0.0123	0.9431	0.0000	0.0006	0.0018	0.0002
7. H	0.0005	0.0009	0.0031	0.0008	0.9423	0.0006	0.0000	0.0114	0.0001
8. N	1.1765	0.0046	0.9653	0.0079	0.0202	0.0018	0.0114	0.0000	0.8194
9. H	0.0027	0.0027	0.0038	0.0057	0.0012	0.0002	0.0001	0.8194	0.0000
10. N	1.5480	0.0029	0.0046	0.0047	0.0041	0.0003	0.0006	0.1215	0.0137
11. H	0.0043	0.0001	0.0010	0.0005	0.0005	0.0000	0.0000	0.0030	0.0003
12. H	0.0049	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0081	0.0002
13. N	1.1313	0.0008	0.0119	0.0012	0.0015	0.0001	0.0005	0.0445	0.0032
14. H	0.0026	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0021	0.0001
15. H	0.0021	0.0001	0.0010	0.0000	0.0002	0.0000	0.0001	0.0098	0.0004
16. O	0.0183	0.0001	0.0012	0.0008	0.0003	0.0001	0.0001	0.0051	0.0002
17. O	0.0096	0.0001	0.0004	0.0001	0.0002	0.0000	0.0000	0.0047	0.0003
18. C	0.0023	0.0001	0.0004	0.0002	0.0001	0.0000	0.0000	0.0015	0.0000
19. C	0.0011	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0003	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0002	0.0123	0.0025	0.0014	0.9432	0.0006	0.0006	0.0013	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.5480	0.0043	0.0049	1.1313	0.0026	0.0021	0.0183	0.0096	0.0023
2. H	0.0029	0.0001	0.0001	0.0008	0.0000	0.0001	0.0001	0.0001	0.0001
3. C	0.0046	0.0010	0.0001	0.0119	0.0002	0.0010	0.0012	0.0004	0.0004
4. H	0.0047	0.0005	0.0001	0.0012	0.0000	0.0000	0.0008	0.0001	0.0002
5. C	0.0041	0.0005	0.0001	0.0015	0.0001	0.0002	0.0003	0.0002	0.0001
6. H	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
7. H	0.0006	0.0000	0.0000	0.0005	0.0000	0.0001	0.0001	0.0000	0.0000
8. N	0.1215	0.0030	0.0081	0.0445	0.0021	0.0098	0.0051	0.0047	0.0015
9. H	0.0137	0.0003	0.0002	0.0032	0.0001	0.0004	0.0002	0.0003	0.0000
10. N	0.0000	0.8486	0.1874	0.0869	0.0182	0.0027	0.0085	0.0428	0.0030
11. H	0.8486	0.0000	0.0002	0.0182	0.0007	0.0005	0.0002	0.0011	0.0001
12. H	0.1874	0.0002	0.0000	0.0013	0.0000	0.0001	0.0014	0.5496	0.0033
13. N	0.0869	0.0182	0.0013	0.0000	0.8273	0.8341	0.0049	0.0031	0.0022
14. H	0.0182	0.0007	0.0000	0.8273	0.0000	0.0002	0.0022	0.0005	0.0002
15. H	0.0027	0.0005	0.0001	0.8341	0.0002	0.0000	0.0002	0.0010	0.0001
16. O	0.0085	0.0002	0.0014	0.0049	0.0022	0.0002	0.0000	0.1698	1.6648

17. O	0.0428	0.0011	0.5496	0.0031	0.0005	0.0010	0.1698	0.0000	1.1489
18. C	0.0030	0.0001	0.0033	0.0022	0.0002	0.0001	1.6648	1.1489	0.0000
19. C	0.0018	0.0001	0.0116	0.0005	0.0003	0.0001	0.0528	0.0213	0.9809
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0149	0.0049	0.0070
21. H	0.0001	0.0000	0.0002	0.0003	0.0000	0.0000	0.0137	0.0022	0.0055
22. H	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000	0.0013	0.0004	0.0094
23. C	0.0004	0.0000	0.0007	0.0001	0.0000	0.0000	0.0050	0.0084	0.0081
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0014
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0004	0.0013
26. H	0.0008	0.0005	0.0000	0.0004	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0011	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0002
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0123
3. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025
4. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9432
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8. N	0.0003	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0013
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0018	0.0001	0.0001	0.0001	0.0004	0.0000	0.0000	0.0008
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005
12. H	0.0116	0.0000	0.0002	0.0003	0.0007	0.0000	0.0000	0.0000
13. N	0.0005	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0004
14. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. O	0.0528	0.0149	0.0137	0.0013	0.0050	0.0008	0.0006	0.0000
17. O	0.0213	0.0049	0.0022	0.0004	0.0084	0.0005	0.0004	0.0001
18. C	0.9809	0.0070	0.0055	0.0094	0.0081	0.0014	0.0013	0.0000
19. C	0.0000	0.9094	0.9156	0.0017	1.0310	0.0022	0.0022	0.0000
20. H	0.9094	0.0000	0.0011	0.0015	0.0029	0.0012	0.0123	0.0000
21. H	0.9156	0.0011	0.0000	0.0013	0.0028	0.0123	0.0013	0.0000
22. H	0.0017	0.0015	0.0013	0.0000	0.9465	0.0005	0.0006	0.0000
23. C	1.0310	0.0029	0.0028	0.9465	0.0000	0.9406	0.9438	0.0000
24. H	0.0022	0.0012	0.0123	0.0005	0.9406	0.0000	0.0007	0.0000
25. H	0.0022	0.0123	0.0013	0.0006	0.9438	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-2: Wiberg index for salt bridge with no water (bridge length=3.2angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0060	0.0111	0.0017	0.0058	0.0001	0.0005	1.1778	0.0027
2. H	0.0060	0.0000	0.9284	0.0013	0.0025	0.0016	0.0009	0.0050	0.0025
3. C	0.0111	0.9284	0.0000	0.9242	1.0232	0.0023	0.0031	0.9662	0.0040
4. H	0.0017	0.0013	0.9242	0.0000	0.0023	0.0122	0.0008	0.0073	0.0063
5. C	0.0058	0.0025	1.0232	0.0023	0.0000	0.9433	0.9422	0.0204	0.0009
6. H	0.0001	0.0016	0.0023	0.0122	0.9433	0.0000	0.0006	0.0017	0.0002
7. H	0.0005	0.0009	0.0031	0.0008	0.9422	0.0006	0.0000	0.0113	0.0001
8. N	1.1778	0.0050	0.9662	0.0073	0.0204	0.0017	0.0113	0.0000	0.8180
9. H	0.0027	0.0025	0.0040	0.0063	0.0009	0.0002	0.0001	0.8180	0.0000
10. N	1.5570	0.0030	0.0046	0.0048	0.0042	0.0003	0.0006	0.1246	0.0138
11. H	0.0043	0.0001	0.0010	0.0006	0.0005	0.0000	0.0000	0.0029	0.0003
12. H	0.0043	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0078	0.0002

13.	N	1.1268	0.0008	0.0118	0.0012	0.0016	0.0001	0.0005	0.0441	0.0032
14.	H	0.0026	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0021	0.0001
15.	H	0.0021	0.0001	0.0010	0.0000	0.0002	0.0000	0.0001	0.0098	0.0004
16.	O	0.0133	0.0001	0.0011	0.0006	0.0003	0.0001	0.0001	0.0040	0.0002
17.	O	0.0094	0.0001	0.0003	0.0001	0.0002	0.0000	0.0000	0.0047	0.0002
18.	C	0.0019	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0012	0.0000
19.	C	0.0010	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0002	0.0123	0.0025	0.0014	0.9431	0.0006	0.0006	0.0013	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.5570	0.0043	0.0043	1.1268	0.0026	0.0021	0.0133	0.0094	0.0019
2.	H	0.0030	0.0001	0.0001	0.0008	0.0000	0.0001	0.0001	0.0001	0.0000
3.	C	0.0046	0.0010	0.0001	0.0118	0.0002	0.0010	0.0011	0.0003	0.0004
4.	H	0.0048	0.0006	0.0001	0.0012	0.0000	0.0000	0.0006	0.0001	0.0001
5.	C	0.0042	0.0005	0.0001	0.0016	0.0001	0.0002	0.0003	0.0002	0.0001
6.	H	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
7.	H	0.0006	0.0000	0.0000	0.0005	0.0000	0.0001	0.0001	0.0000	0.0000
8.	N	0.1246	0.0029	0.0078	0.0441	0.0021	0.0098	0.0040	0.0047	0.0012
9.	H	0.0138	0.0003	0.0002	0.0032	0.0001	0.0004	0.0002	0.0002	0.0000
10.	N	0.0000	0.8500	0.1728	0.0862	0.0184	0.0027	0.0068	0.0397	0.0028
11.	H	0.8500	0.0000	0.0002	0.0186	0.0006	0.0005	0.0002	0.0009	0.0001
12.	H	0.1728	0.0002	0.0000	0.0012	0.0000	0.0001	0.0017	0.5609	0.0033
13.	N	0.0862	0.0186	0.0012	0.0000	0.8259	0.8353	0.0043	0.0030	0.0021
14.	H	0.0184	0.0006	0.0000	0.8259	0.0000	0.0002	0.0023	0.0005	0.0002
15.	H	0.0027	0.0005	0.0001	0.8353	0.0002	0.0000	0.0002	0.0009	0.0001
16.	O	0.0068	0.0002	0.0017	0.0043	0.0023	0.0002	0.0000	0.1694	1.6703
17.	O	0.0397	0.0009	0.5609	0.0030	0.0005	0.0009	0.1694	0.0000	1.1433
18.	C	0.0028	0.0001	0.0033	0.0021	0.0002	0.0001	1.6703	1.1433	0.0000
19.	C	0.0017	0.0001	0.0122	0.0005	0.0003	0.0001	0.0525	0.0206	0.9819
20.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0151	0.0046	0.0068
21.	H	0.0001	0.0000	0.0002	0.0002	0.0000	0.0000	0.0140	0.0023	0.0057
22.	H	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000	0.0014	0.0004	0.0094
23.	C	0.0004	0.0000	0.0007	0.0001	0.0000	0.0000	0.0051	0.0082	0.0082
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0014
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0004	0.0013
26.	H	0.0008	0.0004	0.0000	0.0004	0.0000	0.0000	0.0000	0.0001	0.0000

Atom		19	20	21	22	23	24	25	26
1.	C	0.0010	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0002
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0123
3.	C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025
4.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9431
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8.	N	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0013
9.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

10. N	0.0017	0.0001	0.0001	0.0001	0.0004	0.0000	0.0000	0.0008	
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	
12. H	0.0122	0.0000	0.0002	0.0003	0.0007	0.0000	0.0000	0.0000	
13. N	0.0005	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0004	
14. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
15. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
16. O	0.0525	0.0151	0.0140	0.0014	0.0051	0.0008	0.0006	0.0000	
17. O	0.0206	0.0046	0.0023	0.0004	0.0082	0.0005	0.0004	0.0001	
18. C	0.9819	0.0068	0.0057	0.0094	0.0082	0.0014	0.0013	0.0000	
19. C	0.0000	0.9095	0.9147	0.0017	1.0309	0.0022	0.0022	0.0000	
20. H	0.9095	0.0000	0.0012	0.0015	0.0030	0.0012	0.0123	0.0000	
21. H	0.9147	0.0012	0.0000	0.0013	0.0028	0.0123	0.0013	0.0000	
22. H	0.0017	0.0015	0.0013	0.0000	0.9465	0.0005	0.0006	0.0000	
23. C	1.0309	0.0030	0.0028	0.9465	0.0000	0.9407	0.9435	0.0000	
24. H	0.0022	0.0012	0.0123	0.0005	0.9407	0.0000	0.0007	0.0000	
25. H	0.0022	0.0123	0.0013	0.0006	0.9435	0.0007	0.0000	0.0000	
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	

Table-9C-1-3: Wiberg index for salt bridge with no water (bridge length=3.3angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0063	0.0111	0.0016	0.0060	0.0001	0.0005	1.1776	0.0027
2. H	0.0063	0.0000	0.9281	0.0013	0.0025	0.0016	0.0009	0.0054	0.0023
3. C	0.0111	0.9281	0.0000	0.9243	1.0225	0.0023	0.0031	0.9675	0.0041
4. H	0.0016	0.0013	0.9243	0.0000	0.0024	0.0122	0.0009	0.0066	0.0071
5. C	0.0060	0.0025	1.0225	0.0024	0.0000	0.9435	0.9420	0.0206	0.0007
6. H	0.0001	0.0016	0.0023	0.0122	0.9435	0.0000	0.0006	0.0017	0.0003
7. H	0.0005	0.0009	0.0031	0.0009	0.9420	0.0006	0.0000	0.0113	0.0001
8. N	1.1776	0.0054	0.9675	0.0066	0.0206	0.0017	0.0113	0.0000	0.8164
9. H	0.0027	0.0023	0.0041	0.0071	0.0007	0.0003	0.0001	0.8164	0.0000
10. N	1.5671	0.0029	0.0045	0.0047	0.0045	0.0003	0.0007	0.1274	0.0141
11. H	0.0043	0.0001	0.0010	0.0006	0.0004	0.0000	0.0000	0.0029	0.0003
12. H	0.0036	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0074	0.0001
13. N	1.1221	0.0009	0.0117	0.0012	0.0016	0.0001	0.0005	0.0435	0.0032
14. H	0.0026	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0022	0.0001
15. H	0.0020	0.0001	0.0010	0.0000	0.0002	0.0000	0.0001	0.0098	0.0004
16. O	0.0095	0.0001	0.0009	0.0004	0.0002	0.0000	0.0000	0.0033	0.0002
17. O	0.0090	0.0001	0.0003	0.0001	0.0002	0.0000	0.0000	0.0046	0.0002
18. C	0.0016	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0010	0.0000
19. C	0.0008	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0003	0.0122	0.0025	0.0015	0.9429	0.0006	0.0006	0.0013	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.5671	0.0043	0.0036	1.1221	0.0026	0.0020	0.0095	0.0090	0.0016
2. H	0.0029	0.0001	0.0001	0.0009	0.0000	0.0001	0.0001	0.0001	0.0000
3. C	0.0045	0.0010	0.0001	0.0117	0.0002	0.0010	0.0009	0.0003	0.0003
4. H	0.0047	0.0006	0.0001	0.0012	0.0000	0.0000	0.0004	0.0001	0.0001
5. C	0.0045	0.0004	0.0001	0.0016	0.0001	0.0002	0.0002	0.0002	0.0001

6. H	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. H	0.0007	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000
8. N	0.1274	0.0029	0.0074	0.0435	0.0022	0.0098	0.0033	0.0046	0.0010
9. H	0.0141	0.0003	0.0001	0.0032	0.0001	0.0004	0.0002	0.0002	0.0000
10. N	0.0000	0.8512	0.1585	0.0856	0.0187	0.0027	0.0055	0.0369	0.0025
11. H	0.8512	0.0000	0.0001	0.0189	0.0006	0.0005	0.0002	0.0007	0.0001
12. H	0.1585	0.0001	0.0000	0.0011	0.0000	0.0001	0.0020	0.5718	0.0034
13. N	0.0856	0.0189	0.0011	0.0000	0.8245	0.8364	0.0039	0.0028	0.0020
14. H	0.0187	0.0006	0.0000	0.8245	0.0000	0.0002	0.0023	0.0005	0.0002
15. H	0.0027	0.0005	0.0001	0.8364	0.0002	0.0000	0.0002	0.0007	0.0001
16. O	0.0055	0.0002	0.0020	0.0039	0.0023	0.0002	0.0000	0.1689	1.6756
17. O	0.0369	0.0007	0.5718	0.0028	0.0005	0.0007	0.1689	0.0000	1.1381
18. C	0.0025	0.0001	0.0034	0.0020	0.0002	0.0001	1.6756	1.1381	0.0000
19. C	0.0015	0.0001	0.0126	0.0005	0.0003	0.0001	0.0523	0.0200	0.9828
20. H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0153	0.0043	0.0068
21. H	0.0001	0.0000	0.0002	0.0002	0.0000	0.0000	0.0143	0.0024	0.0058
22. H	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000	0.0015	0.0004	0.0094
23. C	0.0004	0.0000	0.0007	0.0001	0.0000	0.0000	0.0052	0.0080	0.0083
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0004	0.0014
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0004	0.0013
26. H	0.0008	0.0004	0.0000	0.0004	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0008	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0003
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0122
3. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025
4. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9429
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8. N	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0013
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0015	0.0001	0.0001	0.0001	0.0004	0.0000	0.0000	0.0008
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
12. H	0.0126	0.0001	0.0002	0.0004	0.0007	0.0000	0.0000	0.0000
13. N	0.0005	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0004
14. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. O	0.0523	0.0153	0.0143	0.0015	0.0052	0.0008	0.0006	0.0000
17. O	0.0200	0.0043	0.0024	0.0004	0.0080	0.0004	0.0004	0.0001
18. C	0.9828	0.0068	0.0058	0.0094	0.0083	0.0014	0.0013	0.0000
19. C	0.0000	0.9096	0.9141	0.0017	1.0309	0.0022	0.0022	0.0000
20. H	0.9096	0.0000	0.0012	0.0015	0.0030	0.0012	0.0123	0.0000
21. H	0.9141	0.0012	0.0000	0.0013	0.0028	0.0123	0.0013	0.0000
22. H	0.0017	0.0015	0.0013	0.0000	0.9464	0.0005	0.0005	0.0000
23. C	1.0309	0.0030	0.0028	0.9464	0.0000	0.9407	0.9432	0.0000
24. H	0.0022	0.0012	0.0123	0.0005	0.9407	0.0000	0.0007	0.0000
25. H	0.0022	0.0123	0.0013	0.0005	0.9432	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-4: Wiberg index for salt bridge with no water (bridge length=3.4angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0065	0.0111	0.0016	0.0060	0.0001	0.0006	1.1754	0.0027

2. H	0.0065	0.0000	0.9280	0.0013	0.0025	0.0016	0.0009	0.0055	0.0022
3. C	0.0111	0.9280	0.0000	0.9242	1.0219	0.0022	0.0032	0.9686	0.0043
4. H	0.0016	0.0013	0.9242	0.0000	0.0024	0.0122	0.0009	0.0063	0.0077
5. C	0.0060	0.0025	1.0219	0.0024	0.0000	0.9436	0.9417	0.0207	0.0005
6. H	0.0001	0.0016	0.0022	0.0122	0.9436	0.0000	0.0006	0.0017	0.0003
7. H	0.0006	0.0009	0.0032	0.0009	0.9417	0.0006	0.0000	0.0112	0.0000
8. N	1.1754	0.0055	0.9686	0.0063	0.0207	0.0017	0.0112	0.0000	0.8153
9. H	0.0027	0.0022	0.0043	0.0077	0.0005	0.0003	0.0000	0.8153	0.0000
10. N	1.5746	0.0027	0.0044	0.0047	0.0048	0.0003	0.0007	0.1286	0.0144
11. H	0.0043	0.0001	0.0011	0.0006	0.0004	0.0000	0.0000	0.0029	0.0003
12. H	0.0029	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0070	0.0001
13. N	1.1205	0.0008	0.0116	0.0011	0.0017	0.0001	0.0005	0.0430	0.0031
14. H	0.0026	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0022	0.0001
15. H	0.0020	0.0001	0.0010	0.0000	0.0002	0.0000	0.0001	0.0097	0.0004
16. O	0.0067	0.0001	0.0008	0.0003	0.0002	0.0000	0.0000	0.0028	0.0002
17. O	0.0087	0.0001	0.0002	0.0001	0.0002	0.0000	0.0000	0.0045	0.0001
18. C	0.0014	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000	0.0008	0.0000
19. C	0.0007	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0003	0.0121	0.0025	0.0015	0.9427	0.0006	0.0006	0.0013	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.5746	0.0043	0.0029	1.1205	0.0026	0.0020	0.0067	0.0087	0.0014
2. H	0.0027	0.0001	0.0001	0.0008	0.0000	0.0001	0.0001	0.0001	0.0000
3. C	0.0044	0.0011	0.0001	0.0116	0.0002	0.0010	0.0008	0.0002	0.0002
4. H	0.0047	0.0006	0.0001	0.0011	0.0000	0.0000	0.0003	0.0001	0.0001
5. C	0.0048	0.0004	0.0001	0.0017	0.0001	0.0002	0.0002	0.0002	0.0001
6. H	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. H	0.0007	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000
8. N	0.1286	0.0029	0.0070	0.0430	0.0022	0.0097	0.0028	0.0045	0.0008
9. H	0.0144	0.0003	0.0001	0.0031	0.0001	0.0004	0.0002	0.0001	0.0000
10. N	0.0000	0.8518	0.1526	0.0854	0.0189	0.0027	0.0044	0.0358	0.0024
11. H	0.8518	0.0000	0.0001	0.0189	0.0006	0.0005	0.0002	0.0007	0.0001
12. H	0.1526	0.0001	0.0000	0.0011	0.0000	0.0001	0.0023	0.5761	0.0034
13. N	0.0854	0.0189	0.0011	0.0000	0.8237	0.8370	0.0036	0.0027	0.0019
14. H	0.0189	0.0006	0.0000	0.8237	0.0000	0.0002	0.0021	0.0005	0.0002
15. H	0.0027	0.0005	0.0001	0.8370	0.0002	0.0000	0.0002	0.0007	0.0001
16. O	0.0044	0.0002	0.0023	0.0036	0.0021	0.0002	0.0000	0.1687	1.6792
17. O	0.0358	0.0007	0.5761	0.0027	0.0005	0.0007	0.1687	0.0000	1.1350
18. C	0.0024	0.0001	0.0034	0.0019	0.0002	0.0001	1.6792	1.1350	0.0000
19. C	0.0015	0.0001	0.0129	0.0005	0.0003	0.0001	0.0521	0.0197	0.9833
20. H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0154	0.0041	0.0066
21. H	0.0001	0.0000	0.0001	0.0002	0.0000	0.0000	0.0146	0.0025	0.0059
22. H	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000	0.0015	0.0004	0.0094
23. C	0.0004	0.0000	0.0007	0.0001	0.0000	0.0000	0.0054	0.0079	0.0084
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0004	0.0014
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0004	0.0013
26. H	0.0008	0.0004	0.0000	0.0004	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0007	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0003
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0121
3. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9427
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8. N	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0013
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0015	0.0001	0.0001	0.0001	0.0004	0.0000	0.0000	0.0008
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
12. H	0.0129	0.0001	0.0001	0.0004	0.0007	0.0000	0.0000	0.0000
13. N	0.0005	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0004
14. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. O	0.0521	0.0154	0.0146	0.0015	0.0054	0.0008	0.0006	0.0000
17. O	0.0197	0.0041	0.0025	0.0004	0.0079	0.0004	0.0004	0.0001
18. C	0.9833	0.0066	0.0059	0.0094	0.0084	0.0014	0.0013	0.0000
19. C	0.0000	0.9099	0.9136	0.0017	1.0309	0.0022	0.0022	0.0000
20. H	0.9099	0.0000	0.0012	0.0015	0.0030	0.0012	0.0123	0.0000
21. H	0.9136	0.0012	0.0000	0.0013	0.0029	0.0123	0.0013	0.0000
22. H	0.0017	0.0015	0.0013	0.0000	0.9465	0.0005	0.0005	0.0000
23. C	1.0309	0.0030	0.0029	0.9465	0.0000	0.9407	0.9429	0.0000
24. H	0.0022	0.0012	0.0123	0.0005	0.9407	0.0000	0.0007	0.0000
25. H	0.0022	0.0123	0.0013	0.0005	0.9429	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-5: Wiberg index for salt bridge with no water (bridge length=3.5angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0070	0.0108	0.0019	0.0055	0.0001	0.0007	1.1725	0.0020
2. H	0.0070	0.0000	0.9288	0.0011	0.0028	0.0017	0.0010	0.0036	0.0024
3. C	0.0108	0.9288	0.0000	0.9269	1.0229	0.0020	0.0035	0.9661	0.0039
4. H	0.0019	0.0011	0.9269	0.0000	0.0026	0.0122	0.0009	0.0081	0.0076
5. C	0.0055	0.0028	1.0229	0.0026	0.0000	0.9431	0.9399	0.0204	0.0006
6. H	0.0001	0.0017	0.0020	0.0122	0.9431	0.0000	0.0006	0.0015	0.0003
7. H	0.0007	0.0010	0.0035	0.0009	0.9399	0.0006	0.0000	0.0108	0.0001
8. N	1.1725	0.0036	0.9661	0.0081	0.0204	0.0015	0.0108	0.0000	0.8255
9. H	0.0020	0.0024	0.0039	0.0076	0.0006	0.0003	0.0001	0.8255	0.0000
10. N	1.4049	0.0008	0.0041	0.0034	0.0040	0.0002	0.0003	0.0866	0.0108
11. H	0.0029	0.0000	0.0017	0.0018	0.0002	0.0001	0.0000	0.0025	0.0005
12. H	0.0031	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0072	0.0003
13. N	1.2813	0.0004	0.0130	0.0010	0.0031	0.0001	0.0010	0.0628	0.0023
14. H	0.0026	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0028	0.0010
15. H	0.0036	0.0002	0.0005	0.0000	0.0001	0.0000	0.0000	0.0087	0.0002
16. O	0.0055	0.0001	0.0004	0.0001	0.0002	0.0000	0.0000	0.0027	0.0003
17. O	0.0042	0.0002	0.0007	0.0002	0.0001	0.0000	0.0000	0.0029	0.0011
18. C	0.0010	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
19. C	0.0006	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

23.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0005	0.0118	0.0023	0.0015	0.9382	0.0006	0.0006	0.0015	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.4049	0.0029	0.0031	1.2813	0.0026	0.0036	0.0055	0.0042	0.0010
2.	H	0.0008	0.0000	0.0000	0.0004	0.0001	0.0002	0.0001	0.0002	0.0000
3.	C	0.0041	0.0017	0.0002	0.0130	0.0005	0.0005	0.0004	0.0007	0.0001
4.	H	0.0034	0.0018	0.0000	0.0010	0.0000	0.0000	0.0001	0.0002	0.0000
5.	C	0.0040	0.0002	0.0000	0.0031	0.0000	0.0001	0.0002	0.0001	0.0000
6.	H	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0003	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
8.	N	0.0866	0.0025	0.0072	0.0628	0.0028	0.0087	0.0027	0.0029	0.0004
9.	H	0.0108	0.0005	0.0003	0.0023	0.0010	0.0002	0.0003	0.0011	0.0001
10.	N	0.0000	0.8334	0.5504	0.1054	0.0101	0.0020	0.0040	0.0624	0.0043
11.	H	0.8334	0.0000	0.0012	0.0118	0.0009	0.0001	0.0003	0.0025	0.0001
12.	H	0.5504	0.0012	0.0000	0.0012	0.0002	0.0003	0.0012	0.2332	0.0023
13.	N	0.1054	0.0118	0.0012	0.0000	0.8477	0.6466	0.0422	0.0044	0.0051
14.	H	0.0101	0.0009	0.0002	0.8477	0.0000	0.0009	0.0017	0.0003	0.0002
15.	H	0.0020	0.0001	0.0003	0.6466	0.0009	0.0000	0.1407	0.0014	0.0022
16.	O	0.0040	0.0003	0.0012	0.0422	0.0017	0.1407	0.0000	0.1807	1.4576
17.	O	0.0624	0.0025	0.2332	0.0044	0.0003	0.0014	0.1807	0.0000	1.3703
18.	C	0.0043	0.0001	0.0023	0.0051	0.0002	0.0022	1.4576	1.3703	0.0000
19.	C	0.0035	0.0003	0.0083	0.0027	0.0003	0.0064	0.0379	0.0345	0.9695
20.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0120	0.0047	0.0052
21.	H	0.0002	0.0000	0.0001	0.0004	0.0000	0.0002	0.0115	0.0055	0.0062
22.	H	0.0002	0.0000	0.0002	0.0000	0.0000	0.0001	0.0020	0.0011	0.0093
23.	C	0.0007	0.0000	0.0004	0.0002	0.0000	0.0001	0.0055	0.0088	0.0078
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0005	0.0013
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0004	0.0013
26.	H	0.0015	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0001	0.0000

Atom		19	20	21	22	23	24	25	26
1.	C	0.0006	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0005
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0118
3.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9382
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8.	N	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
9.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	N	0.0035	0.0001	0.0002	0.0002	0.0007	0.0000	0.0000	0.0015
11.	H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0083	0.0000	0.0001	0.0002	0.0004	0.0000	0.0000	0.0000
13.	N	0.0027	0.0000	0.0004	0.0000	0.0002	0.0000	0.0000	0.0004
14.	H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	H	0.0064	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000	0.0000
16.	O	0.0379	0.0120	0.0115	0.0020	0.0055	0.0006	0.0009	0.0000
17.	O	0.0345	0.0047	0.0055	0.0011	0.0088	0.0005	0.0004	0.0001
18.	C	0.9695	0.0052	0.0062	0.0093	0.0078	0.0013	0.0013	0.0000
19.	C	0.0000	0.9194	0.9157	0.0018	1.0320	0.0024	0.0024	0.0000

20.	H	0.9194	0.0000	0.0012	0.0013	0.0026	0.0013	0.0127	0.0000
21.	H	0.9157	0.0012	0.0000	0.0014	0.0027	0.0126	0.0013	0.0000
22.	H	0.0018	0.0013	0.0014	0.0000	0.9484	0.0005	0.0005	0.0000
23.	C	1.0320	0.0026	0.0027	0.9484	0.0000	0.9430	0.9423	0.0000
24.	H	0.0024	0.0013	0.0126	0.0005	0.9430	0.0000	0.0007	0.0000
25.	H	0.0024	0.0127	0.0013	0.0005	0.9423	0.0007	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-6: Wiberg index for salt bridge with no water (bridge length=3.6angstroms)

Atom		1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.0071	0.0106	0.0016	0.0054	0.0001	0.0007	1.1672	0.0020
2.	H	0.0071	0.0000	0.9283	0.0011	0.0028	0.0017	0.0010	0.0040	0.0023
3.	C	0.0106	0.9283	0.0000	0.9273	1.0229	0.0020	0.0035	0.9669	0.0040
4.	H	0.0016	0.0011	0.9273	0.0000	0.0026	0.0122	0.0009	0.0074	0.0082
5.	C	0.0054	0.0028	1.0229	0.0026	0.0000	0.9431	0.9397	0.0208	0.0004
6.	H	0.0001	0.0017	0.0020	0.0122	0.9431	0.0000	0.0006	0.0015	0.0003
7.	H	0.0007	0.0010	0.0035	0.0009	0.9397	0.0006	0.0000	0.0109	0.0000
8.	N	1.1672	0.0040	0.9669	0.0074	0.0208	0.0015	0.0109	0.0000	0.8260
9.	H	0.0020	0.0023	0.0040	0.0082	0.0004	0.0003	0.0000	0.8260	0.0000
10.	N	1.3882	0.0008	0.0043	0.0030	0.0038	0.0002	0.0003	0.0818	0.0107
11.	H	0.0028	0.0000	0.0018	0.0018	0.0002	0.0001	0.0000	0.0024	0.0005
12.	H	0.0030	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0071	0.0003
13.	N	1.3073	0.0005	0.0124	0.0010	0.0034	0.0001	0.0010	0.0653	0.0022
14.	H	0.0026	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0026	0.0009
15.	H	0.0032	0.0002	0.0005	0.0000	0.0001	0.0000	0.0000	0.0081	0.0002
16.	O	0.0048	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0028	0.0003
17.	O	0.0031	0.0002	0.0006	0.0002	0.0001	0.0000	0.0000	0.0025	0.0010
18.	C	0.0009	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
19.	C	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
20.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0005	0.0118	0.0023	0.0014	0.9385	0.0006	0.0006	0.0014	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.3882	0.0028	0.0030	1.3073	0.0026	0.0032	0.0048	0.0031	0.0009
2.	H	0.0008	0.0000	0.0000	0.0005	0.0001	0.0002	0.0001	0.0002	0.0000
3.	C	0.0043	0.0018	0.0002	0.0124	0.0005	0.0005	0.0005	0.0006	0.0001
4.	H	0.0030	0.0018	0.0000	0.0010	0.0000	0.0000	0.0001	0.0002	0.0000
5.	C	0.0038	0.0002	0.0000	0.0034	0.0000	0.0001	0.0001	0.0001	0.0000
6.	H	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0003	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
8.	N	0.0818	0.0024	0.0071	0.0653	0.0026	0.0081	0.0028	0.0025	0.0004
9.	H	0.0107	0.0005	0.0003	0.0022	0.0009	0.0002	0.0003	0.0010	0.0001
10.	N	0.0000	0.8334	0.5668	0.1109	0.0103	0.0014	0.0038	0.0592	0.0038
11.	H	0.8334	0.0000	0.0013	0.0108	0.0009	0.0002	0.0002	0.0024	0.0001
12.	H	0.5668	0.0013	0.0000	0.0010	0.0002	0.0004	0.0012	0.2157	0.0021
13.	N	0.1109	0.0108	0.0010	0.0000	0.8451	0.6270	0.0467	0.0037	0.0042
14.	H	0.0103	0.0009	0.0002	0.8451	0.0000	0.0010	0.0019	0.0003	0.0002
15.	H	0.0014	0.0002	0.0004	0.6270	0.0010	0.0000	0.1588	0.0012	0.0020

16. O	0.0038	0.0002	0.0012	0.0467	0.0019	0.1588	0.0000	0.1813	1.4446
17. O	0.0592	0.0024	0.2157	0.0037	0.0003	0.0012	0.1813	0.0000	1.3836
18. C	0.0038	0.0001	0.0021	0.0042	0.0002	0.0020	1.4446	1.3836	0.0000
19. C	0.0035	0.0003	0.0082	0.0031	0.0003	0.0071	0.0354	0.0354	0.9703
20. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0120	0.0056	0.0056
21. H	0.0002	0.0000	0.0001	0.0004	0.0000	0.0002	0.0114	0.0048	0.0057
22. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0001	0.0021	0.0011	0.0093
23. C	0.0006	0.0000	0.0004	0.0002	0.0000	0.0001	0.0055	0.0089	0.0079
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0005	0.0013
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0013
26. H	0.0015	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0005	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0005
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0118
3. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9385
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8. N	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
9. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0035	0.0001	0.0002	0.0001	0.0006	0.0000	0.0000	0.0015
11. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0082	0.0000	0.0001	0.0002	0.0004	0.0000	0.0000	0.0000
13. N	0.0031	0.0000	0.0004	0.0000	0.0002	0.0000	0.0000	0.0004
14. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0071	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000	0.0000
16. O	0.0354	0.0120	0.0114	0.0021	0.0055	0.0007	0.0008	0.0000
17. O	0.0354	0.0056	0.0048	0.0011	0.0089	0.0005	0.0005	0.0001
18. C	0.9703	0.0056	0.0057	0.0093	0.0079	0.0013	0.0013	0.0000
19. C	0.0000	0.9177	0.9173	0.0018	1.0319	0.0024	0.0024	0.0000
20. H	0.9177	0.0000	0.0012	0.0013	0.0027	0.0013	0.0127	0.0000
21. H	0.9173	0.0012	0.0000	0.0013	0.0026	0.0126	0.0013	0.0000
22. H	0.0018	0.0013	0.0013	0.0000	0.9485	0.0005	0.0005	0.0000
23. C	1.0319	0.0027	0.0026	0.9485	0.0000	0.9422	0.9429	0.0000
24. H	0.0024	0.0013	0.0126	0.0005	0.9422	0.0000	0.0007	0.0000
25. H	0.0024	0.0127	0.0013	0.0005	0.9429	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-7: Wiberg index for salt bridge with no water (bridge length=3.7angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0071	0.0105	0.0015	0.0053	0.0001	0.0007	1.1666	0.0020
2. H	0.0071	0.0000	0.9277	0.0011	0.0027	0.0017	0.0010	0.0044	0.0023
3. C	0.0105	0.9277	0.0000	0.9271	1.0229	0.0020	0.0035	0.9674	0.0041
4. H	0.0015	0.0011	0.9271	0.0000	0.0026	0.0122	0.0009	0.0069	0.0085
5. C	0.0053	0.0027	1.0229	0.0026	0.0000	0.9429	0.9394	0.0210	0.0003
6. H	0.0001	0.0017	0.0020	0.0122	0.9429	0.0000	0.0006	0.0015	0.0003
7. H	0.0007	0.0010	0.0035	0.0009	0.9394	0.0006	0.0000	0.0110	0.0000
8. N	1.1666	0.0044	0.9674	0.0069	0.0210	0.0015	0.0110	0.0000	0.8255
9. H	0.0020	0.0023	0.0041	0.0085	0.0003	0.0003	0.0000	0.8255	0.0000
10. N	1.3786	0.0008	0.0041	0.0031	0.0037	0.0002	0.0003	0.0791	0.0108
11. H	0.0027	0.0000	0.0017	0.0016	0.0002	0.0001	0.0000	0.0023	0.0004

12. H	0.0029	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0069	0.0003
13. N	1.3207	0.0007	0.0115	0.0010	0.0035	0.0001	0.0010	0.0665	0.0022
14. H	0.0025	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0025	0.0009
15. H	0.0029	0.0002	0.0006	0.0000	0.0000	0.0000	0.0000	0.0074	0.0002
16. O	0.0035	0.0001	0.0007	0.0001	0.0001	0.0000	0.0000	0.0026	0.0003
17. O	0.0026	0.0002	0.0006	0.0002	0.0001	0.0000	0.0000	0.0023	0.0010
18. C	0.0009	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
19. C	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
20. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0004	0.0118	0.0023	0.0014	0.9391	0.0006	0.0006	0.0014	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3786	0.0027	0.0029	1.3207	0.0025	0.0029	0.0035	0.0026	0.0009
2. H	0.0008	0.0000	0.0000	0.0007	0.0001	0.0002	0.0001	0.0002	0.0000
3. C	0.0041	0.0017	0.0002	0.0115	0.0005	0.0006	0.0007	0.0006	0.0001
4. H	0.0031	0.0016	0.0000	0.0010	0.0000	0.0000	0.0001	0.0002	0.0000
5. C	0.0037	0.0002	0.0000	0.0035	0.0000	0.0000	0.0001	0.0001	0.0000
6. H	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. H	0.0003	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
8. N	0.0791	0.0023	0.0069	0.0665	0.0025	0.0074	0.0026	0.0023	0.0004
9. H	0.0108	0.0004	0.0003	0.0022	0.0009	0.0002	0.0003	0.0010	0.0001
10. N	0.0000	0.8341	0.5747	0.1134	0.0105	0.0010	0.0032	0.0570	0.0033
11. H	0.8341	0.0000	0.0013	0.0102	0.0009	0.0002	0.0002	0.0020	0.0001
12. H	0.5747	0.0013	0.0000	0.0009	0.0002	0.0005	0.0012	0.2061	0.0020
13. N	0.1134	0.0102	0.0009	0.0000	0.8430	0.6219	0.0477	0.0031	0.0032
14. H	0.0105	0.0009	0.0002	0.8430	0.0000	0.0011	0.0018	0.0002	0.0001
15. H	0.0010	0.0002	0.0005	0.6219	0.0011	0.0000	0.1616	0.0011	0.0018
16. O	0.0032	0.0002	0.0012	0.0477	0.0018	0.1616	0.0000	0.1823	1.4421
17. O	0.0570	0.0020	0.2061	0.0031	0.0002	0.0011	0.1823	0.0000	1.3876
18. C	0.0033	0.0001	0.0020	0.0032	0.0001	0.0018	1.4421	1.3876	0.0000
19. C	0.0035	0.0002	0.0082	0.0033	0.0002	0.0076	0.0342	0.0355	0.9709
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0120	0.0051	0.0054
21. H	0.0001	0.0000	0.0001	0.0003	0.0000	0.0002	0.0117	0.0054	0.0058
22. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0001	0.0022	0.0012	0.0093
23. C	0.0006	0.0000	0.0004	0.0002	0.0000	0.0001	0.0056	0.0088	0.0079
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0005	0.0013
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0013
26. H	0.0015	0.0001	0.0000	0.0005	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0003	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0118
3. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9391
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8. N	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014

9.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	N	0.0035	0.0001	0.0001	0.0001	0.0006	0.0000	0.0000	0.0015
11.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
12.	H	0.0082	0.0000	0.0001	0.0002	0.0004	0.0000	0.0000	0.0000
13.	N	0.0033	0.0001	0.0003	0.0000	0.0002	0.0000	0.0000	0.0005
14.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	H	0.0076	0.0001	0.0002	0.0001	0.0001	0.0000	0.0000	0.0000
16.	O	0.0342	0.0120	0.0117	0.0022	0.0056	0.0007	0.0008	0.0000
17.	O	0.0355	0.0051	0.0054	0.0012	0.0088	0.0005	0.0005	0.0001
18.	C	0.9709	0.0054	0.0058	0.0093	0.0079	0.0013	0.0013	0.0000
19.	C	0.0000	0.9184	0.9167	0.0018	1.0318	0.0024	0.0024	0.0000
20.	H	0.9184	0.0000	0.0012	0.0013	0.0026	0.0013	0.0126	0.0000
21.	H	0.9167	0.0012	0.0000	0.0014	0.0027	0.0126	0.0013	0.0000
22.	H	0.0018	0.0013	0.0014	0.0000	0.9486	0.0005	0.0005	0.0000
23.	C	1.0318	0.0026	0.0027	0.9486	0.0000	0.9427	0.9424	0.0000
24.	H	0.0024	0.0013	0.0126	0.0005	0.9427	0.0000	0.0007	0.0000
25.	H	0.0024	0.0126	0.0013	0.0005	0.9424	0.0007	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-8: Wiberg index for salt bridge with no water (bridge length=3.8angstroms)

Atom		1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.0069	0.0106	0.0014	0.0054	0.0001	0.0006	1.1720	0.0021
2.	H	0.0069	0.0000	0.9266	0.0012	0.0027	0.0017	0.0010	0.0053	0.0021
3.	C	0.0106	0.9266	0.0000	0.9263	1.0228	0.0020	0.0035	0.9676	0.0043
4.	H	0.0014	0.0012	0.9263	0.0000	0.0026	0.0121	0.0009	0.0058	0.0089
5.	C	0.0054	0.0027	1.0228	0.0026	0.0000	0.9426	0.9391	0.0210	0.0003
6.	H	0.0001	0.0017	0.0020	0.0121	0.9426	0.0000	0.0006	0.0015	0.0004
7.	H	0.0006	0.0010	0.0035	0.0009	0.9391	0.0006	0.0000	0.0110	0.0000
8.	N	1.1720	0.0053	0.9676	0.0058	0.0210	0.0015	0.0110	0.0000	0.8226
9.	H	0.0021	0.0021	0.0043	0.0089	0.0003	0.0004	0.0000	0.8226	0.0000
10.	N	1.3733	0.0010	0.0036	0.0037	0.0036	0.0002	0.0003	0.0789	0.0116
11.	H	0.0026	0.0000	0.0015	0.0012	0.0003	0.0000	0.0000	0.0022	0.0004
12.	H	0.0028	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0070	0.0003
13.	N	1.3230	0.0010	0.0104	0.0010	0.0035	0.0001	0.0009	0.0682	0.0022
14.	H	0.0025	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0022	0.0006
15.	H	0.0027	0.0002	0.0006	0.0000	0.0000	0.0000	0.0000	0.0067	0.0002
16.	O	0.0021	0.0001	0.0008	0.0000	0.0000	0.0000	0.0000	0.0023	0.0002
17.	O	0.0025	0.0001	0.0006	0.0001	0.0001	0.0000	0.0000	0.0023	0.0009
18.	C	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
19.	C	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
20.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0004	0.0119	0.0023	0.0014	0.9406	0.0006	0.0006	0.0013	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.3733	0.0026	0.0028	1.3230	0.0025	0.0027	0.0021	0.0025	0.0008
2.	H	0.0010	0.0000	0.0000	0.0010	0.0001	0.0002	0.0001	0.0001	0.0000
3.	C	0.0036	0.0015	0.0001	0.0104	0.0004	0.0006	0.0008	0.0006	0.0000
4.	H	0.0037	0.0012	0.0000	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000

5. C	0.0036	0.0003	0.0000	0.0035	0.0000	0.0000	0.0000	0.0001	0.0000
6. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. H	0.0003	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
8. N	0.0789	0.0022	0.0070	0.0682	0.0022	0.0067	0.0023	0.0023	0.0004
9. H	0.0116	0.0004	0.0003	0.0022	0.0006	0.0002	0.0002	0.0009	0.0000
10. N	0.0000	0.8349	0.5796	0.1131	0.0114	0.0009	0.0025	0.0549	0.0027
11. H	0.8349	0.0000	0.0012	0.0103	0.0009	0.0003	0.0002	0.0017	0.0001
12. H	0.5796	0.0012	0.0000	0.0009	0.0002	0.0006	0.0013	0.1984	0.0019
13. N	0.1131	0.0103	0.0009	0.0000	0.8399	0.6289	0.0454	0.0026	0.0024
14. H	0.0114	0.0009	0.0002	0.8399	0.0000	0.0011	0.0017	0.0001	0.0001
15. H	0.0009	0.0003	0.0006	0.6289	0.0011	0.0000	0.1513	0.0011	0.0017
16. O	0.0025	0.0002	0.0013	0.0454	0.0017	0.1513	0.0000	0.1836	1.4464
17. O	0.0549	0.0017	0.1984	0.0026	0.0001	0.0011	0.1836	0.0000	1.3861
18. C	0.0027	0.0001	0.0019	0.0024	0.0001	0.0017	1.4464	1.3861	0.0000
19. C	0.0034	0.0002	0.0084	0.0033	0.0002	0.0077	0.0342	0.0351	0.9713
20. H	0.0001	0.0000	0.0000	0.0002	0.0000	0.0001	0.0120	0.0050	0.0054
21. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0120	0.0056	0.0057
22. H	0.0002	0.0000	0.0003	0.0000	0.0000	0.0001	0.0022	0.0012	0.0093
23. C	0.0006	0.0000	0.0005	0.0001	0.0000	0.0001	0.0056	0.0089	0.0080
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0005	0.0013
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0013
26. H	0.0014	0.0002	0.0000	0.0006	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0003	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119
3. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9406
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8. N	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0013
9. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0034	0.0001	0.0001	0.0002	0.0006	0.0000	0.0000	0.0014
11. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
12. H	0.0084	0.0000	0.0000	0.0003	0.0005	0.0000	0.0000	0.0000
13. N	0.0033	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0006
14. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0077	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
16. O	0.0342	0.0120	0.0120	0.0022	0.0056	0.0007	0.0008	0.0000
17. O	0.0351	0.0050	0.0056	0.0012	0.0089	0.0005	0.0005	0.0001
18. C	0.9713	0.0054	0.0057	0.0093	0.0080	0.0013	0.0013	0.0000
19. C	0.0000	0.9180	0.9170	0.0018	1.0316	0.0024	0.0024	0.0000
20. H	0.9180	0.0000	0.0012	0.0013	0.0026	0.0013	0.0126	0.0000
21. H	0.9170	0.0012	0.0000	0.0014	0.0027	0.0126	0.0013	0.0000
22. H	0.0018	0.0013	0.0014	0.0000	0.9488	0.0005	0.0005	0.0000
23. C	1.0316	0.0026	0.0027	0.9488	0.0000	0.9429	0.9421	0.0000
24. H	0.0024	0.0013	0.0126	0.0005	0.9429	0.0000	0.0007	0.0000
25. H	0.0024	0.0126	0.0013	0.0005	0.9421	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-9: Wiberg index for salt bridge with no water (bridge length=3.9angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0067	0.0108	0.0015	0.0056	0.0001	0.0006	1.1846	0.0021
2. H	0.0067	0.0000	0.9266	0.0012	0.0027	0.0017	0.0010	0.0051	0.0021
3. C	0.0108	0.9266	0.0000	0.9259	1.0232	0.0020	0.0036	0.9647	0.0044
4. H	0.0015	0.0012	0.9259	0.0000	0.0026	0.0121	0.0009	0.0056	0.0086
5. C	0.0056	0.0027	1.0232	0.0026	0.0000	0.9423	0.9386	0.0204	0.0003
6. H	0.0001	0.0017	0.0020	0.0121	0.9423	0.0000	0.0007	0.0016	0.0004
7. H	0.0006	0.0010	0.0036	0.0009	0.9386	0.0007	0.0000	0.0110	0.0000
8. N	1.1846	0.0051	0.9647	0.0056	0.0204	0.0016	0.0110	0.0000	0.8205
9. H	0.0021	0.0021	0.0044	0.0086	0.0003	0.0004	0.0000	0.8205	0.0000
10. N	1.3634	0.0010	0.0035	0.0037	0.0036	0.0002	0.0003	0.0798	0.0116
11. H	0.0025	0.0000	0.0013	0.0009	0.0003	0.0000	0.0000	0.0019	0.0003
12. H	0.0028	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0069	0.0003
13. N	1.3208	0.0011	0.0103	0.0010	0.0035	0.0001	0.0009	0.0701	0.0023
14. H	0.0024	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0019	0.0006
15. H	0.0026	0.0002	0.0006	0.0000	0.0000	0.0000	0.0000	0.0066	0.0002
16. O	0.0018	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0021	0.0002
17. O	0.0023	0.0001	0.0006	0.0001	0.0001	0.0000	0.0000	0.0020	0.0009
18. C	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
19. C	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0004	0.0119	0.0023	0.0015	0.9408	0.0006	0.0006	0.0012	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3634	0.0025	0.0028	1.3208	0.0024	0.0026	0.0018	0.0023	0.0007
2. H	0.0010	0.0000	0.0000	0.0011	0.0001	0.0002	0.0000	0.0001	0.0000
3. C	0.0035	0.0013	0.0001	0.0103	0.0004	0.0006	0.0007	0.0006	0.0000
4. H	0.0037	0.0009	0.0000	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000
5. C	0.0036	0.0003	0.0000	0.0035	0.0000	0.0000	0.0000	0.0001	0.0000
6. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. H	0.0003	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
8. N	0.0798	0.0019	0.0069	0.0701	0.0019	0.0066	0.0021	0.0020	0.0003
9. H	0.0116	0.0003	0.0003	0.0023	0.0006	0.0002	0.0002	0.0009	0.0000
10. N	0.0000	0.8344	0.5985	0.1102	0.0113	0.0009	0.0024	0.0493	0.0024
11. H	0.8344	0.0000	0.0012	0.0105	0.0010	0.0003	0.0002	0.0014	0.0001
12. H	0.5985	0.0012	0.0000	0.0009	0.0003	0.0007	0.0016	0.1743	0.0018
13. N	0.1102	0.0105	0.0009	0.0000	0.8387	0.6409	0.0405	0.0026	0.0020
14. H	0.0113	0.0010	0.0003	0.8387	0.0000	0.0011	0.0015	0.0001	0.0001
15. H	0.0009	0.0003	0.0007	0.6409	0.0011	0.0000	0.1335	0.0014	0.0016
16. O	0.0024	0.0002	0.0016	0.0405	0.0015	0.1335	0.0000	0.1851	1.4475
17. O	0.0493	0.0014	0.1743	0.0026	0.0001	0.0014	0.1851	0.0000	1.3903
18. C	0.0024	0.0001	0.0018	0.0020	0.0001	0.0016	1.4475	1.3903	0.0000
19. C	0.0032	0.0002	0.0083	0.0031	0.0002	0.0076	0.0345	0.0355	0.9715
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0121	0.0050	0.0053
21. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0122	0.0058	0.0057
22. H	0.0001	0.0000	0.0003	0.0000	0.0000	0.0001	0.0023	0.0013	0.0093
23. C	0.0005	0.0000	0.0005	0.0001	0.0000	0.0001	0.0057	0.0091	0.0081
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0005	0.0013

25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0013
26. H	0.0013	0.0002	0.0000	0.0006	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119
3. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9408
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8. N	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012
9. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0032	0.0001	0.0001	0.0001	0.0005	0.0000	0.0000	0.0013
11. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
12. H	0.0083	0.0000	0.0000	0.0003	0.0005	0.0000	0.0000	0.0000
13. N	0.0031	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0006
14. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0076	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
16. O	0.0345	0.0121	0.0122	0.0023	0.0057	0.0007	0.0008	0.0000
17. O	0.0355	0.0050	0.0058	0.0013	0.0091	0.0005	0.0005	0.0001
18. C	0.9715	0.0053	0.0057	0.0093	0.0081	0.0013	0.0013	0.0000
19. C	0.0000	0.9182	0.9168	0.0017	1.0312	0.0024	0.0024	0.0000
20. H	0.9182	0.0000	0.0011	0.0013	0.0026	0.0013	0.0126	0.0000
21. H	0.9168	0.0011	0.0000	0.0014	0.0027	0.0126	0.0013	0.0000
22. H	0.0017	0.0013	0.0014	0.0000	0.9491	0.0005	0.0005	0.0000
23. C	1.0312	0.0026	0.0027	0.9491	0.0000	0.9430	0.9420	0.0000
24. H	0.0024	0.0013	0.0126	0.0005	0.9430	0.0000	0.0007	0.0000
25. H	0.0024	0.0126	0.0013	0.0005	0.9420	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-10: Wiberg index for salt bridge with no water (bridge length=4.0angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0066	0.0109	0.0015	0.0058	0.0001	0.0006	1.1962	0.0021
2. H	0.0066	0.0000	0.9262	0.0012	0.0027	0.0017	0.0010	0.0049	0.0021
3. C	0.0109	0.9262	0.0000	0.9256	1.0238	0.0020	0.0036	0.9617	0.0045
4. H	0.0015	0.0012	0.9256	0.0000	0.0027	0.0121	0.0009	0.0055	0.0084
5. C	0.0058	0.0027	1.0238	0.0027	0.0000	0.9418	0.9377	0.0199	0.0003
6. H	0.0001	0.0017	0.0020	0.0121	0.9418	0.0000	0.0007	0.0015	0.0003
7. H	0.0006	0.0010	0.0036	0.0009	0.9377	0.0007	0.0000	0.0109	0.0000
8. N	1.1962	0.0049	0.9617	0.0055	0.0199	0.0015	0.0109	0.0000	0.8179
9. H	0.0021	0.0021	0.0045	0.0084	0.0003	0.0003	0.0000	0.8179	0.0000
10. N	1.3535	0.0010	0.0034	0.0037	0.0036	0.0002	0.0003	0.0804	0.0114
11. H	0.0024	0.0000	0.0011	0.0008	0.0003	0.0000	0.0000	0.0017	0.0002
12. H	0.0027	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0070	0.0003
13. N	1.3193	0.0011	0.0103	0.0010	0.0035	0.0001	0.0009	0.0719	0.0024
14. H	0.0023	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0018	0.0006
15. H	0.0025	0.0002	0.0007	0.0000	0.0000	0.0000	0.0000	0.0066	0.0002
16. O	0.0017	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0019	0.0002
17. O	0.0021	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0018	0.0008
18. C	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
19. C	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0004	0.0119	0.0023	0.0015	0.9407	0.0006	0.0006	0.0012	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.3535	0.0024	0.0027	1.3193	0.0023	0.0025	0.0017	0.0021	0.0006
2.	H	0.0010	0.0000	0.0000	0.0011	0.0001	0.0002	0.0000	0.0001	0.0000
3.	C	0.0034	0.0011	0.0002	0.0103	0.0003	0.0007	0.0007	0.0005	0.0000
4.	H	0.0037	0.0008	0.0000	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000
5.	C	0.0036	0.0003	0.0000	0.0035	0.0000	0.0000	0.0000	0.0001	0.0000
6.	H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0003	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
8.	N	0.0804	0.0017	0.0070	0.0719	0.0018	0.0066	0.0019	0.0018	0.0003
9.	H	0.0114	0.0002	0.0003	0.0024	0.0006	0.0002	0.0002	0.0008	0.0000
10.	N	0.0000	0.8335	0.6181	0.1073	0.0112	0.0009	0.0023	0.0433	0.0021
11.	H	0.8335	0.0000	0.0011	0.0105	0.0010	0.0003	0.0002	0.0013	0.0001
12.	H	0.6181	0.0011	0.0000	0.0009	0.0003	0.0008	0.0019	0.1493	0.0017
13.	N	0.1073	0.0105	0.0009	0.0000	0.8374	0.6525	0.0358	0.0025	0.0017
14.	H	0.0112	0.0010	0.0003	0.8374	0.0000	0.0010	0.0013	0.0002	0.0001
15.	H	0.0009	0.0003	0.0008	0.6525	0.0010	0.0000	0.1167	0.0017	0.0016
16.	O	0.0023	0.0002	0.0019	0.0358	0.0013	0.1167	0.0000	0.1870	1.4397
17.	O	0.0433	0.0013	0.1493	0.0025	0.0002	0.0017	0.1870	0.0000	1.4046
18.	C	0.0021	0.0001	0.0017	0.0017	0.0001	0.0016	1.4397	1.4046	0.0000
19.	C	0.0030	0.0002	0.0081	0.0029	0.0002	0.0075	0.0348	0.0365	0.9708
20.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0121	0.0051	0.0052
21.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0121	0.0061	0.0056
22.	H	0.0001	0.0000	0.0003	0.0000	0.0000	0.0001	0.0023	0.0014	0.0093
23.	C	0.0005	0.0000	0.0005	0.0001	0.0000	0.0001	0.0058	0.0094	0.0081
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0005	0.0013
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0013
26.	H	0.0013	0.0003	0.0000	0.0006	0.0000	0.0000	0.0000	0.0001	0.0000

Atom		19	20	21	22	23	24	25	26
1.	C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119
3.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9407
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
8.	N	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012
9.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	N	0.0030	0.0001	0.0001	0.0001	0.0005	0.0000	0.0000	0.0013
11.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
12.	H	0.0081	0.0000	0.0000	0.0003	0.0005	0.0000	0.0000	0.0000
13.	N	0.0029	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0006
14.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	H	0.0075	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
16.	O	0.0348	0.0121	0.0121	0.0023	0.0058	0.0007	0.0008	0.0000
17.	O	0.0365	0.0051	0.0061	0.0014	0.0094	0.0005	0.0005	0.0001

18.	C	0.9708	0.0052	0.0056	0.0093	0.0081	0.0013	0.0013	0.0000
19.	C	0.0000	0.9184	0.9168	0.0017	1.0310	0.0025	0.0025	0.0000
20.	H	0.9184	0.0000	0.0011	0.0013	0.0026	0.0013	0.0127	0.0000
21.	H	0.9168	0.0011	0.0000	0.0014	0.0026	0.0127	0.0013	0.0000
22.	H	0.0017	0.0013	0.0014	0.0000	0.9492	0.0005	0.0005	0.0000
23.	C	1.0310	0.0026	0.0026	0.9492	0.0000	0.9430	0.9418	0.0000
24.	H	0.0025	0.0013	0.0127	0.0005	0.9430	0.0000	0.0007	0.0000
25.	H	0.0025	0.0127	0.0013	0.0005	0.9418	0.0007	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-11: Wiberg index for salt bridge with no water (bridge length=4.1angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0066	0.0111	0.0015	0.0060	0.0001	0.0007	1.2076	0.0022
2. H	0.0066	0.0000	0.9259	0.0012	0.0028	0.0017	0.0010	0.0048	0.0021
3. C	0.0111	0.9259	0.0000	0.9256	1.0242	0.0020	0.0037	0.9592	0.0046
4. H	0.0015	0.0012	0.9256	0.0000	0.0027	0.0120	0.0009	0.0053	0.0082
5. C	0.0060	0.0028	1.0242	0.0027	0.0000	0.9415	0.9372	0.0194	0.0003
6. H	0.0001	0.0017	0.0020	0.0120	0.9415	0.0000	0.0007	0.0015	0.0003
7. H	0.0007	0.0010	0.0037	0.0009	0.9372	0.0007	0.0000	0.0109	0.0000
8. N	1.2076	0.0048	0.9592	0.0053	0.0194	0.0015	0.0109	0.0000	0.8160
9. H	0.0022	0.0021	0.0046	0.0082	0.0003	0.0003	0.0000	0.8160	0.0000
10. N	1.3458	0.0010	0.0033	0.0038	0.0036	0.0002	0.0003	0.0812	0.0114
11. H	0.0024	0.0000	0.0011	0.0007	0.0003	0.0000	0.0000	0.0016	0.0002
12. H	0.0026	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0070	0.0004
13. N	1.3156	0.0011	0.0103	0.0010	0.0035	0.0001	0.0009	0.0732	0.0024
14. H	0.0022	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0016	0.0006
15. H	0.0024	0.0002	0.0007	0.0000	0.0001	0.0000	0.0000	0.0066	0.0002
16. O	0.0016	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0017	0.0001
17. O	0.0020	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0017	0.0008
18. C	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
19. C	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0004	0.0119	0.0023	0.0015	0.9407	0.0006	0.0007	0.0012	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3458	0.0024	0.0026	1.3156	0.0022	0.0024	0.0016	0.0020	0.0005
2. H	0.0010	0.0000	0.0000	0.0011	0.0000	0.0002	0.0000	0.0001	0.0000
3. C	0.0033	0.0011	0.0002	0.0103	0.0003	0.0007	0.0006	0.0005	0.0000
4. H	0.0038	0.0007	0.0000	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000
5. C	0.0036	0.0003	0.0000	0.0035	0.0000	0.0001	0.0000	0.0001	0.0000
6. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. H	0.0003	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
8. N	0.0812	0.0016	0.0070	0.0732	0.0016	0.0066	0.0017	0.0017	0.0002
9. H	0.0114	0.0002	0.0004	0.0024	0.0006	0.0002	0.0001	0.0008	0.0000
10. N	0.0000	0.8322	0.6356	0.1043	0.0111	0.0009	0.0022	0.0377	0.0018
11. H	0.8322	0.0000	0.0010	0.0104	0.0010	0.0003	0.0002	0.0011	0.0001
12. H	0.6356	0.0010	0.0000	0.0010	0.0003	0.0009	0.0022	0.1269	0.0017
13. N	0.1043	0.0104	0.0010	0.0000	0.8359	0.6666	0.0307	0.0024	0.0014

14. H	0.0111	0.0010	0.0003	0.8359	0.0000	0.0009	0.0011	0.0002	0.0001
15. H	0.0009	0.0003	0.0009	0.6666	0.0009	0.0000	0.0984	0.0019	0.0015
16. O	0.0022	0.0002	0.0022	0.0307	0.0011	0.0984	0.0000	0.1887	1.4414
17. O	0.0377	0.0011	0.1269	0.0024	0.0002	0.0019	0.1887	0.0000	1.4094
18. C	0.0018	0.0001	0.0017	0.0014	0.0001	0.0015	1.4414	1.4094	0.0000
19. C	0.0028	0.0001	0.0078	0.0027	0.0002	0.0073	0.0357	0.0373	0.9697
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0121	0.0051	0.0051
21. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0122	0.0062	0.0055
22. H	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000	0.0024	0.0015	0.0093
23. C	0.0004	0.0000	0.0005	0.0001	0.0000	0.0001	0.0060	0.0095	0.0082
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0005	0.0012
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0005	0.0013
26. H	0.0012	0.0003	0.0000	0.0005	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119
3. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9407
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007
8. N	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012
9. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0028	0.0001	0.0001	0.0001	0.0004	0.0000	0.0000	0.0012
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
12. H	0.0078	0.0000	0.0000	0.0003	0.0005	0.0000	0.0000	0.0000
13. N	0.0027	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0005
14. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0073	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
16. O	0.0357	0.0121	0.0122	0.0024	0.0060	0.0007	0.0008	0.0000
17. O	0.0373	0.0051	0.0062	0.0015	0.0095	0.0005	0.0005	0.0001
18. C	0.9697	0.0051	0.0055	0.0093	0.0082	0.0012	0.0013	0.0000
19. C	0.0000	0.9187	0.9171	0.0017	1.0309	0.0025	0.0025	0.0000
20. H	0.9187	0.0000	0.0011	0.0013	0.0025	0.0013	0.0127	0.0000
21. H	0.9171	0.0011	0.0000	0.0014	0.0026	0.0127	0.0013	0.0000
22. H	0.0017	0.0013	0.0014	0.0000	0.9495	0.0005	0.0005	0.0000
23. C	1.0309	0.0025	0.0026	0.9495	0.0000	0.9430	0.9418	0.0000
24. H	0.0025	0.0013	0.0127	0.0005	0.9430	0.0000	0.0007	0.0000
25. H	0.0025	0.0127	0.0013	0.0005	0.9418	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-12: Wiberg index for salt bridge with no water (bridge length=4.2 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0065	0.0112	0.0016	0.0061	0.0001	0.0007	1.2175	0.0022
2. H	0.0065	0.0000	0.9256	0.0012	0.0028	0.0017	0.0010	0.0046	0.0022
3. C	0.0112	0.9256	0.0000	0.9255	1.0245	0.0020	0.0037	0.9573	0.0046
4. H	0.0016	0.0012	0.9255	0.0000	0.0027	0.0120	0.0010	0.0052	0.0080
5. C	0.0061	0.0028	1.0245	0.0027	0.0000	0.9412	0.9367	0.0190	0.0003
6. H	0.0001	0.0017	0.0020	0.0120	0.9412	0.0000	0.0007	0.0015	0.0003
7. H	0.0007	0.0010	0.0037	0.0010	0.9367	0.0007	0.0000	0.0108	0.0000
8. N	1.2175	0.0046	0.9573	0.0052	0.0190	0.0015	0.0108	0.0000	0.8149
9. H	0.0022	0.0022	0.0046	0.0080	0.0003	0.0003	0.0000	0.8149	0.0000

10.	N	1.3399	0.0010	0.0033	0.0038	0.0036	0.0002	0.0003	0.0821	0.0113
11.	H	0.0023	0.0000	0.0010	0.0007	0.0003	0.0000	0.0000	0.0015	0.0002
12.	H	0.0025	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0071	0.0004
13.	N	1.3118	0.0011	0.0103	0.0010	0.0035	0.0001	0.0009	0.0743	0.0025
14.	H	0.0022	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0015	0.0006
15.	H	0.0023	0.0002	0.0007	0.0000	0.0001	0.0000	0.0000	0.0067	0.0002
16.	O	0.0014	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0015	0.0001
17.	O	0.0018	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000	0.0015	0.0007
18.	C	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
19.	C	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0004	0.0119	0.0023	0.0015	0.9407	0.0006	0.0007	0.0012	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.3399	0.0023	0.0025	1.3118	0.0022	0.0023	0.0014	0.0018	0.0005
2.	H	0.0010	0.0000	0.0000	0.0011	0.0000	0.0002	0.0000	0.0001	0.0000
3.	C	0.0033	0.0010	0.0002	0.0103	0.0003	0.0007	0.0006	0.0004	0.0000
4.	H	0.0038	0.0007	0.0000	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000
5.	C	0.0036	0.0003	0.0000	0.0035	0.0000	0.0001	0.0000	0.0001	0.0000
6.	H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0003	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
8.	N	0.0821	0.0015	0.0071	0.0743	0.0015	0.0067	0.0015	0.0015	0.0002
9.	H	0.0113	0.0002	0.0004	0.0025	0.0006	0.0002	0.0001	0.0007	0.0000
10.	N	0.0000	0.8309	0.6514	0.1017	0.0111	0.0010	0.0022	0.0325	0.0015
11.	H	0.8309	0.0000	0.0010	0.0104	0.0010	0.0003	0.0002	0.0010	0.0001
12.	H	0.6514	0.0010	0.0000	0.0010	0.0003	0.0010	0.0025	0.1070	0.0017
13.	N	0.1017	0.0104	0.0010	0.0000	0.8341	0.6795	0.0261	0.0024	0.0012
14.	H	0.0111	0.0010	0.0003	0.8341	0.0000	0.0008	0.0010	0.0002	0.0001
15.	H	0.0010	0.0003	0.0010	0.6795	0.0008	0.0000	0.0821	0.0022	0.0015
16.	O	0.0022	0.0002	0.0025	0.0261	0.0010	0.0821	0.0000	0.1909	1.4462
17.	O	0.0325	0.0010	0.1070	0.0024	0.0002	0.0022	0.1909	0.0000	1.4125
18.	C	0.0015	0.0001	0.0017	0.0012	0.0001	0.0015	1.4462	1.4125	0.0000
19.	C	0.0026	0.0001	0.0076	0.0025	0.0001	0.0070	0.0368	0.0383	0.9678
20.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0122	0.0051	0.0050
21.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0122	0.0062	0.0054
22.	H	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000	0.0025	0.0016	0.0093
23.	C	0.0004	0.0000	0.0005	0.0001	0.0000	0.0001	0.0061	0.0097	0.0082
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0006	0.0013
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0005	0.0013
26.	H	0.0011	0.0003	0.0000	0.0005	0.0000	0.0000	0.0000	0.0001	0.0000

Atom		19	20	21	22	23	24	25	26
1.	C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119
3.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9407
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006

7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007
8.	N	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012
9.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	N	0.0026	0.0001	0.0000	0.0001	0.0004	0.0000	0.0000	0.0011
11.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
12.	H	0.0076	0.0000	0.0000	0.0003	0.0005	0.0000	0.0000	0.0000
13.	N	0.0025	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0005
14.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	H	0.0070	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
16.	O	0.0368	0.0122	0.0122	0.0025	0.0061	0.0007	0.0009	0.0000
17.	O	0.0383	0.0051	0.0062	0.0016	0.0097	0.0006	0.0005	0.0001
18.	C	0.9678	0.0050	0.0054	0.0093	0.0082	0.0013	0.0013	0.0000
19.	C	0.0000	0.9193	0.9177	0.0017	1.0309	0.0025	0.0025	0.0000
20.	H	0.9193	0.0000	0.0011	0.0013	0.0025	0.0013	0.0127	0.0000
21.	H	0.9177	0.0011	0.0000	0.0014	0.0026	0.0128	0.0013	0.0000
22.	H	0.0017	0.0013	0.0014	0.0000	0.9497	0.0005	0.0005	0.0000
23.	C	1.0309	0.0025	0.0026	0.9497	0.0000	0.9431	0.9417	0.0000
24.	H	0.0025	0.0013	0.0128	0.0005	0.9431	0.0000	0.0007	0.0000
25.	H	0.0025	0.0127	0.0013	0.0005	0.9417	0.0007	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-13: Wiberg index for salt bridge with no water (bridge length=4.3 angstroms)

Atom		1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.0065	0.0114	0.0016	0.0062	0.0001	0.0007	1.2241	0.0022
2.	H	0.0065	0.0000	0.9255	0.0012	0.0028	0.0017	0.0010	0.0045	0.0022
3.	C	0.0114	0.9255	0.0000	0.9254	1.0248	0.0020	0.0038	0.9554	0.0047
4.	H	0.0016	0.0012	0.9254	0.0000	0.0027	0.0120	0.0010	0.0051	0.0079
5.	C	0.0062	0.0028	1.0248	0.0027	0.0000	0.9410	0.9362	0.0187	0.0004
6.	H	0.0001	0.0017	0.0020	0.0120	0.9410	0.0000	0.0007	0.0015	0.0003
7.	H	0.0007	0.0010	0.0038	0.0010	0.9362	0.0007	0.0000	0.0108	0.0000
8.	N	1.2241	0.0045	0.9554	0.0051	0.0187	0.0015	0.0108	0.0000	0.8140
9.	H	0.0022	0.0022	0.0047	0.0079	0.0004	0.0003	0.0000	0.8140	0.0000
10.	N	1.3367	0.0010	0.0032	0.0038	0.0036	0.0002	0.0003	0.0827	0.0113
11.	H	0.0023	0.0000	0.0010	0.0006	0.0003	0.0000	0.0000	0.0015	0.0002
12.	H	0.0024	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0072	0.0004
13.	N	1.3086	0.0011	0.0103	0.0010	0.0035	0.0001	0.0009	0.0749	0.0025
14.	H	0.0021	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0015	0.0006
15.	H	0.0022	0.0002	0.0007	0.0000	0.0001	0.0000	0.0000	0.0068	0.0002
16.	O	0.0013	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0014	0.0001
17.	O	0.0016	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000	0.0013	0.0007
18.	C	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
19.	C	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0004	0.0119	0.0023	0.0015	0.9406	0.0006	0.0007	0.0012	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.3367	0.0023	0.0024	1.3086	0.0021	0.0022	0.0013	0.0016	0.0004
2.	H	0.0010	0.0000	0.0000	0.0011	0.0000	0.0002	0.0000	0.0001	0.0000

3.	C	0.0032	0.0010	0.0002	0.0103	0.0003	0.0007	0.0005	0.0004	0.0000
4.	H	0.0038	0.0006	0.0000	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000
5.	C	0.0036	0.0003	0.0001	0.0035	0.0000	0.0001	0.0000	0.0001	0.0000
6.	H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0003	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
8.	N	0.0827	0.0015	0.0072	0.0749	0.0015	0.0068	0.0014	0.0013	0.0002
9.	H	0.0113	0.0002	0.0004	0.0025	0.0006	0.0002	0.0001	0.0007	0.0000
10.	N	0.0000	0.8296	0.6644	0.0999	0.0110	0.0011	0.0021	0.0280	0.0013
11.	H	0.8296	0.0000	0.0009	0.0103	0.0010	0.0004	0.0002	0.0009	0.0001
12.	H	0.6644	0.0009	0.0000	0.0011	0.0003	0.0010	0.0029	0.0907	0.0017
13.	N	0.0999	0.0103	0.0011	0.0000	0.8329	0.6928	0.0217	0.0022	0.0010
14.	H	0.0110	0.0010	0.0003	0.8329	0.0000	0.0007	0.0010	0.0002	0.0001
15.	H	0.0011	0.0004	0.0010	0.6928	0.0007	0.0000	0.0668	0.0023	0.0014
16.	O	0.0021	0.0002	0.0029	0.0217	0.0010	0.0668	0.0000	0.1935	1.4498
17.	O	0.0280	0.0009	0.0907	0.0022	0.0002	0.0023	0.1935	0.0000	1.4180
18.	C	0.0013	0.0001	0.0017	0.0010	0.0001	0.0014	1.4498	1.4180	0.0000
19.	C	0.0025	0.0001	0.0074	0.0022	0.0001	0.0065	0.0381	0.0394	0.9656
20.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0123	0.0051	0.0049
21.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0123	0.0062	0.0052
22.	H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0026	0.0017	0.0093
23.	C	0.0003	0.0000	0.0005	0.0001	0.0000	0.0001	0.0063	0.0099	0.0082
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0006	0.0013
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0005	0.0013
26.	H	0.0011	0.0003	0.0000	0.0005	0.0000	0.0000	0.0000	0.0001	0.0000

Atom		19	20	21	22	23	24	25	26
1.	C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119
3.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9406
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007
8.	N	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012
9.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	N	0.0025	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0011
11.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
12.	H	0.0074	0.0000	0.0000	0.0002	0.0005	0.0000	0.0000	0.0000
13.	N	0.0022	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0005
14.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	H	0.0065	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
16.	O	0.0381	0.0123	0.0123	0.0026	0.0063	0.0007	0.0009	0.0000
17.	O	0.0394	0.0051	0.0062	0.0017	0.0099	0.0006	0.0005	0.0001
18.	C	0.9656	0.0049	0.0052	0.0093	0.0082	0.0013	0.0013	0.0000
19.	C	0.0000	0.9197	0.9182	0.0017	1.0308	0.0026	0.0026	0.0000
20.	H	0.9197	0.0000	0.0011	0.0013	0.0025	0.0013	0.0128	0.0000
21.	H	0.9182	0.0011	0.0000	0.0014	0.0026	0.0128	0.0013	0.0000
22.	H	0.0017	0.0013	0.0014	0.0000	0.9500	0.0005	0.0005	0.0000
23.	C	1.0308	0.0025	0.0026	0.9500	0.0000	0.9431	0.9418	0.0000
24.	H	0.0026	0.0013	0.0128	0.0005	0.9431	0.0000	0.0007	0.0000
25.	H	0.0026	0.0128	0.0013	0.0005	0.9418	0.0007	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-1-14: Wiberg index for salt bridge with no water (bridge length=4.4 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0065	0.0115	0.0016	0.0064	0.0001	0.0007	1.2309	0.0022
2. H	0.0065	0.0000	0.9252	0.0012	0.0028	0.0017	0.0010	0.0044	0.0022
3. C	0.0115	0.9252	0.0000	0.9254	1.0251	0.0020	0.0038	0.9540	0.0047
4. H	0.0016	0.0012	0.9254	0.0000	0.0028	0.0120	0.0010	0.0050	0.0078
5. C	0.0064	0.0028	1.0251	0.0028	0.0000	0.9409	0.9358	0.0184	0.0004
6. H	0.0001	0.0017	0.0020	0.0120	0.9409	0.0000	0.0007	0.0015	0.0003
7. H	0.0007	0.0010	0.0038	0.0010	0.9358	0.0007	0.0000	0.0107	0.0000
8. N	1.2309	0.0044	0.9540	0.0050	0.0184	0.0015	0.0107	0.0000	0.8133
9. H	0.0022	0.0022	0.0047	0.0078	0.0004	0.0003	0.0000	0.8133	0.0000
10. N	1.3325	0.0010	0.0032	0.0037	0.0036	0.0002	0.0003	0.0832	0.0112
11. H	0.0023	0.0000	0.0009	0.0006	0.0003	0.0000	0.0000	0.0014	0.0002
12. H	0.0023	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0073	0.0004
13. N	1.3053	0.0011	0.0102	0.0010	0.0034	0.0001	0.0009	0.0754	0.0025
14. H	0.0021	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0014	0.0006
15. H	0.0021	0.0002	0.0008	0.0000	0.0001	0.0000	0.0000	0.0068	0.0002
16. O	0.0012	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0012	0.0001
17. O	0.0015	0.0001	0.0003	0.0001	0.0001	0.0000	0.0000	0.0012	0.0006
18. C	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
19. C	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0004	0.0118	0.0023	0.0015	0.9407	0.0006	0.0007	0.0012	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3325	0.0023	0.0023	1.3053	0.0021	0.0021	0.0012	0.0015	0.0004
2. H	0.0010	0.0000	0.0000	0.0011	0.0000	0.0002	0.0000	0.0001	0.0000
3. C	0.0032	0.0009	0.0002	0.0102	0.0002	0.0008	0.0004	0.0003	0.0000
4. H	0.0037	0.0006	0.0000	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000
5. C	0.0036	0.0003	0.0001	0.0034	0.0000	0.0001	0.0000	0.0001	0.0000
6. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. H	0.0003	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
8. N	0.0832	0.0014	0.0073	0.0754	0.0014	0.0068	0.0012	0.0012	0.0001
9. H	0.0112	0.0002	0.0004	0.0025	0.0006	0.0002	0.0001	0.0006	0.0000
10. N	0.0000	0.8282	0.6784	0.0977	0.0109	0.0011	0.0021	0.0238	0.0011
11. H	0.8282	0.0000	0.0008	0.0102	0.0010	0.0004	0.0002	0.0009	0.0001
12. H	0.6784	0.0008	0.0000	0.0011	0.0003	0.0010	0.0031	0.0755	0.0016
13. N	0.0977	0.0102	0.0011	0.0000	0.8312	0.7051	0.0181	0.0021	0.0008
14. H	0.0109	0.0010	0.0003	0.8312	0.0000	0.0006	0.0009	0.0002	0.0000
15. H	0.0011	0.0004	0.0010	0.7051	0.0006	0.0000	0.0547	0.0025	0.0014
16. O	0.0021	0.0002	0.0031	0.0181	0.0009	0.0547	0.0000	0.1957	1.4532
17. O	0.0238	0.0009	0.0755	0.0021	0.0002	0.0025	0.1957	0.0000	1.4224
18. C	0.0011	0.0001	0.0016	0.0008	0.0000	0.0014	1.4532	1.4224	0.0000
19. C	0.0023	0.0001	0.0071	0.0020	0.0001	0.0061	0.0394	0.0406	0.9631
20. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0123	0.0051	0.0047
21. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0123	0.0063	0.0051
22. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0027	0.0018	0.0094
23. C	0.0003	0.0000	0.0005	0.0001	0.0000	0.0001	0.0064	0.0100	0.0082

24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0006	0.0013
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0006	0.0013
26. H	0.0010	0.0003	0.0000	0.0005	0.0000	0.0000	0.0000	0.0001	0.0000

Atom	19	20	21	22	23	24	25	26
1. C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0118
3. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9407
6. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007
8. N	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012
9. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0023	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0010
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
12. H	0.0071	0.0000	0.0000	0.0002	0.0005	0.0000	0.0000	0.0000
13. N	0.0020	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0005
14. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. H	0.0061	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
16. O	0.0394	0.0123	0.0123	0.0027	0.0064	0.0007	0.0009	0.0000
17. O	0.0406	0.0051	0.0063	0.0018	0.0100	0.0006	0.0006	0.0001
18. C	0.9631	0.0047	0.0051	0.0094	0.0082	0.0013	0.0013	0.0000
19. C	0.0000	0.9204	0.9188	0.0017	1.0309	0.0026	0.0026	0.0000
20. H	0.9204	0.0000	0.0011	0.0013	0.0024	0.0013	0.0128	0.0000
21. H	0.9188	0.0011	0.0000	0.0014	0.0025	0.0128	0.0013	0.0000
22. H	0.0017	0.0013	0.0014	0.0000	0.9502	0.0005	0.0005	0.0000
23. C	1.0309	0.0024	0.0025	0.9502	0.0000	0.9432	0.9417	0.0000
24. H	0.0026	0.0013	0.0128	0.0005	0.9432	0.0000	0.0007	0.0000
25. H	0.0026	0.0128	0.0013	0.0005	0.9417	0.0007	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-9C-2-1: Wiberg index for salt bridge with 5 waters (bridge length=3.8 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0095	0.0027	1.2712	0.0024	1.2603	0.0024	0.0029	1.3258
2. C	0.0095	0.0000	0.9275	0.9603	0.0046	0.0038	0.0018	0.0002	0.0101
3. H	0.0027	0.9275	0.0000	0.0064	0.0058	0.0036	0.0001	0.0000	0.0015
4. N	1.2712	0.9603	0.0064	0.0000	0.7124	0.0734	0.0029	0.0086	0.0882
5. H	0.0024	0.0046	0.0058	0.7124	0.0000	0.0094	0.0002	0.0004	0.0019
6. N	1.2603	0.0038	0.0036	0.0734	0.0094	0.0000	0.8306	0.7396	0.0842
7. H	0.0024	0.0018	0.0001	0.0029	0.0002	0.8306	0.0000	0.0005	0.0105
8. H	0.0029	0.0002	0.0000	0.0086	0.0004	0.7396	0.0005	0.0000	0.0019
9. N	1.3258	0.0101	0.0015	0.0882	0.0019	0.0842	0.0105	0.0019	0.0000
10. H	0.0025	0.0003	0.0000	0.0016	0.0006	0.0096	0.0008	0.0001	0.7852
11. H	0.0028	0.0008	0.0000	0.0089	0.0001	0.0011	0.0001	0.0003	0.7284
12. O	0.0025	0.0003	0.0000	0.0015	0.0001	0.0034	0.0001	0.0024	0.0223
13. O	0.0024	0.0002	0.0001	0.0008	0.0002	0.0173	0.0005	0.0542	0.0027
14. C	0.0004	0.0001	0.0000	0.0005	0.0000	0.0050	0.0001	0.0012	0.0036
15. C	0.0004	0.0000	0.0000	0.0002	0.0000	0.0007	0.0000	0.0016	0.0015
16. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0003
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0000
18. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001
19. O	0.0010	0.0003	0.0001	0.0003	0.0000	0.0010	0.0002	0.0001	0.0004

20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0001	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004
22. O	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0007
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
24. H	0.0060	0.9213	0.0008	0.0135	0.0006	0.0041	0.0005	0.0000	0.0039
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
26. O	0.0007	0.0000	0.0000	0.0003	0.0001	0.0003	0.0001	0.0000	0.0077
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0007
28. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
29. O	0.0019	0.0009	0.0005	0.0233	0.0624	0.0008	0.0000	0.0002	0.0025
30. H	0.0001	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0000	0.0001
31. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
32. O	0.0009	0.0001	0.0000	0.0007	0.0007	0.0002	0.0000	0.0000	0.0010
33. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
34. C	0.0074	1.0311	0.0031	0.0112	0.0023	0.0014	0.0002	0.0001	0.0009
35. H	0.0001	0.0022	0.0120	0.0019	0.0005	0.0001	0.0000	0.0000	0.0001
36. H	0.0005	0.0030	0.0013	0.0087	0.0002	0.0001	0.0000	0.0000	0.0003
37. H	0.0001	0.0024	0.0019	0.0018	0.0001	0.0001	0.0001	0.0000	0.0002
38. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0001
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0025	0.0028	0.0025	0.0024	0.0004	0.0004	0.0000	0.0000	0.0001
2. C	0.0003	0.0008	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0016	0.0089	0.0015	0.0008	0.0005	0.0002	0.0001	0.0000	0.0000
5. H	0.0006	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0096	0.0011	0.0034	0.0173	0.0050	0.0007	0.0002	0.0002	0.0002
7. H	0.0008	0.0001	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0001	0.0003	0.0024	0.0542	0.0012	0.0016	0.0000	0.0001	0.0000
9. N	0.7852	0.7284	0.0223	0.0027	0.0036	0.0015	0.0003	0.0000	0.0001
10. H	0.0000	0.0010	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
11. H	0.0010	0.0000	0.0648	0.0022	0.0023	0.0049	0.0002	0.0000	0.0000
12. O	0.0003	0.0648	0.0000	0.1736	1.4056	0.0370	0.0113	0.0110	0.0001
13. O	0.0002	0.0022	0.1736	0.0000	1.4027	0.0414	0.0071	0.0045	0.0010
14. C	0.0001	0.0023	1.4056	1.4027	0.0000	0.9736	0.0069	0.0055	0.0001
15. C	0.0000	0.0049	0.0370	0.0414	0.9736	0.0000	0.9125	0.9174	0.0001
16. H	0.0000	0.0002	0.0113	0.0071	0.0069	0.9125	0.0000	0.0012	0.0000
17. H	0.0000	0.0000	0.0110	0.0045	0.0055	0.9174	0.0012	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0010	0.0001	0.0001	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0019	0.0173	0.0039	0.0012	0.0001	0.0001	0.7845
20. H	0.0000	0.0001	0.0011	0.0577	0.0012	0.0032	0.0000	0.0000	0.0007
21. H	0.0000	0.0002	0.0625	0.0017	0.0011	0.0023	0.0000	0.0002	0.0000
22. O	0.0001	0.0005	0.0180	0.0021	0.0048	0.0009	0.0001	0.0003	0.0000
23. H	0.0000	0.0001	0.0010	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
24. H	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0167	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
27. H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0031	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0001	0.0001	0.0005	0.0003	0.0002	0.0000	0.0000	0.0000	0.0011
33. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
34. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. C	0.0000	0.0000	0.0055	0.0097	0.0083	1.0305	0.0028	0.0026	0.0000
39. H	0.0000	0.0000	0.0020	0.0015	0.0092	0.0018	0.0015	0.0012	0.0000
40. H	0.0000	0.0000	0.0006	0.0006	0.0013	0.0023	0.0125	0.0013	0.0000
41. H	0.0000	0.0000	0.0008	0.0005	0.0014	0.0023	0.0012	0.0124	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0010	0.0001	0.0000	0.0001	0.0000	0.0060	0.0000	0.0007	0.0000
2. C	0.0003	0.0000	0.0000	0.0000	0.0000	0.9213	0.0000	0.0000	0.0000
3. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000
4. N	0.0003	0.0001	0.0000	0.0001	0.0000	0.0135	0.0000	0.0003	0.0000
5. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0001	0.0000
6. N	0.0010	0.0004	0.0001	0.0001	0.0000	0.0041	0.0000	0.0003	0.0001
7. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000
8. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9. N	0.0004	0.0001	0.0004	0.0007	0.0003	0.0039	0.0002	0.0077	0.0007
10. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0167	0.0001
11. H	0.0001	0.0001	0.0002	0.0005	0.0001	0.0001	0.0000	0.0001	0.0000
12. O	0.0019	0.0011	0.0625	0.0180	0.0010	0.0001	0.0002	0.0004	0.0001
13. O	0.0173	0.0577	0.0017	0.0021	0.0001	0.0001	0.0000	0.0001	0.0000
14. C	0.0039	0.0012	0.0011	0.0048	0.0001	0.0000	0.0000	0.0001	0.0000
15. C	0.0012	0.0032	0.0023	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000
16. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0001	0.0000	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.7845	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.6863	0.0001	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000
20. H	0.6863	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.6658	0.0007	0.0000	0.0001	0.0004	0.0000
22. O	0.0001	0.0000	0.6658	0.0000	0.7725	0.0000	0.0428	0.0142	0.0006
23. H	0.0000	0.0000	0.0007	0.7725	0.0000	0.0000	0.0001	0.0010	0.0000
24. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0001	0.0428	0.0001	0.0000	0.0000	0.7039	0.0007
26. O	0.0000	0.0000	0.0004	0.0142	0.0010	0.0000	0.7039	0.0000	0.7773
27. H	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000	0.0007	0.7773	0.0000
28. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
29. O	0.0002	0.0000	0.0000	0.0002	0.0000	0.0001	0.0005	0.0058	0.0019
30. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0142	0.0001
31. H	0.0386	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0137	0.0005	0.0004	0.0083	0.0011	0.0000	0.0001	0.0005	0.0002
33. H	0.0003	0.0000	0.0001	0.0203	0.0000	0.0000	0.0000	0.0000	0.0000
34. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0126	0.0000	0.0000	0.0000
38. C	0.0003	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

40. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0001	0.0019	0.0001	0.0001	0.0009	0.0000	0.0074	0.0001	0.0005
2. C	0.0000	0.0009	0.0000	0.0000	0.0001	0.0000	1.0311	0.0022	0.0030
3. H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0031	0.0120	0.0013
4. N	0.0003	0.0233	0.0005	0.0001	0.0007	0.0001	0.0112	0.0019	0.0087
5. H	0.0001	0.0624	0.0001	0.0000	0.0007	0.0000	0.0023	0.0005	0.0002
6. N	0.0001	0.0008	0.0001	0.0000	0.0002	0.0000	0.0014	0.0001	0.0001
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
8. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. N	0.0001	0.0025	0.0001	0.0001	0.0010	0.0002	0.0009	0.0001	0.0003
10. H	0.0000	0.0031	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
11. H	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0001
12. O	0.0000	0.0001	0.0000	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000
13. O	0.0000	0.0000	0.0000	0.0001	0.0003	0.0001	0.0001	0.0000	0.0000
14. C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0002	0.0000	0.0386	0.0137	0.0003	0.0000	0.0000	0.0000
20. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000
22. O	0.0001	0.0002	0.0001	0.0002	0.0083	0.0203	0.0000	0.0000	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0026	0.0017	0.0010
25. H	0.0000	0.0005	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
26. O	0.0002	0.0058	0.0142	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0019	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.6979	0.0007	0.0001	0.0506	0.0001	0.0000	0.0000	0.0000
29. O	0.6979	0.0000	0.7478	0.0008	0.0162	0.0004	0.0010	0.0006	0.0001
30. H	0.0007	0.7478	0.0000	0.0000	0.0004	0.0000	0.0001	0.0000	0.0000
31. H	0.0001	0.0008	0.0000	0.0000	0.7128	0.0006	0.0000	0.0000	0.0000
32. O	0.0506	0.0162	0.0004	0.7128	0.0000	0.7438	0.0000	0.0000	0.0000
33. H	0.0001	0.0004	0.0000	0.0006	0.7438	0.0000	0.0000	0.0000	0.0000
34. C	0.0000	0.0010	0.0001	0.0000	0.0000	0.0000	0.0000	0.9356	0.9423
35. H	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.9356	0.0000	0.0007
36. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.9423	0.0007	0.0000
37. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.9406	0.0005	0.0007
38. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41
1. C	0.0001	0.0000	0.0000	0.0000	0.0000
2. C	0.0024	0.0000	0.0000	0.0000	0.0000
3. H	0.0019	0.0000	0.0000	0.0000	0.0000
4. N	0.0018	0.0000	0.0000	0.0000	0.0000
5. H	0.0001	0.0000	0.0000	0.0000	0.0000
6. N	0.0001	0.0001	0.0000	0.0000	0.0000

7.	H	0.0001	0.0000	0.0000	0.0000	0.0000
8.	H	0.0000	0.0001	0.0000	0.0000	0.0000
9.	N	0.0002	0.0001	0.0000	0.0000	0.0001
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000	0.0000	0.0000
12.	O	0.0000	0.0055	0.0020	0.0006	0.0008
13.	O	0.0000	0.0097	0.0015	0.0006	0.0005
14.	C	0.0000	0.0083	0.0092	0.0013	0.0014
15.	C	0.0000	1.0305	0.0018	0.0023	0.0023
16.	H	0.0000	0.0028	0.0015	0.0125	0.0012
17.	H	0.0000	0.0026	0.0012	0.0013	0.0124
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000
19.	O	0.0000	0.0003	0.0001	0.0000	0.0000
20.	H	0.0000	0.0003	0.0001	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0000	0.0001	0.0000	0.0001	0.0001
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0126	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000
26.	O	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000
29.	O	0.0001	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.9406	0.0000	0.0000	0.0000	0.0000
35.	H	0.0005	0.0000	0.0000	0.0000	0.0000
36.	H	0.0007	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000
38.	C	0.0000	0.0000	0.9467	0.9447	0.9407
39.	H	0.0000	0.9467	0.0000	0.0005	0.0005
40.	H	0.0000	0.9447	0.0005	0.0000	0.0006
41.	H	0.0000	0.9407	0.0005	0.0006	0.0000

Table-9C-2-2: Wiberg index for salt bridge with 5 waters (bridge length=4.0 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0095	0.0026	1.2689	0.0025	1.2636	0.0024	0.0027	1.3261
2. C	0.0095	0.0000	0.9275	0.9596	0.0046	0.0037	0.0016	0.0002	0.0102
3. H	0.0026	0.9275	0.0000	0.0060	0.0061	0.0035	0.0000	0.0000	0.0014
4. N	1.2689	0.9596	0.0060	0.0000	0.7141	0.0735	0.0029	0.0084	0.0874
5. H	0.0025	0.0046	0.0061	0.7141	0.0000	0.0097	0.0001	0.0004	0.0020
6. N	1.2636	0.0037	0.0035	0.0735	0.0097	0.0000	0.8301	0.7388	0.0848
7. H	0.0024	0.0016	0.0000	0.0029	0.0001	0.8301	0.0000	0.0005	0.0106
8. H	0.0027	0.0002	0.0000	0.0084	0.0004	0.7388	0.0005	0.0000	0.0019
9. N	1.3261	0.0102	0.0014	0.0874	0.0020	0.0848	0.0106	0.0019	0.0000
10. H	0.0025	0.0002	0.0000	0.0015	0.0006	0.0096	0.0008	0.0002	0.7860
11. H	0.0027	0.0008	0.0000	0.0090	0.0001	0.0012	0.0002	0.0005	0.7262
12. O	0.0020	0.0003	0.0000	0.0014	0.0000	0.0020	0.0001	0.0011	0.0219
13. O	0.0022	0.0002	0.0001	0.0009	0.0002	0.0175	0.0004	0.0516	0.0025
14. C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0026	0.0001	0.0012	0.0018
15. C	0.0004	0.0000	0.0000	0.0002	0.0000	0.0013	0.0001	0.0032	0.0021

16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
18. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
19. O	0.0008	0.0002	0.0001	0.0003	0.0000	0.0011	0.0003	0.0002	0.0003
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0005	0.0000	0.0001	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
22. O	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0006
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
24. H	0.0059	0.9218	0.0008	0.0137	0.0005	0.0041	0.0005	0.0000	0.0038
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
26. O	0.0007	0.0000	0.0000	0.0003	0.0001	0.0003	0.0001	0.0000	0.0079
27. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0007
28. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
29. O	0.0020	0.0009	0.0005	0.0226	0.0605	0.0008	0.0000	0.0002	0.0023
30. H	0.0001	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0000	0.0001
31. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
32. O	0.0009	0.0001	0.0000	0.0007	0.0006	0.0002	0.0000	0.0000	0.0011
33. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
34. C	0.0074	1.0312	0.0031	0.0113	0.0023	0.0013	0.0002	0.0001	0.0009
35. H	0.0001	0.0022	0.0120	0.0019	0.0005	0.0001	0.0000	0.0000	0.0001
36. H	0.0005	0.0030	0.0013	0.0088	0.0002	0.0001	0.0000	0.0000	0.0003
37. H	0.0001	0.0024	0.0019	0.0018	0.0000	0.0001	0.0001	0.0000	0.0002
38. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0001
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0025	0.0027	0.0020	0.0022	0.0003	0.0004	0.0000	0.0000	0.0001
2. C	0.0002	0.0008	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0015	0.0090	0.0014	0.0009	0.0002	0.0002	0.0000	0.0000	0.0000
5. H	0.0006	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0096	0.0012	0.0020	0.0175	0.0026	0.0013	0.0001	0.0001	0.0003
7. H	0.0008	0.0002	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000
8. H	0.0002	0.0005	0.0011	0.0516	0.0012	0.0032	0.0001	0.0001	0.0000
9. N	0.7860	0.7262	0.0219	0.0025	0.0018	0.0021	0.0001	0.0000	0.0000
10. H	0.0000	0.0010	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
11. H	0.0010	0.0000	0.0634	0.0028	0.0016	0.0061	0.0001	0.0000	0.0000
12. O	0.0003	0.0634	0.0000	0.1726	1.4014	0.0368	0.0113	0.0111	0.0001
13. O	0.0002	0.0028	0.1726	0.0000	1.4117	0.0406	0.0076	0.0043	0.0010
14. C	0.0001	0.0016	1.4014	1.4117	0.0000	0.9740	0.0069	0.0053	0.0001
15. C	0.0000	0.0061	0.0368	0.0406	0.9740	0.0000	0.9104	0.9188	0.0001
16. H	0.0000	0.0001	0.0113	0.0076	0.0069	0.9104	0.0000	0.0012	0.0000
17. H	0.0000	0.0000	0.0111	0.0043	0.0053	0.9188	0.0012	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0010	0.0001	0.0001	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0027	0.0148	0.0051	0.0008	0.0002	0.0001	0.7842
20. H	0.0000	0.0000	0.0020	0.0519	0.0013	0.0020	0.0001	0.0000	0.0007
21. H	0.0000	0.0001	0.0642	0.0033	0.0009	0.0008	0.0000	0.0001	0.0000
22. O	0.0001	0.0005	0.0178	0.0031	0.0056	0.0003	0.0001	0.0003	0.0000
23. H	0.0000	0.0001	0.0010	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
24. H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

26. O	0.0173	0.0002	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
27. H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0026	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
32. O	0.0001	0.0003	0.0006	0.0003	0.0003	0.0001	0.0000	0.0000	0.0010
33. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
34. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. C	0.0000	0.0000	0.0055	0.0098	0.0082	1.0304	0.0027	0.0025	0.0000
39. H	0.0000	0.0000	0.0019	0.0015	0.0091	0.0018	0.0016	0.0012	0.0000
40. H	0.0000	0.0000	0.0006	0.0006	0.0012	0.0024	0.0125	0.0013	0.0000
41. H	0.0000	0.0000	0.0009	0.0005	0.0014	0.0023	0.0012	0.0124	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0008	0.0001	0.0000	0.0001	0.0000	0.0059	0.0000	0.0007	0.0001
2. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.9218	0.0000	0.0000	0.0000
3. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000
4. N	0.0003	0.0001	0.0000	0.0001	0.0000	0.0137	0.0000	0.0003	0.0000
5. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000
6. N	0.0011	0.0005	0.0001	0.0001	0.0000	0.0041	0.0000	0.0003	0.0001
7. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000
8. H	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9. N	0.0003	0.0001	0.0002	0.0006	0.0003	0.0038	0.0002	0.0079	0.0007
10. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0173	0.0001
11. H	0.0001	0.0000	0.0001	0.0005	0.0001	0.0001	0.0000	0.0002	0.0000
12. O	0.0027	0.0020	0.0642	0.0178	0.0010	0.0000	0.0002	0.0004	0.0001
13. O	0.0148	0.0519	0.0033	0.0031	0.0001	0.0001	0.0000	0.0000	0.0000
14. C	0.0051	0.0013	0.0009	0.0056	0.0001	0.0000	0.0000	0.0001	0.0000
15. C	0.0008	0.0020	0.0008	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
16. H	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0001	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.7842	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.6934	0.0001	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000
20. H	0.6934	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.6640	0.0007	0.0000	0.0001	0.0004	0.0000
22. O	0.0001	0.0000	0.6640	0.0000	0.7728	0.0000	0.0434	0.0143	0.0006
23. H	0.0000	0.0000	0.0007	0.7728	0.0000	0.0000	0.0001	0.0010	0.0000
24. H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0001	0.0434	0.0001	0.0000	0.0000	0.7026	0.0007
26. O	0.0000	0.0000	0.0004	0.0143	0.0010	0.0000	0.7026	0.0000	0.7770
27. H	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000	0.0007	0.7770	0.0000
28. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
29. O	0.0002	0.0000	0.0000	0.0002	0.0000	0.0001	0.0005	0.0061	0.0019
30. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0150	0.0001
31. H	0.0346	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0124	0.0005	0.0004	0.0080	0.0010	0.0000	0.0001	0.0005	0.0002
33. H	0.0003	0.0000	0.0001	0.0199	0.0000	0.0000	0.0000	0.0000	0.0000
34. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000

36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0126	0.0000	0.0000	0.0000
38. C	0.0002	0.0002	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0001	0.0020	0.0001	0.0001	0.0009	0.0000	0.0074	0.0001	0.0005
2. C	0.0000	0.0009	0.0000	0.0000	0.0001	0.0000	1.0312	0.0022	0.0030
3. H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0031	0.0120	0.0013
4. N	0.0003	0.0226	0.0005	0.0001	0.0007	0.0001	0.0113	0.0019	0.0088
5. H	0.0001	0.0605	0.0001	0.0000	0.0006	0.0000	0.0023	0.0005	0.0002
6. N	0.0001	0.0008	0.0001	0.0000	0.0002	0.0000	0.0013	0.0001	0.0001
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
8. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. N	0.0001	0.0023	0.0001	0.0001	0.0011	0.0002	0.0009	0.0001	0.0003
10. H	0.0000	0.0026	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
11. H	0.0000	0.0002	0.0000	0.0000	0.0003	0.0000	0.0002	0.0000	0.0001
12. O	0.0000	0.0001	0.0000	0.0001	0.0006	0.0001	0.0000	0.0000	0.0000
13. O	0.0000	0.0000	0.0000	0.0001	0.0003	0.0001	0.0001	0.0000	0.0000
14. C	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0002	0.0000	0.0346	0.0124	0.0003	0.0000	0.0000	0.0000
20. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000
22. O	0.0001	0.0002	0.0001	0.0002	0.0080	0.0199	0.0000	0.0000	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0026	0.0017	0.0010
25. H	0.0000	0.0005	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
26. O	0.0002	0.0061	0.0150	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0019	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.7024	0.0007	0.0001	0.0462	0.0001	0.0000	0.0000	0.0000
29. O	0.7024	0.0000	0.7469	0.0008	0.0150	0.0004	0.0009	0.0005	0.0001
30. H	0.0007	0.7469	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000
31. H	0.0001	0.0008	0.0000	0.0000	0.7167	0.0006	0.0000	0.0000	0.0000
32. O	0.0462	0.0150	0.0003	0.7167	0.0000	0.7441	0.0000	0.0000	0.0000
33. H	0.0001	0.0004	0.0000	0.0006	0.7441	0.0000	0.0000	0.0000	0.0000
34. C	0.0000	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.9361	0.9422
35. H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.9361	0.0000	0.0007
36. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.9422	0.0007	0.0000
37. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.9406	0.0005	0.0007
38. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41
1. C	0.0001	0.0000	0.0000	0.0000	0.0000
2. C	0.0024	0.0000	0.0000	0.0000	0.0000

3.	H	0.0019	0.0000	0.0000	0.0000	0.0000
4.	N	0.0018	0.0000	0.0000	0.0000	0.0000
5.	H	0.0000	0.0000	0.0000	0.0000	0.0000
6.	N	0.0001	0.0002	0.0001	0.0000	0.0000
7.	H	0.0001	0.0000	0.0000	0.0000	0.0000
8.	H	0.0000	0.0002	0.0001	0.0000	0.0000
9.	N	0.0002	0.0001	0.0000	0.0000	0.0000
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000	0.0000	0.0000
12.	O	0.0000	0.0055	0.0019	0.0006	0.0009
13.	O	0.0000	0.0098	0.0015	0.0006	0.0005
14.	C	0.0000	0.0082	0.0091	0.0012	0.0014
15.	C	0.0000	1.0304	0.0018	0.0024	0.0023
16.	H	0.0000	0.0027	0.0016	0.0125	0.0012
17.	H	0.0000	0.0025	0.0012	0.0013	0.0124
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000
19.	O	0.0000	0.0002	0.0000	0.0000	0.0000
20.	H	0.0000	0.0002	0.0001	0.0000	0.0000
21.	H	0.0000	0.0001	0.0000	0.0000	0.0000
22.	O	0.0000	0.0003	0.0000	0.0001	0.0001
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0126	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000
26.	O	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000
29.	O	0.0001	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.9406	0.0000	0.0000	0.0000	0.0000
35.	H	0.0005	0.0000	0.0000	0.0000	0.0000
36.	H	0.0007	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000
38.	C	0.0000	0.0000	0.9461	0.9465	0.9401
39.	H	0.0000	0.9461	0.0000	0.0005	0.0005
40.	H	0.0000	0.9465	0.0005	0.0000	0.0006
41.	H	0.0000	0.9401	0.0005	0.0006	0.0000

Table-9C-2-3: Wiberg index for salt bridge with 5 waters (bridge length=4.2 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0097	0.0025	1.2786	0.0026	1.2581	0.0023	0.0025	1.3229
2. C	0.0097	0.0000	0.9275	0.9575	0.0047	0.0037	0.0014	0.0002	0.0103
3. H	0.0025	0.9275	0.0000	0.0054	0.0062	0.0034	0.0000	0.0000	0.0014
4. N	1.2786	0.9575	0.0054	0.0000	0.7103	0.0739	0.0029	0.0085	0.0887
5. H	0.0026	0.0047	0.0062	0.7103	0.0000	0.0098	0.0001	0.0004	0.0021
6. N	1.2581	0.0037	0.0034	0.0739	0.0098	0.0000	0.8277	0.7580	0.0827
7. H	0.0023	0.0014	0.0000	0.0029	0.0001	0.8277	0.0000	0.0004	0.0108
8. H	0.0025	0.0002	0.0000	0.0085	0.0004	0.7580	0.0004	0.0000	0.0020
9. N	1.3229	0.0103	0.0014	0.0887	0.0021	0.0827	0.0108	0.0020	0.0000
10. H	0.0024	0.0002	0.0000	0.0013	0.0005	0.0095	0.0008	0.0002	0.7813
11. H	0.0026	0.0009	0.0000	0.0092	0.0001	0.0013	0.0002	0.0005	0.7435

12. O	0.0015	0.0002	0.0000	0.0010	0.0000	0.0013	0.0001	0.0009	0.0157
13. O	0.0016	0.0001	0.0000	0.0007	0.0001	0.0119	0.0003	0.0331	0.0024
14. C	0.0002	0.0000	0.0000	0.0001	0.0000	0.0015	0.0000	0.0010	0.0012
15. C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0010	0.0000	0.0027	0.0018
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
18. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000
19. O	0.0007	0.0002	0.0001	0.0002	0.0000	0.0011	0.0004	0.0002	0.0004
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0001	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
22. O	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0006
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
24. H	0.0061	0.9221	0.0007	0.0132	0.0004	0.0040	0.0005	0.0000	0.0039
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
26. O	0.0007	0.0000	0.0000	0.0003	0.0001	0.0004	0.0001	0.0000	0.0087
27. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0007
28. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
29. O	0.0021	0.0010	0.0005	0.0230	0.0622	0.0008	0.0000	0.0002	0.0023
30. H	0.0001	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0000	0.0001
31. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
32. O	0.0010	0.0001	0.0000	0.0007	0.0006	0.0002	0.0000	0.0000	0.0011
33. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
34. C	0.0073	1.0313	0.0031	0.0115	0.0022	0.0012	0.0002	0.0001	0.0009
35. H	0.0001	0.0022	0.0119	0.0019	0.0005	0.0001	0.0000	0.0000	0.0001
36. H	0.0005	0.0031	0.0013	0.0089	0.0002	0.0001	0.0000	0.0000	0.0004
37. H	0.0001	0.0024	0.0019	0.0018	0.0000	0.0001	0.0001	0.0000	0.0002
38. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002	0.0001
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0024	0.0026	0.0015	0.0016	0.0002	0.0003	0.0000	0.0000	0.0001
2. C	0.0002	0.0009	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0013	0.0092	0.0010	0.0007	0.0001	0.0002	0.0000	0.0000	0.0000
5. H	0.0005	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0095	0.0013	0.0013	0.0119	0.0015	0.0010	0.0000	0.0001	0.0004
7. H	0.0008	0.0002	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0002	0.0005	0.0009	0.0331	0.0010	0.0027	0.0000	0.0001	0.0000
9. N	0.7813	0.7435	0.0157	0.0024	0.0012	0.0018	0.0001	0.0000	0.0000
10. H	0.0000	0.0008	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0008	0.0000	0.0445	0.0034	0.0016	0.0057	0.0001	0.0000	0.0000
12. O	0.0002	0.0445	0.0000	0.1746	1.4018	0.0377	0.0114	0.0110	0.0001
13. O	0.0002	0.0034	0.1746	0.0000	1.4175	0.0408	0.0078	0.0044	0.0010
14. C	0.0000	0.0016	1.4018	1.4175	0.0000	0.9736	0.0068	0.0052	0.0001
15. C	0.0000	0.0057	0.0377	0.0408	0.9736	0.0000	0.9105	0.9191	0.0001
16. H	0.0000	0.0001	0.0114	0.0078	0.0068	0.9105	0.0000	0.0012	0.0000
17. H	0.0000	0.0000	0.0110	0.0044	0.0052	0.9191	0.0012	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0010	0.0001	0.0001	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0028	0.0159	0.0054	0.0008	0.0002	0.0001	0.7842
20. H	0.0000	0.0000	0.0022	0.0571	0.0014	0.0022	0.0001	0.0000	0.0007
21. H	0.0000	0.0001	0.0714	0.0034	0.0010	0.0010	0.0000	0.0001	0.0000

22. O	0.0001	0.0005	0.0194	0.0033	0.0059	0.0004	0.0001	0.0003	0.0000
23. H	0.0000	0.0001	0.0010	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
24. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0194	0.0002	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
27. H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0025	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
32. O	0.0001	0.0004	0.0006	0.0003	0.0003	0.0001	0.0000	0.0000	0.0010
33. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
34. C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. C	0.0000	0.0000	0.0056	0.0099	0.0082	1.0302	0.0027	0.0025	0.0000
39. H	0.0000	0.0000	0.0020	0.0016	0.0092	0.0018	0.0016	0.0012	0.0000
40. H	0.0000	0.0000	0.0006	0.0006	0.0012	0.0024	0.0126	0.0013	0.0000
41. H	0.0000	0.0000	0.0009	0.0005	0.0014	0.0024	0.0012	0.0124	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0007	0.0001	0.0000	0.0001	0.0000	0.0061	0.0000	0.0007	0.0001
2. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.9221	0.0000	0.0000	0.0000
3. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000
4. N	0.0002	0.0001	0.0000	0.0001	0.0000	0.0132	0.0000	0.0003	0.0000
5. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0001	0.0000
6. N	0.0011	0.0004	0.0000	0.0001	0.0000	0.0040	0.0000	0.0004	0.0001
7. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000
8. H	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9. N	0.0004	0.0001	0.0002	0.0006	0.0002	0.0039	0.0002	0.0087	0.0007
10. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0194	0.0001
11. H	0.0001	0.0000	0.0001	0.0005	0.0001	0.0001	0.0000	0.0002	0.0000
12. O	0.0028	0.0022	0.0714	0.0194	0.0010	0.0000	0.0002	0.0004	0.0001
13. O	0.0159	0.0571	0.0034	0.0033	0.0001	0.0000	0.0000	0.0001	0.0000
14. C	0.0054	0.0014	0.0010	0.0059	0.0001	0.0000	0.0000	0.0001	0.0000
15. C	0.0008	0.0022	0.0010	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
16. H	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0001	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.7842	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.6870	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
20. H	0.6870	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.6551	0.0007	0.0000	0.0001	0.0004	0.0000
22. O	0.0001	0.0001	0.6551	0.0000	0.7727	0.0000	0.0463	0.0151	0.0007
23. H	0.0000	0.0000	0.0007	0.7727	0.0000	0.0000	0.0001	0.0010	0.0000
24. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0001	0.0463	0.0001	0.0000	0.0000	0.6985	0.0007
26. O	0.0000	0.0000	0.0004	0.0151	0.0010	0.0000	0.6985	0.0000	0.7765
27. H	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000	0.0007	0.7765	0.0000
28. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
29. O	0.0002	0.0000	0.0000	0.0002	0.0000	0.0001	0.0005	0.0061	0.0018
30. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0149	0.0001
31. H	0.0350	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000

32. O	0.0125	0.0005	0.0004	0.0083	0.0010	0.0000	0.0001	0.0005	0.0002
33. H	0.0003	0.0000	0.0001	0.0210	0.0000	0.0000	0.0000	0.0000	0.0000
34. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0126	0.0000	0.0000	0.0000
38. C	0.0002	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0001	0.0021	0.0001	0.0001	0.0010	0.0000	0.0073	0.0001	0.0005
2. C	0.0000	0.0010	0.0000	0.0000	0.0001	0.0000	1.0313	0.0022	0.0031
3. H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0031	0.0119	0.0013
4. N	0.0003	0.0230	0.0005	0.0001	0.0007	0.0001	0.0115	0.0019	0.0089
5. H	0.0001	0.0622	0.0001	0.0000	0.0006	0.0000	0.0022	0.0005	0.0002
6. N	0.0001	0.0008	0.0001	0.0000	0.0002	0.0000	0.0012	0.0001	0.0001
7. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
8. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. N	0.0001	0.0023	0.0001	0.0001	0.0011	0.0002	0.0009	0.0001	0.0004
10. H	0.0000	0.0025	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
11. H	0.0000	0.0002	0.0000	0.0000	0.0004	0.0000	0.0002	0.0000	0.0001
12. O	0.0000	0.0001	0.0000	0.0001	0.0006	0.0001	0.0000	0.0000	0.0000
13. O	0.0000	0.0000	0.0000	0.0001	0.0003	0.0001	0.0000	0.0000	0.0000
14. C	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0002	0.0000	0.0350	0.0125	0.0003	0.0000	0.0000	0.0000
20. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000
22. O	0.0001	0.0002	0.0001	0.0002	0.0083	0.0210	0.0000	0.0000	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0026	0.0017	0.0010
25. H	0.0000	0.0005	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
26. O	0.0002	0.0061	0.0149	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0018	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.7012	0.0007	0.0001	0.0465	0.0001	0.0000	0.0000	0.0000
29. O	0.7012	0.0000	0.7466	0.0009	0.0150	0.0004	0.0008	0.0005	0.0001
30. H	0.0007	0.7466	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000
31. H	0.0001	0.0009	0.0000	0.0000	0.7159	0.0006	0.0000	0.0000	0.0000
32. O	0.0465	0.0150	0.0003	0.7159	0.0000	0.7422	0.0000	0.0000	0.0000
33. H	0.0001	0.0004	0.0000	0.0006	0.7422	0.0000	0.0000	0.0000	0.0000
34. C	0.0000	0.0008	0.0001	0.0000	0.0000	0.0000	0.0000	0.9364	0.9418
35. H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.9364	0.0000	0.0007
36. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.9418	0.0007	0.0000
37. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.9405	0.0005	0.0007
38. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41
1. C	0.0001	0.0000	0.0000	0.0000	0.0000
2. C	0.0024	0.0000	0.0000	0.0000	0.0000
3. H	0.0019	0.0000	0.0000	0.0000	0.0000
4. N	0.0018	0.0000	0.0000	0.0000	0.0000
5. H	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0001	0.0001	0.0000	0.0000	0.0000
7. H	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0002	0.0001	0.0000	0.0000
9. N	0.0002	0.0001	0.0000	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0000	0.0056	0.0020	0.0006	0.0009
13. O	0.0000	0.0099	0.0016	0.0006	0.0005
14. C	0.0000	0.0082	0.0092	0.0012	0.0014
15. C	0.0000	1.0302	0.0018	0.0024	0.0024
16. H	0.0000	0.0027	0.0016	0.0126	0.0012
17. H	0.0000	0.0025	0.0012	0.0013	0.0124
18. H	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0002	0.0000	0.0000	0.0000
20. H	0.0000	0.0002	0.0001	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0002	0.0000	0.0001	0.0001
23. H	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0126	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0001	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0000
34. C	0.9405	0.0000	0.0000	0.0000	0.0000
35. H	0.0005	0.0000	0.0000	0.0000	0.0000
36. H	0.0007	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000
38. C	0.0000	0.0000	0.9464	0.9466	0.9401
39. H	0.0000	0.9464	0.0000	0.0005	0.0005
40. H	0.0000	0.9466	0.0005	0.0000	0.0006
41. H	0.0000	0.9401	0.0005	0.0006	0.0000

Table-9C-3-1: Wiberg index for salt bridge with 6 waters (bridge length=3.8 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0093	0.0025	1.2294	0.0018	1.3032	0.0026	0.0031	1.3255
2. C	0.0093	0.0000	0.9255	0.9621	0.0051	0.0038	0.0019	0.0002	0.0102
3. H	0.0025	0.9255	0.0000	0.0073	0.0062	0.0043	0.0001	0.0000	0.0013
4. N	1.2294	0.9621	0.0073	0.0000	0.7803	0.0767	0.0027	0.0079	0.0811
5. H	0.0018	0.0051	0.0062	0.7803	0.0000	0.0098	0.0003	0.0004	0.0017
6. N	1.3032	0.0038	0.0043	0.0767	0.0098	0.0000	0.8289	0.6785	0.0935
7. H	0.0026	0.0019	0.0001	0.0027	0.0003	0.8289	0.0000	0.0009	0.0107

8. H	0.0031	0.0002	0.0000	0.0079	0.0004	0.6785	0.0009	0.0000	0.0015
9. N	1.3255	0.0102	0.0013	0.0811	0.0017	0.0935	0.0107	0.0015	0.0000
10. H	0.0026	0.0003	0.0000	0.0021	0.0007	0.0099	0.0008	0.0001	0.7975
11. H	0.0030	0.0007	0.0000	0.0087	0.0001	0.0014	0.0001	0.0004	0.6859
12. O	0.0031	0.0004	0.0001	0.0022	0.0001	0.0025	0.0001	0.0013	0.0346
13. O	0.0039	0.0003	0.0001	0.0020	0.0005	0.0360	0.0004	0.1143	0.0029
14. C	0.0005	0.0000	0.0000	0.0004	0.0000	0.0027	0.0001	0.0016	0.0029
15. C	0.0008	0.0000	0.0000	0.0005	0.0001	0.0026	0.0001	0.0061	0.0027
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
18. H	0.0053	0.9177	0.0009	0.0146	0.0009	0.0041	0.0003	0.0000	0.0036
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004
20. O	0.0006	0.0000	0.0000	0.0007	0.0001	0.0001	0.0000	0.0000	0.0014
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
22. O	0.0003	0.0002	0.0001	0.0004	0.0000	0.0019	0.0008	0.0003	0.0003
23. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0006	0.0000	0.0000	0.0001
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0001
25. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
26. O	0.0018	0.0005	0.0001	0.0015	0.0004	0.0005	0.0001	0.0000	0.0003
27. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
28. O	0.0005	0.0001	0.0000	0.0008	0.0005	0.0004	0.0001	0.0000	0.0076
29. H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0003
30. H	0.0001	0.0000	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000	0.0011
31. H	0.0001	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0002	0.0009	0.0002	0.0012	0.0004	0.0002	0.0000	0.0000	0.0001
33. H	0.0000	0.0001	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0001	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000
35. O	0.0004	0.0003	0.0001	0.0069	0.0156	0.0003	0.0000	0.0000	0.0004
36. H	0.0000	0.0001	0.0001	0.0006	0.0001	0.0001	0.0000	0.0000	0.0001
37. C	0.0071	1.0306	0.0028	0.0114	0.0027	0.0016	0.0002	0.0001	0.0011
38. H	0.0001	0.0025	0.0119	0.0016	0.0005	0.0001	0.0000	0.0000	0.0001
39. H	0.0005	0.0032	0.0014	0.0085	0.0003	0.0001	0.0000	0.0000	0.0004
40. H	0.0001	0.0026	0.0018	0.0016	0.0001	0.0001	0.0001	0.0000	0.0001
41. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0003	0.0001
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0026	0.0030	0.0031	0.0039	0.0005	0.0008	0.0000	0.0000	0.0053
2. C	0.0003	0.0007	0.0004	0.0003	0.0000	0.0000	0.0000	0.0000	0.9177
3. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0009
4. N	0.0021	0.0087	0.0022	0.0020	0.0004	0.0005	0.0000	0.0000	0.0146
5. H	0.0007	0.0001	0.0001	0.0005	0.0000	0.0001	0.0000	0.0000	0.0009
6. N	0.0099	0.0014	0.0025	0.0360	0.0027	0.0026	0.0000	0.0001	0.0041
7. H	0.0008	0.0001	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000	0.0003
8. H	0.0001	0.0004	0.0013	0.1143	0.0016	0.0061	0.0000	0.0000	0.0000
9. N	0.7975	0.6859	0.0346	0.0029	0.0029	0.0027	0.0003	0.0000	0.0036
10. H	0.0000	0.0011	0.0006	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
11. H	0.0011	0.0000	0.1068	0.0010	0.0016	0.0059	0.0002	0.0000	0.0001
12. O	0.0006	0.1068	0.0000	0.1715	1.4396	0.0377	0.0108	0.0113	0.0001
13. O	0.0001	0.0010	0.1715	0.0000	1.3740	0.0374	0.0035	0.0074	0.0001
14. C	0.0001	0.0016	1.4396	1.3740	0.0000	0.9700	0.0048	0.0070	0.0000

15. C	0.0001	0.0059	0.0377	0.0374	0.9700	0.0000	0.9206	0.9141	0.0000
16. H	0.0000	0.0002	0.0108	0.0035	0.0048	0.9206	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0113	0.0074	0.0070	0.9141	0.0011	0.0000	0.0000
18. H	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0002	0.0088	0.0022	0.0041	0.0002	0.0001	0.0002	0.0000
21. H	0.0000	0.0001	0.0262	0.0022	0.0006	0.0004	0.0000	0.0001	0.0000
22. O	0.0000	0.0000	0.0030	0.0137	0.0048	0.0004	0.0001	0.0003	0.0002
23. H	0.0000	0.0000	0.0001	0.0010	0.0002	0.0001	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0033	0.0467	0.0008	0.0006	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
26. O	0.0001	0.0000	0.0005	0.0004	0.0004	0.0001	0.0000	0.0000	0.0004
27. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
28. O	0.0172	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0023
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0018
39. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0123
41. C	0.0000	0.0000	0.0056	0.0096	0.0082	1.0307	0.0025	0.0030	0.0000
42. H	0.0000	0.0001	0.0019	0.0013	0.0094	0.0018	0.0013	0.0015	0.0000
43. H	0.0000	0.0000	0.0009	0.0004	0.0013	0.0023	0.0125	0.0012	0.0000
44. H	0.0000	0.0000	0.0005	0.0006	0.0013	0.0022	0.0013	0.0125	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0000	0.0006	0.0000	0.0003	0.0001	0.0000	0.0001	0.0018	0.0001
2. C	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0005	0.0000
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
4. N	0.0000	0.0007	0.0000	0.0004	0.0001	0.0000	0.0001	0.0015	0.0001
5. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
6. N	0.0001	0.0001	0.0000	0.0019	0.0006	0.0005	0.0002	0.0005	0.0000
7. H	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0001	0.0000
8. H	0.0000	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
9. N	0.0004	0.0014	0.0003	0.0003	0.0001	0.0001	0.0000	0.0003	0.0001
10. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
11. H	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0005	0.0088	0.0262	0.0030	0.0001	0.0033	0.0001	0.0005	0.0001
13. O	0.0001	0.0022	0.0022	0.0137	0.0010	0.0467	0.0001	0.0004	0.0001
14. C	0.0001	0.0041	0.0006	0.0048	0.0002	0.0008	0.0001	0.0004	0.0001
15. C	0.0000	0.0002	0.0004	0.0004	0.0001	0.0006	0.0000	0.0001	0.0001
16. H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0002	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0004	0.0000
19. H	0.0000	0.7392	0.0006	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001
20. O	0.7392	0.0000	0.7280	0.0001	0.0000	0.0001	0.0005	0.0171	0.0547
21. H	0.0006	0.7280	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0001

22. O	0.0000	0.0001	0.0001	0.0000	0.7822	0.6988	0.0369	0.0128	0.0003
23. H	0.0000	0.0000	0.0000	0.7822	0.0000	0.0007	0.0001	0.0012	0.0000
24. H	0.0000	0.0001	0.0000	0.6988	0.0007	0.0000	0.0001	0.0005	0.0000
25. H	0.0000	0.0005	0.0000	0.0369	0.0001	0.0001	0.0000	0.7074	0.0006
26. O	0.0005	0.0171	0.0004	0.0128	0.0012	0.0005	0.7074	0.0000	0.6892
27. H	0.0001	0.0547	0.0001	0.0003	0.0000	0.0000	0.0006	0.6892	0.0000
28. O	0.0218	0.0089	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
29. H	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0001	0.0943	0.0001
32. O	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0015	0.0270	0.0007
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
35. O	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
37. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
41. C	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0005	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000	0.0004	0.0000
2. C	0.0001	0.0000	0.0000	0.0000	0.0009	0.0001	0.0001	0.0003	0.0001
3. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0001
4. N	0.0008	0.0001	0.0001	0.0003	0.0012	0.0003	0.0004	0.0069	0.0006
5. H	0.0005	0.0001	0.0001	0.0000	0.0004	0.0001	0.0001	0.0156	0.0001
6. N	0.0004	0.0001	0.0002	0.0000	0.0002	0.0000	0.0001	0.0003	0.0001
7. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9. N	0.0076	0.0003	0.0011	0.0000	0.0001	0.0000	0.0000	0.0004	0.0001
10. H	0.0172	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000	0.0001	0.0000
19. H	0.0218	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
20. O	0.0089	0.0005	0.0010	0.0002	0.0002	0.0000	0.0000	0.0002	0.0000
21. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0001	0.0015	0.0000	0.0000	0.0000	0.0000
26. O	0.0002	0.0000	0.0000	0.0943	0.0270	0.0009	0.0002	0.0003	0.0001
27. H	0.0000	0.0000	0.0000	0.0001	0.0007	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.6982	0.7762	0.0000	0.0002	0.0000	0.0006	0.0158	0.0010

29. H	0.6982	0.0000	0.0007	0.0000	0.0001	0.0000	0.0001	0.0480	0.0001
30. H	0.7762	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6424	0.0008	0.0001	0.0005	0.0000
32. O	0.0002	0.0001	0.0000	0.6424	0.0000	0.7785	0.0838	0.0242	0.0008
33. H	0.0000	0.0000	0.0000	0.0008	0.7785	0.0000	0.0001	0.0012	0.0000
34. H	0.0006	0.0001	0.0000	0.0001	0.0838	0.0001	0.0000	0.6545	0.0007
35. O	0.0158	0.0480	0.0007	0.0005	0.0242	0.0012	0.6545	0.0000	0.7747
36. H	0.0010	0.0001	0.0000	0.0000	0.0008	0.0000	0.0007	0.7747	0.0000
37. C	0.0001	0.0001	0.0000	0.0000	0.0006	0.0001	0.0001	0.0016	0.0001
38. H	0.0001	0.0000	0.0000	0.0000	0.0006	0.0000	0.0001	0.0013	0.0001
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000
41. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44
1. C	0.0071	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000
2. C	1.0306	0.0025	0.0032	0.0026	0.0000	0.0000	0.0000	0.0000
3. H	0.0028	0.0119	0.0014	0.0018	0.0000	0.0000	0.0000	0.0000
4. N	0.0114	0.0016	0.0085	0.0016	0.0000	0.0000	0.0000	0.0000
5. H	0.0027	0.0005	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
6. N	0.0016	0.0001	0.0001	0.0001	0.0005	0.0001	0.0000	0.0000
7. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0001	0.0000	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000
9. N	0.0011	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000
10. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0002	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
12. O	0.0000	0.0000	0.0000	0.0000	0.0056	0.0019	0.0009	0.0005
13. O	0.0001	0.0000	0.0000	0.0000	0.0096	0.0013	0.0004	0.0006
14. C	0.0000	0.0000	0.0000	0.0000	0.0082	0.0094	0.0013	0.0013
15. C	0.0000	0.0000	0.0000	0.0000	1.0307	0.0018	0.0023	0.0022
16. H	0.0000	0.0000	0.0000	0.0000	0.0025	0.0013	0.0125	0.0013
17. H	0.0000	0.0000	0.0000	0.0000	0.0030	0.0015	0.0012	0.0125
18. H	0.0023	0.0018	0.0010	0.0123	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0006	0.0006	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0016	0.0013	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000

36.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	C	0.0000	0.9374	0.9407	0.9422	0.0000	0.0000	0.0000	0.0000
38.	H	0.9374	0.0000	0.0007	0.0005	0.0000	0.0000	0.0000	0.0000
39.	H	0.9407	0.0007	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000
40.	H	0.9422	0.0005	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.9473	0.9404	0.9437
42.	H	0.0000	0.0000	0.0000	0.0000	0.9473	0.0000	0.0005	0.0005
43.	H	0.0000	0.0000	0.0000	0.0000	0.9404	0.0005	0.0000	0.0006
44.	H	0.0000	0.0000	0.0000	0.0000	0.9437	0.0005	0.0006	0.0000

Table-9C-3-2: Wiberg index for salt bridge with 6 waters (bridge length=4.0 angstroms)

Atom		1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.0094	0.0024	1.2415	0.0020	1.2986	0.0024	0.0026	1.3220
2.	C	0.0094	0.0000	0.9258	0.9577	0.0051	0.0038	0.0016	0.0002	0.0101
3.	H	0.0024	0.9258	0.0000	0.0068	0.0065	0.0037	0.0001	0.0000	0.0013
4.	N	1.2415	0.9577	0.0068	0.0000	0.7748	0.0769	0.0026	0.0079	0.0818
5.	H	0.0020	0.0051	0.0065	0.7748	0.0000	0.0101	0.0002	0.0004	0.0021
6.	N	1.2986	0.0038	0.0037	0.0769	0.0101	0.0000	0.8244	0.7064	0.0916
7.	H	0.0024	0.0016	0.0001	0.0026	0.0002	0.8244	0.0000	0.0007	0.0100
8.	H	0.0026	0.0002	0.0000	0.0079	0.0004	0.7064	0.0007	0.0000	0.0015
9.	N	1.3220	0.0101	0.0013	0.0818	0.0021	0.0916	0.0100	0.0015	0.0000
10.	H	0.0024	0.0002	0.0000	0.0018	0.0006	0.0094	0.0009	0.0002	0.7918
11.	H	0.0026	0.0007	0.0000	0.0083	0.0001	0.0014	0.0002	0.0006	0.7100
12.	O	0.0021	0.0003	0.0000	0.0017	0.0001	0.0021	0.0001	0.0016	0.0252
13.	O	0.0024	0.0002	0.0001	0.0014	0.0004	0.0255	0.0003	0.0778	0.0023
14.	C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0016	0.0000	0.0015	0.0017
15.	C	0.0004	0.0000	0.0000	0.0004	0.0000	0.0021	0.0001	0.0056	0.0022
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	H	0.0051	0.9183	0.0008	0.0139	0.0007	0.0043	0.0004	0.0000	0.0035
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004
20.	O	0.0007	0.0000	0.0000	0.0006	0.0000	0.0002	0.0000	0.0000	0.0016
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
22.	O	0.0004	0.0001	0.0001	0.0004	0.0000	0.0019	0.0008	0.0004	0.0002
23.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0006	0.0000	0.0001	0.0001
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0002	0.0001
25.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
26.	O	0.0019	0.0004	0.0001	0.0014	0.0003	0.0006	0.0001	0.0000	0.0004
27.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
28.	O	0.0006	0.0001	0.0000	0.0007	0.0004	0.0005	0.0001	0.0000	0.0083
29.	H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0003
30.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0012
31.	H	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0002	0.0009	0.0002	0.0009	0.0004	0.0001	0.0000	0.0000	0.0001
33.	H	0.0000	0.0001	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000
35.	O	0.0005	0.0003	0.0001	0.0072	0.0168	0.0004	0.0000	0.0000	0.0005
36.	H	0.0001	0.0001	0.0001	0.0006	0.0001	0.0001	0.0000	0.0000	0.0001
37.	C	0.0070	1.0317	0.0029	0.0111	0.0027	0.0014	0.0002	0.0001	0.0009
38.	H	0.0001	0.0025	0.0119	0.0015	0.0005	0.0001	0.0000	0.0000	0.0001
39.	H	0.0005	0.0033	0.0016	0.0086	0.0002	0.0001	0.0000	0.0000	0.0003
40.	H	0.0001	0.0026	0.0016	0.0017	0.0001	0.0001	0.0001	0.0000	0.0002

41. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0003	0.0001
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0024	0.0026	0.0021	0.0024	0.0003	0.0004	0.0000	0.0000	0.0051
2. C	0.0002	0.0007	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.9183
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0008
4. N	0.0018	0.0083	0.0017	0.0014	0.0002	0.0004	0.0000	0.0000	0.0139
5. H	0.0006	0.0001	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0007
6. N	0.0094	0.0014	0.0021	0.0255	0.0016	0.0021	0.0000	0.0000	0.0043
7. H	0.0009	0.0002	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0004
8. H	0.0002	0.0006	0.0016	0.0778	0.0015	0.0056	0.0000	0.0000	0.0000
9. N	0.7918	0.7100	0.0252	0.0023	0.0017	0.0022	0.0002	0.0000	0.0035
10. H	0.0000	0.0009	0.0005	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
11. H	0.0009	0.0000	0.0751	0.0014	0.0014	0.0056	0.0002	0.0000	0.0001
12. O	0.0005	0.0751	0.0000	0.1728	1.4430	0.0380	0.0113	0.0117	0.0001
13. O	0.0001	0.0014	0.1728	0.0000	1.3755	0.0376	0.0036	0.0076	0.0001
14. C	0.0001	0.0014	1.4430	1.3755	0.0000	0.9734	0.0049	0.0070	0.0000
15. C	0.0001	0.0056	0.0380	0.0376	0.9734	0.0000	0.9196	0.9132	0.0000
16. H	0.0000	0.0002	0.0113	0.0036	0.0049	0.9196	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0117	0.0076	0.0070	0.9132	0.0011	0.0000	0.0000
18. H	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0004	0.0093	0.0023	0.0042	0.0003	0.0000	0.0003	0.0000
21. H	0.0000	0.0001	0.0294	0.0023	0.0007	0.0005	0.0000	0.0001	0.0000
22. O	0.0000	0.0000	0.0033	0.0156	0.0054	0.0005	0.0001	0.0003	0.0001
23. H	0.0000	0.0000	0.0001	0.0010	0.0002	0.0001	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0035	0.0556	0.0009	0.0008	0.0000	0.0001	0.0000
25. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
26. O	0.0001	0.0000	0.0004	0.0004	0.0003	0.0001	0.0000	0.0000	0.0004
27. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
28. O	0.0189	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0024
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0020
39. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0124
41. C	0.0000	0.0000	0.0057	0.0099	0.0084	1.0300	0.0026	0.0030	0.0000
42. H	0.0000	0.0000	0.0019	0.0014	0.0093	0.0017	0.0012	0.0016	0.0000
43. H	0.0000	0.0000	0.0010	0.0005	0.0014	0.0023	0.0124	0.0012	0.0000
44. H	0.0000	0.0000	0.0005	0.0006	0.0013	0.0022	0.0013	0.0125	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0000	0.0007	0.0000	0.0004	0.0001	0.0000	0.0001	0.0019	0.0001

2. C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0000
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
4. N	0.0000	0.0006	0.0000	0.0004	0.0001	0.0000	0.0001	0.0014	0.0001
5. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
6. N	0.0001	0.0002	0.0000	0.0019	0.0006	0.0004	0.0002	0.0006	0.0000
7. H	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0001	0.0000
8. H	0.0000	0.0000	0.0000	0.0004	0.0001	0.0002	0.0000	0.0000	0.0000
9. N	0.0004	0.0016	0.0004	0.0002	0.0001	0.0001	0.0000	0.0004	0.0002
10. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
11. H	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0005	0.0093	0.0294	0.0033	0.0001	0.0035	0.0001	0.0004	0.0001
13. O	0.0001	0.0023	0.0023	0.0156	0.0010	0.0556	0.0001	0.0004	0.0001
14. C	0.0001	0.0042	0.0007	0.0054	0.0002	0.0009	0.0001	0.0003	0.0001
15. C	0.0000	0.0003	0.0005	0.0005	0.0001	0.0008	0.0000	0.0001	0.0000
16. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0003	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0000
19. H	0.0000	0.7436	0.0006	0.0000	0.0000	0.0000	0.0000	0.0006	0.0001
20. O	0.7436	0.0000	0.7207	0.0001	0.0000	0.0001	0.0005	0.0174	0.0557
21. H	0.0006	0.7207	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0001
22. O	0.0000	0.0001	0.0001	0.0000	0.7824	0.6863	0.0406	0.0138	0.0003
23. H	0.0000	0.0000	0.0000	0.7824	0.0000	0.0007	0.0001	0.0012	0.0000
24. H	0.0000	0.0001	0.0000	0.6863	0.0007	0.0000	0.0001	0.0004	0.0000
25. H	0.0000	0.0005	0.0000	0.0406	0.0001	0.0001	0.0000	0.7025	0.0006
26. O	0.0006	0.0174	0.0004	0.0138	0.0012	0.0004	0.7025	0.0000	0.6873
27. H	0.0001	0.0557	0.0001	0.0003	0.0000	0.0000	0.0006	0.6873	0.0000
28. O	0.0192	0.0081	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
29. H	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0002	0.0000	0.0003	0.0000	0.0000	0.0001	0.0991	0.0001
32. O	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0016	0.0283	0.0007
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
35. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
37. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
41. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0006	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000	0.0005	0.0001
2. C	0.0001	0.0000	0.0000	0.0001	0.0009	0.0001	0.0000	0.0003	0.0001
3. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0001
4. N	0.0007	0.0001	0.0001	0.0002	0.0009	0.0002	0.0004	0.0072	0.0006
5. H	0.0004	0.0001	0.0000	0.0000	0.0004	0.0001	0.0001	0.0168	0.0001
6. N	0.0005	0.0001	0.0002	0.0000	0.0001	0.0000	0.0001	0.0004	0.0001
7. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

9.	N	0.0083	0.0003	0.0012	0.0000	0.0001	0.0000	0.0000	0.0005	0.0001
10.	H	0.0189	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
11.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	O	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	H	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000	0.0001	0.0000
19.	H	0.0192	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	O	0.0081	0.0006	0.0009	0.0002	0.0002	0.0000	0.0000	0.0002	0.0000
21.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0000	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0001	0.0016	0.0000	0.0000	0.0000	0.0000
26.	O	0.0002	0.0000	0.0000	0.0991	0.0283	0.0010	0.0002	0.0003	0.0001
27.	H	0.0000	0.0000	0.0000	0.0001	0.0007	0.0000	0.0000	0.0000	0.0000
28.	O	0.0000	0.7018	0.7753	0.0000	0.0002	0.0000	0.0005	0.0148	0.0009
29.	H	0.7018	0.0000	0.0007	0.0000	0.0001	0.0000	0.0001	0.0445	0.0001
30.	H	0.7753	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.6383	0.0008	0.0001	0.0005	0.0000
32.	O	0.0002	0.0001	0.0000	0.6383	0.0000	0.7783	0.0840	0.0242	0.0008
33.	H	0.0000	0.0000	0.0000	0.0008	0.7783	0.0000	0.0001	0.0012	0.0000
34.	H	0.0005	0.0001	0.0000	0.0001	0.0840	0.0001	0.0000	0.6541	0.0007
35.	O	0.0148	0.0445	0.0007	0.0005	0.0242	0.0012	0.6541	0.0000	0.7754
36.	H	0.0009	0.0001	0.0000	0.0000	0.0008	0.0000	0.0007	0.7754	0.0000
37.	C	0.0001	0.0000	0.0000	0.0000	0.0006	0.0001	0.0001	0.0016	0.0001
38.	H	0.0001	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0013	0.0001
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44
1. C	0.0070	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
2. C	1.0317	0.0025	0.0033	0.0026	0.0000	0.0000	0.0000	0.0000
3. H	0.0029	0.0119	0.0016	0.0016	0.0000	0.0000	0.0000	0.0000
4. N	0.0111	0.0015	0.0086	0.0017	0.0000	0.0000	0.0000	0.0000
5. H	0.0027	0.0005	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
6. N	0.0014	0.0001	0.0001	0.0001	0.0003	0.0001	0.0000	0.0000
7. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0001	0.0000	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000
9. N	0.0009	0.0001	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000
10. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0000	0.0000	0.0000	0.0000	0.0057	0.0019	0.0010	0.0005
13. O	0.0001	0.0000	0.0000	0.0000	0.0099	0.0014	0.0005	0.0006
14. C	0.0000	0.0000	0.0000	0.0000	0.0084	0.0093	0.0014	0.0013
15. C	0.0000	0.0000	0.0000	0.0000	1.0300	0.0017	0.0023	0.0022

16.	H	0.0000	0.0000	0.0000	0.0000	0.0026	0.0012	0.0124	0.0013
17.	H	0.0000	0.0000	0.0000	0.0000	0.0030	0.0016	0.0012	0.0125
18.	H	0.0024	0.0020	0.0009	0.0124	0.0000	0.0000	0.0000	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0001
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	O	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	O	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0006	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	O	0.0016	0.0013	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
36.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	C	0.0000	0.9375	0.9400	0.9415	0.0000	0.0000	0.0000	0.0000
38.	H	0.9375	0.0000	0.0007	0.0005	0.0000	0.0000	0.0000	0.0000
39.	H	0.9400	0.0007	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000
40.	H	0.9415	0.0005	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.9479	0.9400	0.9437
42.	H	0.0000	0.0000	0.0000	0.0000	0.9479	0.0000	0.0005	0.0005
43.	H	0.0000	0.0000	0.0000	0.0000	0.9400	0.0005	0.0000	0.0007
44.	H	0.0000	0.0000	0.0000	0.0000	0.9437	0.0005	0.0007	0.0000

Table-9C-3-3: Wiberg index for salt bridge with 6 waters (bridge length=4.2 angstroms)

Atom		1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.0095	0.0024	1.2531	0.0021	1.2893	0.0023	0.0024	1.3207
2.	C	0.0095	0.0000	0.9259	0.9549	0.0051	0.0038	0.0015	0.0002	0.0101
3.	H	0.0024	0.9259	0.0000	0.0063	0.0065	0.0035	0.0001	0.0000	0.0013
4.	N	1.2531	0.9549	0.0063	0.0000	0.7692	0.0769	0.0026	0.0080	0.0835
5.	H	0.0021	0.0051	0.0065	0.7692	0.0000	0.0103	0.0001	0.0004	0.0022
6.	N	1.2893	0.0038	0.0035	0.0769	0.0103	0.0000	0.8227	0.7278	0.0888
7.	H	0.0023	0.0015	0.0001	0.0026	0.0001	0.8227	0.0000	0.0005	0.0100
8.	H	0.0024	0.0002	0.0000	0.0080	0.0004	0.7278	0.0005	0.0000	0.0017
9.	N	1.3207	0.0101	0.0013	0.0835	0.0022	0.0888	0.0100	0.0017	0.0000
10.	H	0.0024	0.0002	0.0000	0.0016	0.0005	0.0092	0.0009	0.0002	0.7867
11.	H	0.0024	0.0008	0.0000	0.0084	0.0001	0.0015	0.0002	0.0007	0.7299
12.	O	0.0016	0.0003	0.0000	0.0014	0.0001	0.0018	0.0001	0.0019	0.0183
13.	O	0.0018	0.0001	0.0000	0.0012	0.0003	0.0183	0.0003	0.0540	0.0019
14.	C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0012	0.0000	0.0014	0.0012
15.	C	0.0003	0.0000	0.0000	0.0003	0.0000	0.0017	0.0001	0.0049	0.0019
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	H	0.0052	0.9186	0.0008	0.0132	0.0006	0.0042	0.0004	0.0000	0.0035
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004
20.	O	0.0007	0.0000	0.0000	0.0006	0.0000	0.0002	0.0000	0.0000	0.0018
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003

22. O	0.0004	0.0001	0.0001	0.0004	0.0000	0.0018	0.0008	0.0005	0.0002
23. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0006	0.0000	0.0001	0.0001
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002	0.0000
25. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
26. O	0.0018	0.0004	0.0001	0.0014	0.0003	0.0006	0.0001	0.0000	0.0004
27. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
28. O	0.0006	0.0001	0.0000	0.0007	0.0003	0.0005	0.0001	0.0000	0.0089
29. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0003
30. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0013
31. H	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0002	0.0008	0.0002	0.0009	0.0004	0.0001	0.0000	0.0000	0.0001
33. H	0.0000	0.0001	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0000
35. O	0.0006	0.0003	0.0001	0.0080	0.0192	0.0004	0.0000	0.0001	0.0005
36. H	0.0001	0.0001	0.0001	0.0006	0.0001	0.0001	0.0000	0.0000	0.0001
37. C	0.0070	1.0320	0.0029	0.0111	0.0027	0.0013	0.0002	0.0001	0.0009
38. H	0.0001	0.0024	0.0119	0.0015	0.0005	0.0001	0.0000	0.0000	0.0001
39. H	0.0005	0.0033	0.0016	0.0086	0.0002	0.0001	0.0000	0.0000	0.0003
40. H	0.0001	0.0025	0.0016	0.0018	0.0001	0.0001	0.0001	0.0000	0.0002
41. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0003	0.0001
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0024	0.0024	0.0016	0.0018	0.0003	0.0003	0.0000	0.0000	0.0052
2. C	0.0002	0.0008	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.9186
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008
4. N	0.0016	0.0084	0.0014	0.0012	0.0002	0.0003	0.0000	0.0000	0.0132
5. H	0.0005	0.0001	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0006
6. N	0.0092	0.0015	0.0018	0.0183	0.0012	0.0017	0.0000	0.0000	0.0042
7. H	0.0009	0.0002	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0004
8. H	0.0002	0.0007	0.0019	0.0540	0.0014	0.0049	0.0000	0.0000	0.0000
9. N	0.7867	0.7299	0.0183	0.0019	0.0012	0.0019	0.0002	0.0000	0.0035
10. H	0.0000	0.0008	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0008	0.0000	0.0528	0.0016	0.0013	0.0050	0.0002	0.0000	0.0001
12. O	0.0003	0.0528	0.0000	0.1748	1.4469	0.0390	0.0116	0.0118	0.0000
13. O	0.0001	0.0016	0.1748	0.0000	1.3789	0.0385	0.0037	0.0077	0.0000
14. C	0.0000	0.0013	1.4469	1.3789	0.0000	0.9728	0.0048	0.0070	0.0000
15. C	0.0000	0.0050	0.0390	0.0385	0.9728	0.0000	0.9200	0.9134	0.0000
16. H	0.0000	0.0002	0.0116	0.0037	0.0048	0.9200	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0118	0.0077	0.0070	0.9134	0.0011	0.0000	0.0000
18. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0004	0.0095	0.0023	0.0042	0.0003	0.0000	0.0003	0.0000
21. H	0.0000	0.0002	0.0309	0.0023	0.0007	0.0007	0.0000	0.0001	0.0000
22. O	0.0000	0.0000	0.0034	0.0166	0.0055	0.0005	0.0001	0.0003	0.0001
23. H	0.0000	0.0000	0.0001	0.0011	0.0002	0.0001	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0035	0.0600	0.0010	0.0010	0.0000	0.0001	0.0000
25. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
26. O	0.0001	0.0000	0.0004	0.0004	0.0003	0.0001	0.0000	0.0000	0.0004
27. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
28. O	0.0207	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000

29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0024
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0020
39. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0123
41. C	0.0000	0.0000	0.0058	0.0101	0.0085	1.0297	0.0025	0.0029	0.0000
42. H	0.0000	0.0000	0.0020	0.0015	0.0093	0.0017	0.0012	0.0015	0.0000
43. H	0.0000	0.0000	0.0010	0.0005	0.0014	0.0023	0.0124	0.0012	0.0000
44. H	0.0000	0.0000	0.0005	0.0006	0.0013	0.0023	0.0013	0.0125	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0000	0.0007	0.0000	0.0004	0.0001	0.0000	0.0000	0.0018	0.0001
2. C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0000
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
4. N	0.0000	0.0006	0.0000	0.0004	0.0001	0.0000	0.0001	0.0014	0.0000
5. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
6. N	0.0001	0.0002	0.0000	0.0018	0.0006	0.0003	0.0002	0.0006	0.0000
7. H	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0001	0.0000
8. H	0.0000	0.0000	0.0000	0.0005	0.0001	0.0002	0.0000	0.0000	0.0000
9. N	0.0004	0.0018	0.0003	0.0002	0.0001	0.0000	0.0000	0.0004	0.0002
10. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
11. H	0.0000	0.0004	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0005	0.0095	0.0309	0.0034	0.0001	0.0035	0.0001	0.0004	0.0001
13. O	0.0001	0.0023	0.0023	0.0166	0.0011	0.0600	0.0001	0.0004	0.0001
14. C	0.0001	0.0042	0.0007	0.0055	0.0002	0.0010	0.0001	0.0003	0.0001
15. C	0.0000	0.0003	0.0007	0.0005	0.0001	0.0010	0.0000	0.0001	0.0000
16. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0003	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0000
19. H	0.0000	0.7467	0.0006	0.0000	0.0000	0.0000	0.0000	0.0006	0.0001
20. O	0.7467	0.0000	0.7159	0.0002	0.0000	0.0001	0.0005	0.0175	0.0561
21. H	0.0006	0.7159	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0001
22. O	0.0000	0.0002	0.0001	0.0000	0.7829	0.6794	0.0414	0.0140	0.0003
23. H	0.0000	0.0000	0.0000	0.7829	0.0000	0.0007	0.0001	0.0011	0.0000
24. H	0.0000	0.0001	0.0000	0.6794	0.0007	0.0000	0.0001	0.0004	0.0000
25. H	0.0000	0.0005	0.0000	0.0414	0.0001	0.0001	0.0000	0.7011	0.0006
26. O	0.0006	0.0175	0.0004	0.0140	0.0011	0.0004	0.7011	0.0000	0.6864
27. H	0.0001	0.0561	0.0001	0.0003	0.0000	0.0000	0.0006	0.6864	0.0000
28. O	0.0175	0.0075	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
29. H	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0002	0.0000	0.0003	0.0000	0.0000	0.0001	0.1006	0.0001
32. O	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0015	0.0285	0.0007
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
35. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000

36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
37. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
41. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0006	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000	0.0006	0.0001
2. C	0.0001	0.0000	0.0000	0.0001	0.0008	0.0001	0.0000	0.0003	0.0001
3. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0001
4. N	0.0007	0.0001	0.0001	0.0002	0.0009	0.0002	0.0003	0.0080	0.0006
5. H	0.0003	0.0000	0.0000	0.0000	0.0004	0.0001	0.0001	0.0192	0.0001
6. N	0.0005	0.0001	0.0002	0.0000	0.0001	0.0000	0.0001	0.0004	0.0001
7. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
9. N	0.0089	0.0003	0.0013	0.0000	0.0001	0.0000	0.0000	0.0005	0.0001
10. H	0.0207	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
11. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000	0.0001	0.0000
19. H	0.0175	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0075	0.0005	0.0009	0.0002	0.0002	0.0000	0.0000	0.0002	0.0000
21. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0001	0.0015	0.0000	0.0000	0.0000	0.0000
26. O	0.0002	0.0000	0.0000	0.1006	0.0285	0.0011	0.0003	0.0003	0.0001
27. H	0.0000	0.0000	0.0000	0.0001	0.0007	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.7026	0.7748	0.0000	0.0002	0.0000	0.0005	0.0148	0.0009
29. H	0.7026	0.0000	0.0007	0.0000	0.0001	0.0000	0.0001	0.0443	0.0000
30. H	0.7748	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6362	0.0008	0.0001	0.0005	0.0000
32. O	0.0002	0.0001	0.0000	0.6362	0.0000	0.7778	0.0864	0.0248	0.0007
33. H	0.0000	0.0000	0.0000	0.0008	0.7778	0.0000	0.0001	0.0012	0.0000
34. H	0.0005	0.0001	0.0000	0.0001	0.0864	0.0001	0.0000	0.6516	0.0007
35. O	0.0148	0.0443	0.0007	0.0005	0.0248	0.0012	0.6516	0.0000	0.7751
36. H	0.0009	0.0000	0.0000	0.0000	0.0007	0.0000	0.0007	0.7751	0.0000
37. C	0.0001	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0015	0.0001
38. H	0.0001	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0012	0.0001
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000
41. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		37	38	39	40	41	42	43	44
1.	C	0.0070	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
2.	C	1.0320	0.0024	0.0033	0.0025	0.0000	0.0000	0.0000	0.0000
3.	H	0.0029	0.0119	0.0016	0.0016	0.0000	0.0000	0.0000	0.0000
4.	N	0.0111	0.0015	0.0086	0.0018	0.0000	0.0000	0.0000	0.0000
5.	H	0.0027	0.0005	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
6.	N	0.0013	0.0001	0.0001	0.0001	0.0002	0.0001	0.0000	0.0000
7.	H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8.	H	0.0001	0.0000	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000
9.	N	0.0009	0.0001	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000
10.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	H	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12.	O	0.0000	0.0000	0.0000	0.0000	0.0058	0.0020	0.0010	0.0005
13.	O	0.0001	0.0000	0.0000	0.0000	0.0101	0.0015	0.0005	0.0006
14.	C	0.0000	0.0000	0.0000	0.0000	0.0085	0.0093	0.0014	0.0013
15.	C	0.0000	0.0000	0.0000	0.0000	1.0297	0.0017	0.0023	0.0023
16.	H	0.0000	0.0000	0.0000	0.0000	0.0025	0.0012	0.0124	0.0013
17.	H	0.0000	0.0000	0.0000	0.0000	0.0029	0.0015	0.0012	0.0125
18.	H	0.0024	0.0020	0.0009	0.0123	0.0000	0.0000	0.0000	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	O	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	O	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0005	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	O	0.0015	0.0012	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
36.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	C	0.0000	0.9379	0.9396	0.9412	0.0000	0.0000	0.0000	0.0000
38.	H	0.9379	0.0000	0.0007	0.0005	0.0000	0.0000	0.0000	0.0000
39.	H	0.9396	0.0007	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000
40.	H	0.9412	0.0005	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.9484	0.9400	0.9438
42.	H	0.0000	0.0000	0.0000	0.0000	0.9484	0.0000	0.0005	0.0005
43.	H	0.0000	0.0000	0.0000	0.0000	0.9400	0.0005	0.0000	0.0007
44.	H	0.0000	0.0000	0.0000	0.0000	0.9438	0.0005	0.0007	0.0000

Table-9C-4-1: Wiberg index for salt bridge with 7 waters (bridge length=3.8 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0095	0.0031	1.2588	0.0023	1.2685	0.0025	0.0028	1.3301
2. C	0.0095	0.0000	0.9254	0.9607	0.0047	0.0033	0.0013	0.0002	0.0106
3. H	0.0031	0.9254	0.0000	0.0071	0.0052	0.0035	0.0000	0.0000	0.0018
4. N	1.2588	0.9607	0.0071	0.0000	0.7227	0.0744	0.0023	0.0091	0.0875
5. H	0.0023	0.0047	0.0052	0.7227	0.0000	0.0095	0.0001	0.0005	0.0017
6. N	1.2685	0.0033	0.0035	0.0744	0.0095	0.0000	0.7962	0.7578	0.0876
7. H	0.0025	0.0013	0.0000	0.0023	0.0001	0.7962	0.0000	0.0006	0.0108
8. H	0.0028	0.0002	0.0000	0.0091	0.0005	0.7578	0.0006	0.0000	0.0020
9. N	1.3301	0.0106	0.0018	0.0875	0.0017	0.0876	0.0108	0.0020	0.0000
10. H	0.0026	0.0003	0.0000	0.0016	0.0006	0.0101	0.0007	0.0002	0.7872
11. H	0.0029	0.0007	0.0000	0.0093	0.0001	0.0012	0.0001	0.0004	0.7047
12. O	0.0027	0.0003	0.0000	0.0018	0.0000	0.0024	0.0001	0.0010	0.0298
13. O	0.0023	0.0002	0.0001	0.0009	0.0002	0.0152	0.0002	0.0429	0.0024
14. C	0.0004	0.0000	0.0000	0.0003	0.0000	0.0030	0.0000	0.0010	0.0031
15. C	0.0005	0.0000	0.0000	0.0002	0.0000	0.0010	0.0000	0.0026	0.0023
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0003
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
18. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0001
19. O	0.0025	0.0004	0.0001	0.0009	0.0002	0.0012	0.0002	0.0000	0.0005
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
22. O	0.0004	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0015
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
24. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0009	0.0001	0.0000	0.0001
25. O	0.0006	0.0014	0.0001	0.0005	0.0000	0.0066	0.0148	0.0001	0.0004
26. H	0.0000	0.0002	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000
27. O	0.0001	0.0001	0.0000	0.0000	0.0000	0.0003	0.0001	0.0002	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0056	0.9208	0.0007	0.0133	0.0009	0.0040	0.0005	0.0000	0.0035
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
32. O	0.0006	0.0000	0.0000	0.0004	0.0002	0.0004	0.0001	0.0000	0.0081
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0009
34. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
35. O	0.0017	0.0008	0.0004	0.0217	0.0562	0.0007	0.0000	0.0002	0.0017
36. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
37. H	0.0001	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0003	0.0001	0.0000	0.0006	0.0003	0.0002	0.0000	0.0000	0.0004
39. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
40. C	0.0072	1.0313	0.0028	0.0107	0.0025	0.0012	0.0002	0.0001	0.0009
41. H	0.0001	0.0023	0.0121	0.0020	0.0005	0.0001	0.0000	0.0000	0.0002
42. H	0.0006	0.0029	0.0012	0.0085	0.0003	0.0001	0.0000	0.0000	0.0004
43. H	0.0001	0.0025	0.0020	0.0017	0.0001	0.0001	0.0000	0.0000	0.0001
44. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0001
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0026	0.0029	0.0027	0.0023	0.0004	0.0005	0.0000	0.0000	0.0001
2. C	0.0003	0.0007	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

4. N	0.0016	0.0093	0.0018	0.0009	0.0003	0.0002	0.0000	0.0000	0.0001
5. H	0.0006	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0101	0.0012	0.0024	0.0152	0.0030	0.0010	0.0001	0.0001	0.0002
7. H	0.0007	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0002	0.0004	0.0010	0.0429	0.0010	0.0026	0.0001	0.0001	0.0000
9. N	0.7872	0.7047	0.0298	0.0024	0.0031	0.0023	0.0003	0.0000	0.0001
10. H	0.0000	0.0011	0.0004	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
11. H	0.0011	0.0000	0.0886	0.0016	0.0016	0.0058	0.0001	0.0000	0.0000
12. O	0.0004	0.0886	0.0000	0.1696	1.4691	0.0379	0.0121	0.0124	0.0001
13. O	0.0001	0.0016	0.1696	0.0000	1.3347	0.0386	0.0049	0.0052	0.0004
14. C	0.0001	0.0016	1.4691	1.3347	0.0000	0.9745	0.0060	0.0063	0.0001
15. C	0.0001	0.0058	0.0379	0.0386	0.9745	0.0000	0.9153	0.9154	0.0000
16. H	0.0000	0.0001	0.0121	0.0049	0.0060	0.9153	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0124	0.0052	0.0063	0.9154	0.0011	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0022	0.0121	0.0037	0.0008	0.0001	0.0002	0.7330
20. H	0.0000	0.0000	0.0015	0.0411	0.0010	0.0021	0.0001	0.0001	0.0006
21. H	0.0000	0.0001	0.0220	0.0016	0.0005	0.0005	0.0000	0.0000	0.0000
22. O	0.0002	0.0003	0.0083	0.0018	0.0037	0.0002	0.0001	0.0002	0.0000
23. H	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
25. O	0.0001	0.0000	0.0001	0.0009	0.0001	0.0001	0.0000	0.0000	0.0193
26. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
27. O	0.0000	0.0000	0.0017	0.0194	0.0023	0.0005	0.0001	0.0001	0.0001
28. H	0.0000	0.0000	0.0031	0.0564	0.0003	0.0002	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0002	0.0011	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
31. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0179	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0015	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0000	0.0000	0.0004	0.0003	0.0002	0.0000	0.0000	0.0000	0.0014
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. C	0.0000	0.0000	0.0054	0.0097	0.0085	1.0303	0.0029	0.0028	0.0000
45. H	0.0000	0.0000	0.0020	0.0014	0.0093	0.0017	0.0013	0.0013	0.0000
46. H	0.0000	0.0000	0.0007	0.0005	0.0013	0.0021	0.0123	0.0012	0.0000
47. H	0.0000	0.0000	0.0006	0.0005	0.0014	0.0021	0.0012	0.0123	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0025	0.0001	0.0000	0.0004	0.0000	0.0001	0.0006	0.0000	0.0001
2. C	0.0004	0.0000	0.0000	0.0000	0.0000	0.0001	0.0014	0.0002	0.0001
3. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
4. N	0.0009	0.0001	0.0000	0.0001	0.0000	0.0001	0.0005	0.0001	0.0000
5. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0012	0.0003	0.0000	0.0001	0.0000	0.0009	0.0066	0.0003	0.0003
7. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0148	0.0000	0.0001

8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
9.	N	0.0005	0.0001	0.0002	0.0015	0.0002	0.0001	0.0004	0.0000	0.0000
10.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
11.	H	0.0001	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
12.	O	0.0022	0.0015	0.0220	0.0083	0.0004	0.0000	0.0001	0.0000	0.0017
13.	O	0.0121	0.0411	0.0016	0.0018	0.0001	0.0002	0.0009	0.0002	0.0194
14.	C	0.0037	0.0010	0.0005	0.0037	0.0001	0.0000	0.0001	0.0000	0.0023
15.	C	0.0008	0.0021	0.0005	0.0002	0.0000	0.0000	0.0001	0.0000	0.0005
16.	H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
17.	H	0.0002	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
18.	H	0.7330	0.0006	0.0000	0.0000	0.0000	0.0001	0.0193	0.0001	0.0001
19.	O	0.0000	0.7055	0.0000	0.0002	0.0001	0.0014	0.0072	0.0004	0.0007
20.	H	0.7055	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002
21.	H	0.0000	0.0000	0.0000	0.7268	0.0006	0.0000	0.0000	0.0000	0.0000
22.	O	0.0002	0.0000	0.7268	0.0000	0.7259	0.0000	0.0000	0.0000	0.0000
23.	H	0.0001	0.0000	0.0006	0.7259	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.7784	0.0007	0.0008
25.	O	0.0072	0.0002	0.0000	0.0000	0.0000	0.7784	0.0000	0.6857	0.0180
26.	H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0007	0.6857	0.0000	0.0588
27.	O	0.0007	0.0002	0.0000	0.0000	0.0000	0.0008	0.0180	0.0588	0.0000
28.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.6815
29.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0001	0.7817
30.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0013	0.0002	0.0001
31.	H	0.0000	0.0000	0.0001	0.0747	0.0001	0.0000	0.0000	0.0000	0.0000
32.	O	0.0000	0.0000	0.0005	0.0227	0.0003	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35.	O	0.0002	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0700	0.0001	0.0000	0.0004	0.0001	0.0000	0.0001	0.0000	0.0000
38.	O	0.0210	0.0006	0.0003	0.0109	0.0299	0.0001	0.0001	0.0000	0.0000
39.	H	0.0008	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000
40.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
44.	C	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
45.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0000	0.0056	0.0000	0.0006	0.0001	0.0001	0.0017	0.0001
2. C	0.0000	0.0000	0.9208	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
3. H	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
4. N	0.0000	0.0000	0.0133	0.0000	0.0004	0.0000	0.0003	0.0217	0.0003
5. H	0.0000	0.0000	0.0009	0.0000	0.0002	0.0000	0.0001	0.0562	0.0001
6. N	0.0001	0.0000	0.0040	0.0000	0.0004	0.0001	0.0001	0.0007	0.0001
7. H	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
9. N	0.0000	0.0000	0.0035	0.0002	0.0081	0.0009	0.0001	0.0017	0.0001
10. H	0.0000	0.0000	0.0000	0.0001	0.0179	0.0001	0.0000	0.0015	0.0001
11. H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000

12. O	0.0031	0.0002	0.0001	0.0002	0.0003	0.0000	0.0000	0.0001	0.0000
13. O	0.0564	0.0011	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0003	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0747	0.0227	0.0017	0.0001	0.0004	0.0001
23. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0001	0.0000
24. H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0003	0.0011	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.6815	0.7817	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6722	0.0007	0.0000	0.0004	0.0001
32. O	0.0000	0.0000	0.0000	0.6722	0.0000	0.7739	0.0002	0.0100	0.0273
33. H	0.0000	0.0000	0.0000	0.0007	0.7739	0.0000	0.0000	0.0022	0.0001
34. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.7329	0.0007
35. O	0.0000	0.0000	0.0001	0.0004	0.0100	0.0022	0.7329	0.0000	0.7285
36. H	0.0000	0.0000	0.0000	0.0001	0.0273	0.0001	0.0007	0.7285	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000
38. O	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001	0.0256	0.0098	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000
40. C	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0001	0.0010	0.0001
41. H	0.0000	0.0000	0.0016	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000
42. H	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
43. H	0.0000	0.0000	0.0125	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
44. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0001	0.0003	0.0001	0.0072	0.0001	0.0006	0.0001	0.0000	0.0000
2. C	0.0000	0.0001	0.0000	1.0313	0.0023	0.0029	0.0025	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0028	0.0121	0.0012	0.0020	0.0000	0.0000
4. N	0.0002	0.0006	0.0001	0.0107	0.0020	0.0085	0.0017	0.0000	0.0000
5. H	0.0000	0.0003	0.0000	0.0025	0.0005	0.0003	0.0001	0.0000	0.0000
6. N	0.0000	0.0002	0.0000	0.0012	0.0001	0.0001	0.0001	0.0002	0.0000
7. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0001
9. N	0.0001	0.0004	0.0002	0.0009	0.0002	0.0004	0.0001	0.0001	0.0000
10. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000
12. O	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054	0.0020
13. O	0.0002	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0097	0.0014
14. C	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0085	0.0093
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0303	0.0017

16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0029	0.0013
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0013
18. H	0.0001	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0700	0.0210	0.0008	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
20. H	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
21. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
22. O	0.0004	0.0109	0.0008	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
23. H	0.0001	0.0299	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0024	0.0016	0.0011	0.0125	0.0000	0.0000
31. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0256	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0005	0.0098	0.0011	0.0010	0.0006	0.0001	0.0001	0.0000	0.0000
36. H	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.6679	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.6679	0.0000	0.7762	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0007	0.7762	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0000	0.0000	0.0000	0.0000	0.9369	0.9430	0.9405	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.9369	0.0000	0.0007	0.0005	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.9430	0.0007	0.0000	0.0006	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.9405	0.0005	0.0006	0.0000	0.0000	0.0000
44. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9464
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9464	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9413	0.0005
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9413	0.0005

Atom	46	47
1. C	0.0000	0.0000
2. C	0.0000	0.0000
3. H	0.0000	0.0000
4. N	0.0000	0.0000
5. H	0.0000	0.0000
6. N	0.0000	0.0000
7. H	0.0000	0.0000
8. H	0.0000	0.0000
9. N	0.0000	0.0000
10. H	0.0000	0.0000
11. H	0.0000	0.0000
12. O	0.0007	0.0006
13. O	0.0005	0.0005
14. C	0.0013	0.0014
15. C	0.0021	0.0021
16. H	0.0123	0.0012
17. H	0.0012	0.0123
18. H	0.0000	0.0000
19. O	0.0000	0.0000

20.	H	0.0000	0.0000
21.	H	0.0000	0.0000
22.	O	0.0001	0.0001
23.	H	0.0000	0.0000
24.	H	0.0000	0.0000
25.	O	0.0000	0.0000
26.	H	0.0000	0.0000
27.	O	0.0000	0.0000
28.	H	0.0000	0.0000
29.	H	0.0000	0.0000
30.	H	0.0000	0.0000
31.	H	0.0000	0.0000
32.	O	0.0000	0.0000
33.	H	0.0000	0.0000
34.	H	0.0000	0.0000
35.	O	0.0000	0.0000
36.	H	0.0000	0.0000
37.	H	0.0000	0.0000
38.	O	0.0000	0.0000
39.	H	0.0000	0.0000
40.	C	0.0000	0.0000
41.	H	0.0000	0.0000
42.	H	0.0000	0.0000
43.	H	0.0000	0.0000
44.	C	0.9413	0.9413
45.	H	0.0005	0.0005
46.	H	0.0000	0.0007
47.	H	0.0007	0.0000

Table-9C-4-2: Wiberg index for salt bridge with 7 waters (bridge length=4.0 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0095	0.0031	1.2637	0.0025	1.2685	0.0025	0.0026	1.3270
2. C	0.0095	0.0000	0.9253	0.9591	0.0047	0.0035	0.0013	0.0002	0.0104
3. H	0.0031	0.9253	0.0000	0.0070	0.0053	0.0032	0.0000	0.0000	0.0019
4. N	1.2637	0.9591	0.0070	0.0000	0.7213	0.0744	0.0023	0.0091	0.0876
5. H	0.0025	0.0047	0.0053	0.7213	0.0000	0.0097	0.0001	0.0005	0.0019
6. N	1.2685	0.0035	0.0032	0.0744	0.0097	0.0000	0.7916	0.7668	0.0867
7. H	0.0025	0.0013	0.0000	0.0023	0.0001	0.7916	0.0000	0.0005	0.0106
8. H	0.0026	0.0002	0.0000	0.0091	0.0005	0.7668	0.0005	0.0000	0.0021
9. N	1.3270	0.0104	0.0019	0.0876	0.0019	0.0867	0.0106	0.0021	0.0000
10. H	0.0025	0.0002	0.0000	0.0014	0.0005	0.0099	0.0007	0.0002	0.7831
11. H	0.0027	0.0007	0.0000	0.0091	0.0001	0.0012	0.0001	0.0005	0.7207
12. O	0.0021	0.0003	0.0000	0.0015	0.0000	0.0018	0.0001	0.0009	0.0239
13. O	0.0018	0.0001	0.0000	0.0008	0.0002	0.0120	0.0002	0.0329	0.0022
14. C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0020	0.0000	0.0009	0.0022
15. C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0010	0.0000	0.0025	0.0021
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
18. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0001
19. O	0.0023	0.0004	0.0001	0.0007	0.0002	0.0013	0.0002	0.0001	0.0005
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0001	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
22. O	0.0005	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0016

23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
24. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0009	0.0001	0.0000	0.0001
25. O	0.0007	0.0013	0.0001	0.0005	0.0000	0.0073	0.0164	0.0001	0.0004
26. H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000
27. O	0.0001	0.0001	0.0000	0.0000	0.0000	0.0003	0.0001	0.0002	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0054	0.9216	0.0007	0.0130	0.0009	0.0040	0.0007	0.0000	0.0034
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
32. O	0.0006	0.0000	0.0000	0.0004	0.0002	0.0004	0.0001	0.0000	0.0088
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0010
34. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
35. O	0.0019	0.0008	0.0004	0.0213	0.0556	0.0008	0.0000	0.0002	0.0018
36. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
37. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0003	0.0001	0.0000	0.0005	0.0003	0.0002	0.0000	0.0000	0.0004
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
40. C	0.0071	1.0320	0.0028	0.0105	0.0025	0.0011	0.0002	0.0001	0.0008
41. H	0.0001	0.0023	0.0121	0.0019	0.0005	0.0001	0.0000	0.0000	0.0002
42. H	0.0005	0.0030	0.0012	0.0085	0.0003	0.0001	0.0000	0.0000	0.0003
43. H	0.0001	0.0025	0.0019	0.0018	0.0001	0.0001	0.0001	0.0000	0.0001
44. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0001
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0025	0.0027	0.0021	0.0018	0.0003	0.0003	0.0000	0.0000	0.0001
2. C	0.0002	0.0007	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0014	0.0091	0.0015	0.0008	0.0002	0.0002	0.0000	0.0000	0.0000
5. H	0.0005	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0099	0.0012	0.0018	0.0120	0.0020	0.0010	0.0001	0.0001	0.0003
7. H	0.0007	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0002	0.0005	0.0009	0.0329	0.0009	0.0025	0.0000	0.0001	0.0000
9. N	0.7831	0.7207	0.0239	0.0022	0.0022	0.0021	0.0002	0.0000	0.0001
10. H	0.0000	0.0010	0.0003	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
11. H	0.0010	0.0000	0.0691	0.0020	0.0016	0.0057	0.0001	0.0000	0.0000
12. O	0.0003	0.0691	0.0000	0.1704	1.4755	0.0384	0.0124	0.0125	0.0001
13. O	0.0001	0.0020	0.1704	0.0000	1.3310	0.0377	0.0049	0.0053	0.0004
14. C	0.0001	0.0016	1.4755	1.3310	0.0000	0.9757	0.0060	0.0062	0.0001
15. C	0.0000	0.0057	0.0384	0.0377	0.9757	0.0000	0.9151	0.9151	0.0000
16. H	0.0000	0.0001	0.0124	0.0049	0.0060	0.9151	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0125	0.0053	0.0062	0.9151	0.0011	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0023	0.0124	0.0037	0.0008	0.0001	0.0002	0.7333
20. H	0.0000	0.0000	0.0015	0.0430	0.0011	0.0022	0.0001	0.0001	0.0006
21. H	0.0000	0.0001	0.0249	0.0016	0.0005	0.0005	0.0000	0.0000	0.0000
22. O	0.0002	0.0004	0.0090	0.0018	0.0039	0.0003	0.0001	0.0002	0.0000
23. H	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
25. O	0.0001	0.0000	0.0001	0.0008	0.0001	0.0001	0.0000	0.0000	0.0199
26. H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001

27. O	0.0000	0.0000	0.0018	0.0203	0.0024	0.0004	0.0001	0.0001	0.0001
28. H	0.0000	0.0000	0.0033	0.0601	0.0004	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0002	0.0011	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0198	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0015	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0000	0.0000	0.0003	0.0003	0.0001	0.0000	0.0000	0.0000	0.0014
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. C	0.0000	0.0000	0.0054	0.0097	0.0086	1.0300	0.0028	0.0028	0.0000
45. H	0.0000	0.0000	0.0020	0.0014	0.0093	0.0017	0.0014	0.0013	0.0000
46. H	0.0000	0.0000	0.0007	0.0005	0.0013	0.0021	0.0123	0.0013	0.0000
47. H	0.0000	0.0000	0.0006	0.0005	0.0014	0.0021	0.0012	0.0123	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0023	0.0001	0.0000	0.0005	0.0000	0.0001	0.0007	0.0000	0.0001
2. C	0.0004	0.0000	0.0000	0.0000	0.0000	0.0001	0.0013	0.0001	0.0001
3. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
4. N	0.0007	0.0001	0.0000	0.0001	0.0000	0.0001	0.0005	0.0001	0.0000
5. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0013	0.0004	0.0000	0.0001	0.0000	0.0009	0.0073	0.0003	0.0003
7. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0164	0.0000	0.0001
8. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
9. N	0.0005	0.0001	0.0002	0.0016	0.0002	0.0001	0.0004	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0001	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0023	0.0015	0.0249	0.0090	0.0004	0.0000	0.0001	0.0001	0.0018
13. O	0.0124	0.0430	0.0016	0.0018	0.0001	0.0002	0.0008	0.0002	0.0203
14. C	0.0037	0.0011	0.0005	0.0039	0.0001	0.0000	0.0001	0.0000	0.0024
15. C	0.0008	0.0022	0.0005	0.0003	0.0000	0.0000	0.0001	0.0000	0.0004
16. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0002	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
18. H	0.7333	0.0006	0.0000	0.0000	0.0000	0.0001	0.0199	0.0001	0.0001
19. O	0.0000	0.7026	0.0000	0.0002	0.0001	0.0014	0.0074	0.0004	0.0008
20. H	0.7026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002
21. H	0.0000	0.0000	0.0000	0.7212	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0002	0.0000	0.7212	0.0000	0.7266	0.0000	0.0000	0.0000	0.0000
23. H	0.0001	0.0000	0.0006	0.7266	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.7777	0.0007	0.0008
25. O	0.0074	0.0002	0.0000	0.0000	0.0000	0.7777	0.0000	0.6818	0.0188
26. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0007	0.6818	0.0000	0.0620
27. O	0.0008	0.0002	0.0000	0.0000	0.0000	0.0008	0.0188	0.0620	0.0000
28. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.6758
29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0001	0.7822
30. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0011	0.0001	0.0001

31. H	0.0000	0.0000	0.0001	0.0769	0.0001	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0006	0.0232	0.0003	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0002	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0699	0.0001	0.0000	0.0004	0.0001	0.0000	0.0001	0.0000	0.0000
38. O	0.0211	0.0006	0.0003	0.0108	0.0295	0.0000	0.0001	0.0000	0.0000
39. H	0.0008	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
44. C	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
45. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0000	0.0054	0.0000	0.0006	0.0001	0.0001	0.0019	0.0001
2. C	0.0000	0.0000	0.9216	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
3. H	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
4. N	0.0000	0.0000	0.0130	0.0000	0.0004	0.0000	0.0003	0.0213	0.0003
5. H	0.0000	0.0000	0.0009	0.0000	0.0002	0.0000	0.0001	0.0556	0.0001
6. N	0.0001	0.0000	0.0040	0.0000	0.0004	0.0001	0.0001	0.0008	0.0001
7. H	0.0000	0.0000	0.0007	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
9. N	0.0000	0.0000	0.0034	0.0002	0.0088	0.0010	0.0001	0.0018	0.0001
10. H	0.0000	0.0000	0.0000	0.0001	0.0198	0.0001	0.0000	0.0015	0.0001
11. H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000
12. O	0.0033	0.0002	0.0001	0.0002	0.0003	0.0000	0.0000	0.0001	0.0000
13. O	0.0601	0.0011	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0004	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0769	0.0232	0.0018	0.0001	0.0003	0.0001
23. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0001	0.0000
24. H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0003	0.0011	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.6758	0.7822	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6693	0.0007	0.0000	0.0004	0.0001
32. O	0.0000	0.0000	0.0000	0.6693	0.0000	0.7735	0.0002	0.0098	0.0270
33. H	0.0000	0.0000	0.0000	0.0007	0.7735	0.0000	0.0000	0.0021	0.0001
34. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.7311	0.0007

35. O	0.0000	0.0000	0.0001	0.0004	0.0098	0.0021	0.7311	0.0000	0.7289
36. H	0.0000	0.0000	0.0000	0.0001	0.0270	0.0001	0.0007	0.7289	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000
38. O	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001	0.0261	0.0100	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000
40. C	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0001	0.0010	0.0001
41. H	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
42. H	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
43. H	0.0000	0.0000	0.0125	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
44. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0001	0.0003	0.0000	0.0071	0.0001	0.0005	0.0001	0.0000	0.0000
2. C	0.0000	0.0001	0.0000	1.0320	0.0023	0.0030	0.0025	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0028	0.0121	0.0012	0.0019	0.0000	0.0000
4. N	0.0001	0.0005	0.0000	0.0105	0.0019	0.0085	0.0018	0.0000	0.0000
5. H	0.0000	0.0003	0.0000	0.0025	0.0005	0.0003	0.0001	0.0000	0.0000
6. N	0.0000	0.0002	0.0000	0.0011	0.0001	0.0001	0.0001	0.0002	0.0000
7. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0001
9. N	0.0001	0.0004	0.0002	0.0008	0.0002	0.0003	0.0001	0.0001	0.0000
10. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000
12. O	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054	0.0020
13. O	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0097	0.0014
14. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086	0.0093
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0300	0.0017
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0014
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0013
18. H	0.0001	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0699	0.0211	0.0008	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
20. H	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
21. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0004	0.0108	0.0009	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
23. H	0.0001	0.0295	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0024	0.0017	0.0010	0.0125	0.0000	0.0000
31. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0261	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0006	0.0100	0.0011	0.0010	0.0005	0.0001	0.0001	0.0000	0.0000
36. H	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.6678	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.6678	0.0000	0.7761	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

39. H	0.0007	0.7761	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0000	0.0000	0.0000	0.0000	0.9369	0.9425	0.9402	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.9369	0.0000	0.0007	0.0005	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.9425	0.0007	0.0000	0.0007	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.9402	0.0005	0.0007	0.0000	0.0000	0.0000
44. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9466
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9466	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9413	0.0005
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9412	0.0005

Atom	46	47
1. C	0.0000	0.0000
2. C	0.0000	0.0000
3. H	0.0000	0.0000
4. N	0.0000	0.0000
5. H	0.0000	0.0000
6. N	0.0000	0.0000
7. H	0.0000	0.0000
8. H	0.0000	0.0000
9. N	0.0000	0.0000
10. H	0.0000	0.0000
11. H	0.0000	0.0000
12. O	0.0007	0.0006
13. O	0.0005	0.0005
14. C	0.0013	0.0014
15. C	0.0021	0.0021
16. H	0.0123	0.0012
17. H	0.0013	0.0123
18. H	0.0000	0.0000
19. O	0.0000	0.0000
20. H	0.0000	0.0000
21. H	0.0000	0.0000
22. O	0.0001	0.0001
23. H	0.0000	0.0000
24. H	0.0000	0.0000
25. O	0.0000	0.0000
26. H	0.0000	0.0000
27. O	0.0000	0.0000
28. H	0.0000	0.0000
29. H	0.0000	0.0000
30. H	0.0000	0.0000
31. H	0.0000	0.0000
32. O	0.0000	0.0000
33. H	0.0000	0.0000
34. H	0.0000	0.0000
35. O	0.0000	0.0000
36. H	0.0000	0.0000
37. H	0.0000	0.0000
38. O	0.0000	0.0000
39. H	0.0000	0.0000
40. C	0.0000	0.0000
41. H	0.0000	0.0000
42. H	0.0000	0.0000

43.	H	0.0000	0.0000
44.	C	0.9413	0.9412
45.	H	0.0005	0.0005
46.	H	0.0000	0.0007
47.	H	0.0007	0.0000

Table-9C-4-3: Wiberg index for salt bridge with 7 waters (bridge length=4.2 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0096	0.0031	1.2697	0.0026	1.2693	0.0024	0.0024	1.3216
2. C	0.0096	0.0000	0.9255	0.9571	0.0047	0.0035	0.0012	0.0002	0.0104
3. H	0.0031	0.9255	0.0000	0.0066	0.0054	0.0031	0.0000	0.0000	0.0018
4. N	1.2697	0.9571	0.0066	0.0000	0.7190	0.0752	0.0023	0.0090	0.0872
5. H	0.0026	0.0047	0.0054	0.7190	0.0000	0.0099	0.0001	0.0005	0.0020
6. N	1.2693	0.0035	0.0031	0.0752	0.0099	0.0000	0.7889	0.7790	0.0856
7. H	0.0024	0.0012	0.0000	0.0023	0.0001	0.7889	0.0000	0.0004	0.0104
8. H	0.0024	0.0002	0.0000	0.0090	0.0005	0.7790	0.0004	0.0000	0.0022
9. N	1.3216	0.0104	0.0018	0.0872	0.0020	0.0856	0.0104	0.0022	0.0000
10. H	0.0024	0.0002	0.0000	0.0013	0.0005	0.0097	0.0007	0.0002	0.7798
11. H	0.0026	0.0008	0.0000	0.0094	0.0001	0.0013	0.0001	0.0005	0.7405
12. O	0.0014	0.0002	0.0000	0.0010	0.0000	0.0013	0.0000	0.0008	0.0166
13. O	0.0014	0.0001	0.0000	0.0007	0.0001	0.0081	0.0002	0.0215	0.0019
14. C	0.0002	0.0000	0.0000	0.0001	0.0000	0.0013	0.0000	0.0008	0.0014
15. C	0.0002	0.0000	0.0000	0.0002	0.0000	0.0008	0.0000	0.0021	0.0017
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
18. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001
19. O	0.0020	0.0003	0.0001	0.0006	0.0001	0.0013	0.0002	0.0001	0.0005
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0001	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
22. O	0.0005	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0015
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
24. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0009	0.0001	0.0000	0.0001
25. O	0.0008	0.0011	0.0001	0.0005	0.0000	0.0074	0.0164	0.0001	0.0004
26. H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000
27. O	0.0001	0.0001	0.0000	0.0000	0.0000	0.0003	0.0001	0.0002	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0054	0.9220	0.0007	0.0128	0.0008	0.0040	0.0006	0.0000	0.0033
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
32. O	0.0006	0.0000	0.0000	0.0003	0.0002	0.0004	0.0001	0.0000	0.0089
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0010
34. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
35. O	0.0019	0.0009	0.0004	0.0211	0.0557	0.0008	0.0000	0.0002	0.0020
36. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
37. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0003	0.0001	0.0000	0.0004	0.0003	0.0002	0.0000	0.0000	0.0005
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
40. C	0.0071	1.0324	0.0029	0.0106	0.0025	0.0011	0.0001	0.0001	0.0008
41. H	0.0001	0.0023	0.0121	0.0019	0.0005	0.0001	0.0000	0.0000	0.0001
42. H	0.0005	0.0031	0.0013	0.0086	0.0002	0.0001	0.0000	0.0000	0.0003
43. H	0.0001	0.0025	0.0019	0.0018	0.0001	0.0001	0.0001	0.0000	0.0001
44. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0001
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000

46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Atom	10	11	12	13	14	15	16	17	18
1. C	0.0024	0.0026	0.0014	0.0014	0.0002	0.0002	0.0000	0.0000	0.0001
2. C	0.0002	0.0008	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0013	0.0094	0.0010	0.0007	0.0001	0.0002	0.0000	0.0000	0.0000
5. H	0.0005	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0097	0.0013	0.0013	0.0081	0.0013	0.0008	0.0000	0.0001	0.0002
7. H	0.0007	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0002	0.0005	0.0008	0.0215	0.0008	0.0021	0.0000	0.0000	0.0000
9. N	0.7798	0.7405	0.0166	0.0019	0.0014	0.0017	0.0001	0.0000	0.0001
10. H	0.0000	0.0009	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0009	0.0000	0.0476	0.0022	0.0015	0.0052	0.0001	0.0000	0.0000
12. O	0.0002	0.0476	0.0000	0.1729	1.4830	0.0398	0.0126	0.0126	0.0001
13. O	0.0001	0.0022	0.1729	0.0000	1.3310	0.0378	0.0049	0.0054	0.0004
14. C	0.0000	0.0015	1.4830	1.3310	0.0000	0.9755	0.0059	0.0062	0.0001
15. C	0.0000	0.0052	0.0398	0.0378	0.9755	0.0000	0.9151	0.9152	0.0000
16. H	0.0000	0.0001	0.0126	0.0049	0.0059	0.9151	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0126	0.0054	0.0062	0.9152	0.0011	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0002	0.0021	0.0118	0.0033	0.0008	0.0001	0.0001	0.7333
20. H	0.0000	0.0000	0.0015	0.0410	0.0011	0.0023	0.0001	0.0001	0.0006
21. H	0.0000	0.0001	0.0248	0.0016	0.0005	0.0006	0.0000	0.0000	0.0000
22. O	0.0002	0.0007	0.0086	0.0018	0.0037	0.0003	0.0001	0.0002	0.0000
23. H	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
25. O	0.0001	0.0000	0.0001	0.0008	0.0001	0.0001	0.0000	0.0000	0.0198
26. H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
27. O	0.0000	0.0000	0.0020	0.0212	0.0026	0.0004	0.0001	0.0001	0.0001
28. H	0.0000	0.0000	0.0035	0.0642	0.0004	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0002	0.0011	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0206	0.0002	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0016	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0000	0.0000	0.0003	0.0003	0.0001	0.0000	0.0000	0.0000	0.0014
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. C	0.0000	0.0000	0.0054	0.0099	0.0086	1.0300	0.0028	0.0028	0.0000
45. H	0.0000	0.0000	0.0020	0.0014	0.0093	0.0017	0.0014	0.0013	0.0000
46. H	0.0000	0.0000	0.0007	0.0005	0.0013	0.0022	0.0124	0.0013	0.0000
47. H	0.0000	0.0000	0.0006	0.0005	0.0014	0.0022	0.0012	0.0124	0.0000
Atom	19	20	21	22	23	24	25	26	27

1. C	0.0020	0.0001	0.0000	0.0005	0.0000	0.0001	0.0008	0.0000	0.0001
2. C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0001	0.0011	0.0001	0.0001
3. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
4. N	0.0006	0.0001	0.0000	0.0001	0.0000	0.0001	0.0005	0.0001	0.0000
5. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0013	0.0003	0.0000	0.0001	0.0000	0.0009	0.0074	0.0003	0.0003
7. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0164	0.0000	0.0001
8. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
9. N	0.0005	0.0001	0.0002	0.0015	0.0002	0.0001	0.0004	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0002	0.0000	0.0001	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0021	0.0015	0.0248	0.0086	0.0004	0.0000	0.0001	0.0001	0.0020
13. O	0.0118	0.0410	0.0016	0.0018	0.0001	0.0002	0.0008	0.0002	0.0212
14. C	0.0033	0.0011	0.0005	0.0037	0.0001	0.0000	0.0001	0.0000	0.0026
15. C	0.0008	0.0023	0.0006	0.0003	0.0000	0.0000	0.0001	0.0000	0.0004
16. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
18. H	0.7333	0.0006	0.0000	0.0000	0.0000	0.0001	0.0198	0.0001	0.0001
19. O	0.0000	0.7020	0.0000	0.0002	0.0001	0.0014	0.0074	0.0004	0.0008
20. H	0.7020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0003
21. H	0.0000	0.0000	0.0000	0.7181	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0002	0.0000	0.7181	0.0000	0.7275	0.0000	0.0000	0.0000	0.0000
23. H	0.0001	0.0000	0.0006	0.7275	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.7780	0.0007	0.0008
25. O	0.0074	0.0002	0.0000	0.0000	0.0000	0.7780	0.0000	0.6793	0.0192
26. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0007	0.6793	0.0000	0.0636
27. O	0.0008	0.0003	0.0000	0.0000	0.0000	0.0008	0.0192	0.0636	0.0000
28. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.6694
29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0001	0.7824
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0001	0.0001
31. H	0.0000	0.0000	0.0001	0.0786	0.0001	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0006	0.0236	0.0003	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0002	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0697	0.0001	0.0000	0.0004	0.0001	0.0000	0.0001	0.0000	0.0000
38. O	0.0210	0.0007	0.0003	0.0106	0.0288	0.0000	0.0001	0.0000	0.0001
39. H	0.0009	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
44. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
45. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0000	0.0054	0.0000	0.0006	0.0001	0.0001	0.0019	0.0001
2. C	0.0000	0.0000	0.9220	0.0000	0.0000	0.0000	0.0000	0.0009	0.0000
3. H	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
4. N	0.0000	0.0000	0.0128	0.0000	0.0003	0.0000	0.0003	0.0211	0.0003

5. H	0.0000	0.0000	0.0008	0.0000	0.0002	0.0000	0.0001	0.0557	0.0001
6. N	0.0001	0.0000	0.0040	0.0000	0.0004	0.0001	0.0001	0.0008	0.0001
7. H	0.0000	0.0000	0.0006	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
9. N	0.0000	0.0000	0.0033	0.0002	0.0089	0.0010	0.0001	0.0020	0.0001
10. H	0.0000	0.0000	0.0000	0.0001	0.0206	0.0001	0.0000	0.0016	0.0001
11. H	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0002	0.0000
12. O	0.0035	0.0002	0.0000	0.0002	0.0003	0.0000	0.0000	0.0001	0.0000
13. O	0.0642	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0004	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0786	0.0236	0.0018	0.0001	0.0003	0.0001
23. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0001	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0004	0.0011	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.6694	0.7824	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6666	0.0007	0.0000	0.0004	0.0001
32. O	0.0000	0.0000	0.0000	0.6666	0.0000	0.7731	0.0002	0.0099	0.0273
33. H	0.0000	0.0000	0.0000	0.0007	0.7731	0.0000	0.0000	0.0021	0.0001
34. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.7299	0.0006
35. O	0.0000	0.0000	0.0001	0.0004	0.0099	0.0021	0.7299	0.0000	0.7282
36. H	0.0000	0.0000	0.0000	0.0001	0.0273	0.0001	0.0006	0.7282	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000
38. O	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001	0.0263	0.0100	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000
40. C	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0001	0.0009	0.0001
41. H	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
42. H	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
43. H	0.0000	0.0000	0.0125	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
44. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0001	0.0003	0.0000	0.0071	0.0001	0.0005	0.0001	0.0000	0.0000
2. C	0.0000	0.0001	0.0000	1.0324	0.0023	0.0031	0.0025	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0029	0.0121	0.0013	0.0019	0.0000	0.0000
4. N	0.0001	0.0004	0.0000	0.0106	0.0019	0.0086	0.0018	0.0000	0.0000
5. H	0.0000	0.0003	0.0000	0.0025	0.0005	0.0002	0.0001	0.0000	0.0000
6. N	0.0000	0.0002	0.0000	0.0011	0.0001	0.0001	0.0001	0.0001	0.0000
7. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0001

9. N	0.0001	0.0005	0.0002	0.0008	0.0001	0.0003	0.0001	0.0001	0.0000
10. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000
12. O	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054	0.0020
13. O	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0099	0.0014
14. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086	0.0093
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0300	0.0017
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0014
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0013
18. H	0.0001	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0697	0.0210	0.0009	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
20. H	0.0001	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001
21. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0004	0.0106	0.0009	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
23. H	0.0001	0.0288	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0024	0.0018	0.0010	0.0125	0.0000	0.0000
31. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0263	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0006	0.0100	0.0011	0.0009	0.0005	0.0001	0.0001	0.0000	0.0000
36. H	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.6676	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.6676	0.0000	0.7762	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0007	0.7762	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. C	0.0000	0.0000	0.0000	0.0000	0.9371	0.9420	0.9400	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.9371	0.0000	0.0007	0.0005	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.9420	0.0007	0.0000	0.0007	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.9400	0.0005	0.0007	0.0000	0.0000	0.0000
44. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9471
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9471	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9414	0.0005
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9413	0.0005

Atom	46	47
1. C	0.0000	0.0000
2. C	0.0000	0.0000
3. H	0.0000	0.0000
4. N	0.0000	0.0000
5. H	0.0000	0.0000
6. N	0.0000	0.0000
7. H	0.0000	0.0000
8. H	0.0000	0.0000
9. N	0.0000	0.0000
10. H	0.0000	0.0000
11. H	0.0000	0.0000
12. O	0.0007	0.0006

13.	O	0.0005	0.0005
14.	C	0.0013	0.0014
15.	C	0.0022	0.0022
16.	H	0.0124	0.0012
17.	H	0.0013	0.0124
18.	H	0.0000	0.0000
19.	O	0.0000	0.0000
20.	H	0.0000	0.0000
21.	H	0.0000	0.0000
22.	O	0.0001	0.0001
23.	H	0.0000	0.0000
24.	H	0.0000	0.0000
25.	O	0.0000	0.0000
26.	H	0.0000	0.0000
27.	O	0.0000	0.0000
28.	H	0.0000	0.0000
29.	H	0.0000	0.0000
30.	H	0.0000	0.0000
31.	H	0.0000	0.0000
32.	O	0.0000	0.0000
33.	H	0.0000	0.0000
34.	H	0.0000	0.0000
35.	O	0.0000	0.0000
36.	H	0.0000	0.0000
37.	H	0.0000	0.0000
38.	O	0.0000	0.0000
39.	H	0.0000	0.0000
40.	C	0.0000	0.0000
41.	H	0.0000	0.0000
42.	H	0.0000	0.0000
43.	H	0.0000	0.0000
44.	C	0.9414	0.9413
45.	H	0.0005	0.0005
46.	H	0.0000	0.0007
47.	H	0.0007	0.0000

Table-9C-5-1: Wiberg index for salt bridge with 8 waters (bridge length=3.8 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0095	0.0032	1.2580	0.0023	1.2684	0.0024	0.0028	1.3318
2. C	0.0095	0.0000	0.9273	0.9591	0.0046	0.0034	0.0016	0.0002	0.0100
3. H	0.0032	0.9273	0.0000	0.0078	0.0052	0.0035	0.0001	0.0000	0.0019
4. N	1.2580	0.9591	0.0078	0.0000	0.7283	0.0740	0.0022	0.0089	0.0872
5. H	0.0023	0.0046	0.0052	0.7283	0.0000	0.0094	0.0002	0.0004	0.0018
6. N	1.2684	0.0034	0.0035	0.0740	0.0094	0.0000	0.8044	0.7488	0.0879
7. H	0.0024	0.0016	0.0001	0.0022	0.0002	0.8044	0.0000	0.0007	0.0099
8. H	0.0028	0.0002	0.0000	0.0089	0.0004	0.7488	0.0007	0.0000	0.0019
9. N	1.3318	0.0100	0.0019	0.0872	0.0018	0.0879	0.0099	0.0019	0.0000
10. H	0.0026	0.0003	0.0000	0.0016	0.0006	0.0097	0.0007	0.0001	0.7848
11. H	0.0029	0.0007	0.0000	0.0088	0.0001	0.0012	0.0001	0.0004	0.7062
12. O	0.0025	0.0003	0.0000	0.0018	0.0000	0.0024	0.0001	0.0010	0.0299
13. O	0.0023	0.0002	0.0001	0.0010	0.0002	0.0176	0.0003	0.0498	0.0024
14. C	0.0004	0.0000	0.0000	0.0003	0.0000	0.0031	0.0001	0.0010	0.0028
15. C	0.0005	0.0000	0.0000	0.0002	0.0000	0.0012	0.0000	0.0029	0.0025

16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0002
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0001
18. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001
19. O	0.0020	0.0003	0.0000	0.0007	0.0002	0.0009	0.0001	0.0000	0.0004
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
22. O	0.0004	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0014
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0001
25. O	0.0006	0.0004	0.0001	0.0003	0.0000	0.0053	0.0097	0.0001	0.0003
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
27. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0002	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0051	0.9126	0.0006	0.0120	0.0010	0.0039	0.0005	0.0000	0.0033
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
32. O	0.0007	0.0000	0.0000	0.0003	0.0002	0.0004	0.0001	0.0000	0.0083
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0009
34. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
35. O	0.0017	0.0008	0.0004	0.0199	0.0508	0.0007	0.0000	0.0001	0.0022
36. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
37. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0003	0.0000	0.0000	0.0004	0.0003	0.0002	0.0000	0.0000	0.0005
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
40. H	0.0000	0.0002	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
41. O	0.0002	0.0029	0.0001	0.0003	0.0000	0.0006	0.0003	0.0000	0.0002
42. H	0.0000	0.0004	0.0000	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000
43. C	0.0072	1.0314	0.0028	0.0102	0.0026	0.0012	0.0002	0.0001	0.0008
44. H	0.0001	0.0023	0.0123	0.0019	0.0005	0.0001	0.0000	0.0000	0.0002
45. H	0.0005	0.0030	0.0013	0.0085	0.0003	0.0001	0.0000	0.0000	0.0003
46. H	0.0001	0.0027	0.0019	0.0019	0.0001	0.0001	0.0000	0.0000	0.0002
47. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0001
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0026	0.0029	0.0025	0.0023	0.0004	0.0005	0.0000	0.0000	0.0001
2. C	0.0003	0.0007	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
3. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0016	0.0088	0.0018	0.0010	0.0003	0.0002	0.0000	0.0000	0.0000
5. H	0.0006	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0097	0.0012	0.0024	0.0176	0.0031	0.0012	0.0001	0.0001	0.0002
7. H	0.0007	0.0001	0.0001	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0001	0.0004	0.0010	0.0498	0.0010	0.0029	0.0001	0.0001	0.0000
9. N	0.7848	0.7062	0.0299	0.0024	0.0028	0.0025	0.0002	0.0001	0.0001
10. H	0.0000	0.0012	0.0004	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
11. H	0.0012	0.0000	0.0876	0.0015	0.0016	0.0059	0.0001	0.0000	0.0000
12. O	0.0004	0.0876	0.0000	0.1681	1.4796	0.0383	0.0123	0.0123	0.0001
13. O	0.0001	0.0015	0.1681	0.0000	1.3238	0.0378	0.0054	0.0045	0.0005
14. C	0.0001	0.0016	1.4796	1.3238	0.0000	0.9740	0.0063	0.0058	0.0001
15. C	0.0001	0.0059	0.0383	0.0378	0.9740	0.0000	0.9137	0.9174	0.0000
16. H	0.0000	0.0001	0.0123	0.0054	0.0063	0.9137	0.0000	0.0011	0.0000

17. H	0.0000	0.0000	0.0123	0.0045	0.0058	0.9174	0.0011	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0023	0.0117	0.0036	0.0007	0.0001	0.0001	0.7115
20. H	0.0000	0.0000	0.0016	0.0368	0.0009	0.0017	0.0001	0.0001	0.0006
21. H	0.0000	0.0001	0.0217	0.0016	0.0004	0.0003	0.0000	0.0000	0.0000
22. O	0.0002	0.0003	0.0083	0.0018	0.0038	0.0002	0.0001	0.0002	0.0000
23. H	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0001	0.0000	0.0001	0.0008	0.0001	0.0001	0.0000	0.0000	0.0001
26. H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0000	0.0019	0.0222	0.0025	0.0008	0.0002	0.0001	0.0001
28. H	0.0000	0.0000	0.0035	0.0685	0.0004	0.0002	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0002	0.0011	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0185	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0025	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0001
38. O	0.0000	0.0000	0.0004	0.0003	0.0002	0.0000	0.0000	0.0000	0.0009
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
41. O	0.0000	0.0000	0.0001	0.0002	0.0001	0.0000	0.0000	0.0000	0.0377
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
43. C	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. C	0.0000	0.0000	0.0054	0.0097	0.0085	1.0302	0.0029	0.0028	0.0000
48. H	0.0000	0.0000	0.0020	0.0013	0.0093	0.0017	0.0014	0.0012	0.0000
49. H	0.0000	0.0000	0.0006	0.0005	0.0013	0.0021	0.0122	0.0013	0.0000
50. H	0.0000	0.0000	0.0007	0.0005	0.0014	0.0021	0.0012	0.0123	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0020	0.0001	0.0000	0.0004	0.0000	0.0000	0.0006	0.0000	0.0001
2. C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
4. N	0.0007	0.0001	0.0000	0.0001	0.0000	0.0000	0.0003	0.0000	0.0000
5. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0009	0.0003	0.0000	0.0001	0.0000	0.0004	0.0053	0.0002	0.0002
7. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0097	0.0000	0.0001
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
9. N	0.0004	0.0001	0.0002	0.0014	0.0002	0.0001	0.0003	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0001	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0023	0.0016	0.0217	0.0083	0.0004	0.0000	0.0001	0.0001	0.0019
13. O	0.0117	0.0368	0.0016	0.0018	0.0001	0.0001	0.0008	0.0003	0.0222
14. C	0.0036	0.0009	0.0004	0.0038	0.0001	0.0000	0.0001	0.0000	0.0025
15. C	0.0007	0.0017	0.0003	0.0002	0.0000	0.0000	0.0001	0.0000	0.0008
16. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
17. H	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001

18. H	0.7115	0.0006	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
19. O	0.0000	0.7113	0.0000	0.0002	0.0001	0.0000	0.0002	0.0000	0.0005
20. H	0.7113	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
21. H	0.0000	0.0000	0.0000	0.7284	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0002	0.0000	0.7284	0.0000	0.7218	0.0000	0.0000	0.0000	0.0000
23. H	0.0001	0.0000	0.0006	0.7218	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7736	0.0007	0.0011
25. O	0.0002	0.0000	0.0000	0.0000	0.0000	0.7736	0.0000	0.6679	0.0221
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.6679	0.0000	0.0732
27. O	0.0005	0.0002	0.0000	0.0000	0.0000	0.0011	0.0221	0.0732	0.0000
28. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.6687
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0001	0.7811
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
31. H	0.0000	0.0000	0.0001	0.0758	0.0001	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0006	0.0229	0.0003	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0002	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0815	0.0001	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
38. O	0.0242	0.0007	0.0003	0.0119	0.0333	0.0000	0.0000	0.0000	0.0000
39. H	0.0009	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0001	0.0460	0.0000	0.0002
41. O	0.0132	0.0003	0.0000	0.0000	0.0000	0.0015	0.0155	0.0004	0.0003
42. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000
43. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. C	0.0001	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0000	0.0051	0.0000	0.0007	0.0000	0.0001	0.0017	0.0001
2. C	0.0000	0.0000	0.9126	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
3. H	0.0000	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
4. N	0.0000	0.0000	0.0120	0.0000	0.0003	0.0000	0.0003	0.0199	0.0003
5. H	0.0000	0.0000	0.0010	0.0000	0.0002	0.0000	0.0001	0.0508	0.0001
6. N	0.0001	0.0000	0.0039	0.0000	0.0004	0.0001	0.0001	0.0007	0.0001
7. H	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
9. N	0.0000	0.0000	0.0033	0.0002	0.0083	0.0009	0.0001	0.0022	0.0001
10. H	0.0000	0.0000	0.0000	0.0001	0.0185	0.0001	0.0000	0.0025	0.0001
11. H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000
12. O	0.0035	0.0002	0.0001	0.0002	0.0003	0.0000	0.0000	0.0001	0.0000
13. O	0.0685	0.0011	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0004	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

19. O	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0758	0.0229	0.0018	0.0000	0.0003	0.0001
23. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0001	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0004	0.0012	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.6687	0.7811	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6714	0.0007	0.0000	0.0004	0.0001
32. O	0.0000	0.0000	0.0000	0.6714	0.0000	0.7747	0.0002	0.0093	0.0255
33. H	0.0000	0.0000	0.0000	0.0007	0.7747	0.0000	0.0000	0.0022	0.0001
34. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.7309	0.0007
35. O	0.0000	0.0000	0.0001	0.0004	0.0093	0.0022	0.7309	0.0000	0.7314
36. H	0.0000	0.0000	0.0000	0.0001	0.0255	0.0001	0.0007	0.7314	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000
38. O	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001	0.0265	0.0102	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000
40. H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0000	0.0001	0.0046	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. C	0.0000	0.0000	0.0025	0.0000	0.0000	0.0000	0.0001	0.0009	0.0001
44. H	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
45. H	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
46. H	0.0000	0.0000	0.0120	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
47. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0001	0.0003	0.0000	0.0000	0.0002	0.0000	0.0072	0.0001	0.0005
2. C	0.0000	0.0000	0.0000	0.0002	0.0029	0.0004	1.0314	0.0023	0.0030
3. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0028	0.0123	0.0013
4. N	0.0001	0.0004	0.0000	0.0001	0.0003	0.0001	0.0102	0.0019	0.0085
5. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0026	0.0005	0.0003
6. N	0.0000	0.0002	0.0000	0.0002	0.0006	0.0004	0.0012	0.0001	0.0001
7. H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. N	0.0001	0.0005	0.0002	0.0000	0.0002	0.0000	0.0008	0.0002	0.0003
10. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
12. O	0.0001	0.0004	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
13. O	0.0001	0.0003	0.0000	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000
14. C	0.0001	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0001	0.0009	0.0000	0.0001	0.0377	0.0001	0.0000	0.0000	0.0000
19. O	0.0815	0.0242	0.0009	0.0005	0.0132	0.0011	0.0000	0.0000	0.0000

20.	H	0.0001	0.0007	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0004	0.0119	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0001	0.0333	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0001	0.0015	0.0000	0.0000	0.0000	0.0000
25.	O	0.0000	0.0000	0.0000	0.0460	0.0155	0.0007	0.0001	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
27.	O	0.0000	0.0000	0.0000	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0002	0.0046	0.0003	0.0025	0.0017	0.0010
31.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0001	0.0265	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
35.	O	0.0005	0.0102	0.0010	0.0000	0.0000	0.0000	0.0009	0.0005	0.0001
36.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
37.	H	0.0000	0.6584	0.0008	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
38.	O	0.6584	0.0000	0.7772	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
39.	H	0.0008	0.7772	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.7038	0.0007	0.0000	0.0000	0.0000
41.	O	0.0001	0.0002	0.0000	0.7038	0.0000	0.7815	0.0002	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0007	0.7815	0.0000	0.0000	0.0000	0.0000
43.	C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.9370	0.9430
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9370	0.0000	0.0007
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9430	0.0007	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.9415	0.0005	0.0006
47.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50
1. C	0.0001	0.0000	0.0000	0.0000	0.0000
2. C	0.0027	0.0000	0.0000	0.0000	0.0000
3. H	0.0019	0.0000	0.0000	0.0000	0.0000
4. N	0.0019	0.0000	0.0000	0.0000	0.0000
5. H	0.0001	0.0000	0.0000	0.0000	0.0000
6. N	0.0001	0.0002	0.0000	0.0000	0.0000
7. H	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0002	0.0001	0.0000	0.0000
9. N	0.0002	0.0001	0.0000	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0000	0.0054	0.0020	0.0006	0.0007
13. O	0.0000	0.0097	0.0013	0.0005	0.0005
14. C	0.0000	0.0085	0.0093	0.0013	0.0014
15. C	0.0000	1.0302	0.0017	0.0021	0.0021
16. H	0.0000	0.0029	0.0014	0.0122	0.0012
17. H	0.0000	0.0028	0.0012	0.0013	0.0123
18. H	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0000	0.0000	0.0000
20. H	0.0000	0.0001	0.0000	0.0000	0.0000

21.	H	0.0000	0.0001	0.0000	0.0000	0.0000
22.	O	0.0000	0.0002	0.0000	0.0002	0.0001
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000
25.	O	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000
27.	O	0.0000	0.0001	0.0000	0.0000	0.0000
28.	H	0.0000	0.0001	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0120	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000
35.	O	0.0001	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000
38.	O	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000
41.	O	0.0001	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000
43.	C	0.9415	0.0000	0.0000	0.0000	0.0000
44.	H	0.0005	0.0000	0.0000	0.0000	0.0000
45.	H	0.0006	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000
47.	C	0.0000	0.0000	0.9463	0.9420	0.9404
48.	H	0.0000	0.9463	0.0000	0.0005	0.0005
49.	H	0.0000	0.9420	0.0005	0.0000	0.0007
50.	H	0.0000	0.9404	0.0005	0.0007	0.0000

Table-9C-5-2: Wiberg index for salt bridge with 8 waters (bridge length=4.0 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0095	0.0031	1.2645	0.0025	1.2703	0.0023	0.0026	1.3253
2. C	0.0095	0.0000	0.9275	0.9564	0.0046	0.0034	0.0014	0.0002	0.0101
3. H	0.0031	0.9275	0.0000	0.0074	0.0053	0.0032	0.0001	0.0000	0.0019
4. N	1.2645	0.9564	0.0074	0.0000	0.7267	0.0749	0.0020	0.0088	0.0865
5. H	0.0025	0.0046	0.0053	0.7267	0.0000	0.0097	0.0001	0.0004	0.0020
6. N	1.2703	0.0034	0.0032	0.0749	0.0097	0.0000	0.8018	0.7566	0.0869
7. H	0.0023	0.0014	0.0001	0.0020	0.0001	0.8018	0.0000	0.0006	0.0098
8. H	0.0026	0.0002	0.0000	0.0088	0.0004	0.7566	0.0006	0.0000	0.0020
9. N	1.3253	0.0101	0.0019	0.0865	0.0020	0.0869	0.0098	0.0020	0.0000
10. H	0.0025	0.0002	0.0000	0.0013	0.0005	0.0094	0.0008	0.0002	0.7819
11. H	0.0026	0.0008	0.0000	0.0087	0.0001	0.0013	0.0002	0.0005	0.7249
12. O	0.0020	0.0003	0.0000	0.0014	0.0000	0.0019	0.0001	0.0010	0.0230
13. O	0.0020	0.0001	0.0000	0.0010	0.0002	0.0145	0.0003	0.0399	0.0023
14. C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0021	0.0000	0.0010	0.0020
15. C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0011	0.0000	0.0029	0.0021
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
18. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001
19. O	0.0017	0.0003	0.0000	0.0006	0.0001	0.0010	0.0001	0.0001	0.0004
20. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0001	0.0001

21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
22. O	0.0004	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0015
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0001
25. O	0.0007	0.0003	0.0001	0.0002	0.0000	0.0055	0.0102	0.0001	0.0003
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
27. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0002	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0050	0.9137	0.0006	0.0117	0.0009	0.0038	0.0005	0.0000	0.0031
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
32. O	0.0006	0.0000	0.0000	0.0003	0.0002	0.0004	0.0001	0.0000	0.0087
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0009
34. H	0.0001	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0001
35. O	0.0018	0.0008	0.0004	0.0193	0.0498	0.0007	0.0000	0.0001	0.0022
36. H	0.0001	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000	0.0001
37. H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0003	0.0000	0.0000	0.0003	0.0003	0.0002	0.0000	0.0000	0.0005
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
40. H	0.0000	0.0002	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
41. O	0.0002	0.0027	0.0001	0.0003	0.0000	0.0007	0.0003	0.0000	0.0002
42. H	0.0000	0.0004	0.0000	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000
43. C	0.0071	1.0321	0.0029	0.0101	0.0026	0.0010	0.0002	0.0001	0.0007
44. H	0.0001	0.0023	0.0122	0.0018	0.0005	0.0001	0.0000	0.0000	0.0001
45. H	0.0005	0.0030	0.0014	0.0085	0.0003	0.0001	0.0000	0.0000	0.0003
46. H	0.0001	0.0027	0.0018	0.0020	0.0001	0.0001	0.0000	0.0000	0.0002
47. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0001
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0025	0.0026	0.0020	0.0020	0.0003	0.0003	0.0000	0.0000	0.0000
2. C	0.0002	0.0008	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0013	0.0087	0.0014	0.0010	0.0002	0.0002	0.0000	0.0000	0.0000
5. H	0.0005	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0094	0.0013	0.0019	0.0145	0.0021	0.0011	0.0001	0.0001	0.0002
7. H	0.0008	0.0002	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0002	0.0005	0.0010	0.0399	0.0010	0.0029	0.0000	0.0001	0.0000
9. N	0.7819	0.7249	0.0230	0.0023	0.0020	0.0021	0.0002	0.0000	0.0001
10. H	0.0000	0.0010	0.0003	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
11. H	0.0010	0.0000	0.0653	0.0019	0.0015	0.0056	0.0001	0.0000	0.0000
12. O	0.0003	0.0653	0.0000	0.1695	1.4866	0.0391	0.0127	0.0126	0.0001
13. O	0.0001	0.0019	0.1695	0.0000	1.3200	0.0370	0.0054	0.0046	0.0005
14. C	0.0001	0.0015	1.4866	1.3200	0.0000	0.9760	0.0064	0.0059	0.0001
15. C	0.0000	0.0056	0.0391	0.0370	0.9760	0.0000	0.9130	0.9166	0.0000
16. H	0.0000	0.0001	0.0127	0.0054	0.0064	0.9130	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0126	0.0046	0.0059	0.9166	0.0011	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0022	0.0110	0.0033	0.0007	0.0001	0.0001	0.7128
20. H	0.0000	0.0000	0.0015	0.0347	0.0009	0.0017	0.0001	0.0001	0.0006
21. H	0.0000	0.0001	0.0232	0.0016	0.0005	0.0004	0.0000	0.0000	0.0000

22. O	0.0003	0.0003	0.0086	0.0018	0.0038	0.0002	0.0001	0.0002	0.0000
23. H	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0001	0.0000	0.0001	0.0007	0.0001	0.0001	0.0000	0.0000	0.0001
26. H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0000	0.0021	0.0239	0.0027	0.0007	0.0002	0.0001	0.0001
28. H	0.0000	0.0000	0.0038	0.0754	0.0004	0.0002	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0002	0.0011	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0196	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0024	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0001
38. O	0.0000	0.0000	0.0004	0.0003	0.0002	0.0000	0.0000	0.0000	0.0009
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
41. O	0.0000	0.0000	0.0001	0.0002	0.0001	0.0000	0.0000	0.0000	0.0367
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
43. C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. C	0.0000	0.0000	0.0054	0.0097	0.0086	1.0301	0.0029	0.0028	0.0000
48. H	0.0000	0.0000	0.0019	0.0013	0.0093	0.0017	0.0015	0.0012	0.0000
49. H	0.0000	0.0000	0.0006	0.0005	0.0013	0.0021	0.0123	0.0013	0.0000
50. H	0.0000	0.0000	0.0007	0.0005	0.0014	0.0021	0.0012	0.0123	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0017	0.0001	0.0000	0.0004	0.0000	0.0000	0.0007	0.0000	0.0001
2. C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
4. N	0.0006	0.0001	0.0000	0.0001	0.0000	0.0000	0.0002	0.0000	0.0000
5. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0010	0.0003	0.0000	0.0001	0.0000	0.0004	0.0055	0.0002	0.0002
7. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0102	0.0000	0.0001
8. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
9. N	0.0004	0.0001	0.0002	0.0015	0.0002	0.0001	0.0003	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0001	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0022	0.0015	0.0232	0.0086	0.0004	0.0000	0.0001	0.0001	0.0021
13. O	0.0110	0.0347	0.0016	0.0018	0.0001	0.0001	0.0007	0.0003	0.0239
14. C	0.0033	0.0009	0.0005	0.0038	0.0001	0.0000	0.0001	0.0000	0.0027
15. C	0.0007	0.0017	0.0004	0.0002	0.0000	0.0000	0.0001	0.0000	0.0007
16. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
17. H	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
18. H	0.7128	0.0006	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
19. O	0.0000	0.7120	0.0000	0.0002	0.0001	0.0000	0.0002	0.0000	0.0006
20. H	0.7120	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
21. H	0.0000	0.0000	0.0000	0.7238	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0002	0.0000	0.7238	0.0000	0.7231	0.0000	0.0000	0.0000	0.0000

23. H	0.0001	0.0000	0.0006	0.7231	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7736	0.0007	0.0011
25. O	0.0002	0.0000	0.0000	0.0000	0.0000	0.7736	0.0000	0.6637	0.0230
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.6637	0.0000	0.0768
27. O	0.0006	0.0002	0.0000	0.0000	0.0000	0.0011	0.0230	0.0768	0.0000
28. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.6597
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0001	0.7813
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
31. H	0.0000	0.0000	0.0001	0.0781	0.0001	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0006	0.0235	0.0003	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0002	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0793	0.0001	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
38. O	0.0236	0.0008	0.0003	0.0117	0.0323	0.0000	0.0000	0.0000	0.0000
39. H	0.0009	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0001	0.0465	0.0000	0.0002
41. O	0.0130	0.0003	0.0000	0.0000	0.0000	0.0015	0.0157	0.0004	0.0003
42. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000
43. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. C	0.0001	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0000	0.0050	0.0000	0.0006	0.0000	0.0001	0.0018	0.0001
2. C	0.0000	0.0000	0.9137	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
3. H	0.0000	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
4. N	0.0000	0.0000	0.0117	0.0000	0.0003	0.0000	0.0003	0.0193	0.0003
5. H	0.0000	0.0000	0.0009	0.0000	0.0002	0.0000	0.0000	0.0498	0.0001
6. N	0.0001	0.0000	0.0038	0.0000	0.0004	0.0001	0.0001	0.0007	0.0001
7. H	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
9. N	0.0000	0.0000	0.0031	0.0002	0.0087	0.0009	0.0001	0.0022	0.0001
10. H	0.0000	0.0000	0.0000	0.0001	0.0196	0.0001	0.0000	0.0024	0.0001
11. H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000
12. O	0.0038	0.0002	0.0000	0.0002	0.0003	0.0000	0.0000	0.0001	0.0000
13. O	0.0754	0.0011	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0004	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0781	0.0235	0.0018	0.0000	0.0003	0.0001
23. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0001	0.0000

24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0004	0.0012	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.6597	0.7813	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6687	0.0007	0.0000	0.0004	0.0001
32. O	0.0000	0.0000	0.0000	0.6687	0.0000	0.7745	0.0002	0.0092	0.0252
33. H	0.0000	0.0000	0.0000	0.0007	0.7745	0.0000	0.0000	0.0021	0.0001
34. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.7300	0.0007
35. O	0.0000	0.0000	0.0001	0.0004	0.0092	0.0021	0.7300	0.0000	0.7314
36. H	0.0000	0.0000	0.0000	0.0001	0.0252	0.0001	0.0007	0.7314	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000
38. O	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001	0.0266	0.0101	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000
40. H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0000	0.0001	0.0041	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. C	0.0000	0.0000	0.0025	0.0000	0.0000	0.0000	0.0001	0.0008	0.0001
44. H	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
45. H	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
46. H	0.0000	0.0000	0.0121	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
47. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0001	0.0003	0.0000	0.0000	0.0002	0.0000	0.0071	0.0001	0.0005
2. C	0.0000	0.0000	0.0000	0.0002	0.0027	0.0004	1.0321	0.0023	0.0030
3. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0029	0.0122	0.0014
4. N	0.0001	0.0003	0.0000	0.0001	0.0003	0.0001	0.0101	0.0018	0.0085
5. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0026	0.0005	0.0003
6. N	0.0000	0.0002	0.0000	0.0002	0.0007	0.0004	0.0010	0.0001	0.0001
7. H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. N	0.0001	0.0005	0.0003	0.0000	0.0002	0.0000	0.0007	0.0001	0.0003
10. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
12. O	0.0001	0.0004	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
13. O	0.0001	0.0003	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
14. C	0.0001	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0001	0.0009	0.0000	0.0001	0.0367	0.0001	0.0000	0.0000	0.0000
19. O	0.0793	0.0236	0.0009	0.0005	0.0130	0.0011	0.0000	0.0000	0.0000
20. H	0.0001	0.0008	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0004	0.0117	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. H	0.0001	0.0323	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0001	0.0015	0.0000	0.0000	0.0000	0.0000

25. O	0.0000	0.0000	0.0000	0.0465	0.0157	0.0007	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0000	0.0000	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0002	0.0041	0.0002	0.0025	0.0018	0.0009
31. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0266	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
35. O	0.0005	0.0101	0.0010	0.0000	0.0000	0.0000	0.0008	0.0004	0.0001
36. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
37. H	0.0000	0.6599	0.0008	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
38. O	0.6599	0.0000	0.7771	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
39. H	0.0008	0.7771	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.7039	0.0007	0.0000	0.0000	0.0000
41. O	0.0001	0.0002	0.0000	0.7039	0.0000	0.7818	0.0002	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0007	0.7818	0.0000	0.0000	0.0000	0.0000
43. C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.9372	0.9425
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9372	0.0000	0.0007
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9425	0.0007	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.9412	0.0005	0.0007
47. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50
1. C	0.0001	0.0000	0.0000	0.0000	0.0000
2. C	0.0027	0.0000	0.0000	0.0000	0.0000
3. H	0.0018	0.0000	0.0000	0.0000	0.0000
4. N	0.0020	0.0000	0.0000	0.0000	0.0000
5. H	0.0001	0.0000	0.0000	0.0000	0.0000
6. N	0.0001	0.0002	0.0000	0.0000	0.0000
7. H	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0002	0.0001	0.0000	0.0000
9. N	0.0002	0.0001	0.0000	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0000	0.0054	0.0019	0.0006	0.0007
13. O	0.0000	0.0097	0.0013	0.0005	0.0005
14. C	0.0000	0.0086	0.0093	0.0013	0.0014
15. C	0.0000	1.0301	0.0017	0.0021	0.0021
16. H	0.0000	0.0029	0.0015	0.0123	0.0012
17. H	0.0000	0.0028	0.0012	0.0013	0.0123
18. H	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0000	0.0000	0.0000
20. H	0.0000	0.0001	0.0000	0.0000	0.0000
21. H	0.0000	0.0001	0.0000	0.0000	0.0000
22. O	0.0000	0.0002	0.0000	0.0001	0.0001
23. H	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0000	0.0000	0.0000	0.0000	0.0000

26.	H	0.0000	0.0000	0.0000	0.0000	0.0000
27.	O	0.0000	0.0001	0.0000	0.0000	0.0000
28.	H	0.0000	0.0001	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0121	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000
35.	O	0.0001	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000
38.	O	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000
41.	O	0.0001	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000
43.	C	0.9412	0.0000	0.0000	0.0000	0.0000
44.	H	0.0005	0.0000	0.0000	0.0000	0.0000
45.	H	0.0007	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000
47.	C	0.0000	0.0000	0.9466	0.9419	0.9404
48.	H	0.0000	0.9466	0.0000	0.0005	0.0005
49.	H	0.0000	0.9419	0.0005	0.0000	0.0007
50.	H	0.0000	0.9404	0.0005	0.0007	0.0000

Table-9C-5-3: Wiberg index for salt bridge with 8 waters (bridge length=4.2 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0096	0.0031	1.2704	0.0026	1.2719	0.0023	0.0024	1.3191
2. C	0.0096	0.0000	0.9276	0.9545	0.0046	0.0034	0.0013	0.0002	0.0101
3. H	0.0031	0.9276	0.0000	0.0070	0.0053	0.0031	0.0000	0.0000	0.0018
4. N	1.2704	0.9545	0.0070	0.0000	0.7254	0.0760	0.0020	0.0087	0.0858
5. H	0.0026	0.0046	0.0053	0.7254	0.0000	0.0099	0.0001	0.0004	0.0022
6. N	1.2719	0.0034	0.0031	0.0760	0.0099	0.0000	0.7998	0.7690	0.0858
7. H	0.0023	0.0013	0.0000	0.0020	0.0001	0.7998	0.0000	0.0005	0.0095
8. H	0.0024	0.0002	0.0000	0.0087	0.0004	0.7690	0.0005	0.0000	0.0021
9. N	1.3191	0.0101	0.0018	0.0858	0.0022	0.0858	0.0095	0.0021	0.0000
10. H	0.0024	0.0002	0.0000	0.0012	0.0005	0.0092	0.0008	0.0002	0.7789
11. H	0.0026	0.0009	0.0000	0.0091	0.0001	0.0014	0.0002	0.0005	0.7456
12. O	0.0013	0.0002	0.0000	0.0010	0.0000	0.0014	0.0000	0.0009	0.0154
13. O	0.0015	0.0001	0.0000	0.0008	0.0001	0.0101	0.0003	0.0268	0.0019
14. C	0.0002	0.0000	0.0000	0.0001	0.0000	0.0014	0.0000	0.0008	0.0013
15. C	0.0002	0.0000	0.0000	0.0002	0.0000	0.0009	0.0000	0.0024	0.0017
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
19. O	0.0016	0.0003	0.0000	0.0005	0.0001	0.0010	0.0001	0.0001	0.0004
20. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0001	0.0001
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
22. O	0.0004	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0014
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0001
25. O	0.0007	0.0003	0.0001	0.0002	0.0000	0.0054	0.0098	0.0001	0.0003

26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
27. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0050	0.9144	0.0006	0.0116	0.0009	0.0039	0.0005	0.0000	0.0031
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
32. O	0.0007	0.0000	0.0000	0.0003	0.0002	0.0004	0.0001	0.0000	0.0087
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0009
34. H	0.0001	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0001
35. O	0.0019	0.0008	0.0004	0.0189	0.0489	0.0008	0.0000	0.0002	0.0024
36. H	0.0001	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0001
37. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0002	0.0000	0.0000	0.0003	0.0003	0.0002	0.0000	0.0000	0.0005
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
40. H	0.0000	0.0002	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
41. O	0.0002	0.0025	0.0001	0.0003	0.0000	0.0007	0.0003	0.0000	0.0002
42. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000
43. C	0.0070	1.0324	0.0029	0.0101	0.0026	0.0010	0.0002	0.0001	0.0007
44. H	0.0001	0.0023	0.0122	0.0018	0.0005	0.0001	0.0000	0.0000	0.0001
45. H	0.0005	0.0031	0.0014	0.0086	0.0002	0.0001	0.0000	0.0000	0.0003
46. H	0.0001	0.0026	0.0017	0.0020	0.0001	0.0001	0.0000	0.0000	0.0002
47. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002	0.0001
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0024	0.0026	0.0013	0.0015	0.0002	0.0002	0.0000	0.0000	0.0000
2. C	0.0002	0.0009	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4. N	0.0012	0.0091	0.0010	0.0008	0.0001	0.0002	0.0000	0.0000	0.0000
5. H	0.0005	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0092	0.0014	0.0014	0.0101	0.0014	0.0009	0.0000	0.0001	0.0002
7. H	0.0008	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0002	0.0005	0.0009	0.0268	0.0008	0.0024	0.0000	0.0001	0.0000
9. N	0.7789	0.7456	0.0154	0.0019	0.0013	0.0017	0.0001	0.0000	0.0000
10. H	0.0000	0.0009	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0009	0.0000	0.0435	0.0022	0.0015	0.0050	0.0001	0.0000	0.0000
12. O	0.0002	0.0435	0.0000	0.1719	1.4948	0.0404	0.0129	0.0127	0.0001
13. O	0.0001	0.0022	0.1719	0.0000	1.3198	0.0371	0.0054	0.0047	0.0005
14. C	0.0000	0.0015	1.4948	1.3198	0.0000	0.9755	0.0062	0.0058	0.0001
15. C	0.0000	0.0050	0.0404	0.0371	0.9755	0.0000	0.9136	0.9168	0.0000
16. H	0.0000	0.0001	0.0129	0.0054	0.0062	0.9136	0.0000	0.0011	0.0000
17. H	0.0000	0.0000	0.0127	0.0047	0.0058	0.9168	0.0011	0.0000	0.0000
18. H	0.0000	0.0000	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0002	0.0020	0.0103	0.0030	0.0007	0.0001	0.0001	0.7136
20. H	0.0000	0.0000	0.0015	0.0331	0.0009	0.0018	0.0001	0.0001	0.0006
21. H	0.0000	0.0001	0.0234	0.0016	0.0005	0.0005	0.0000	0.0000	0.0000
22. O	0.0002	0.0007	0.0083	0.0017	0.0036	0.0002	0.0001	0.0002	0.0000
23. H	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0001	0.0000	0.0001	0.0007	0.0001	0.0001	0.0000	0.0000	0.0001
26. H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000

27. O	0.0000	0.0000	0.0022	0.0249	0.0029	0.0006	0.0002	0.0001	0.0001
28. H	0.0000	0.0000	0.0040	0.0802	0.0004	0.0002	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0002	0.0011	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0200	0.0002	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0026	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
38. O	0.0000	0.0000	0.0003	0.0003	0.0001	0.0000	0.0000	0.0000	0.0009
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
41. O	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0359
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
43. C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. C	0.0000	0.0000	0.0055	0.0099	0.0086	1.0299	0.0029	0.0028	0.0000
48. H	0.0000	0.0000	0.0020	0.0014	0.0093	0.0017	0.0015	0.0012	0.0000
49. H	0.0000	0.0000	0.0006	0.0005	0.0013	0.0022	0.0123	0.0013	0.0000
50. H	0.0000	0.0000	0.0007	0.0005	0.0014	0.0021	0.0012	0.0124	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0016	0.0000	0.0000	0.0004	0.0000	0.0000	0.0007	0.0000	0.0001
2. C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
3. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
4. N	0.0005	0.0001	0.0000	0.0001	0.0000	0.0000	0.0002	0.0000	0.0000
5. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6. N	0.0010	0.0003	0.0000	0.0001	0.0000	0.0004	0.0054	0.0002	0.0002
7. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0098	0.0000	0.0001
8. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
9. N	0.0004	0.0001	0.0001	0.0014	0.0002	0.0001	0.0003	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0002	0.0000	0.0001	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0020	0.0015	0.0234	0.0083	0.0004	0.0000	0.0001	0.0001	0.0022
13. O	0.0103	0.0331	0.0016	0.0017	0.0001	0.0001	0.0007	0.0003	0.0249
14. C	0.0030	0.0009	0.0005	0.0036	0.0001	0.0000	0.0001	0.0000	0.0029
15. C	0.0007	0.0018	0.0005	0.0002	0.0000	0.0000	0.0001	0.0000	0.0006
16. H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002
17. H	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
18. H	0.7136	0.0006	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
19. O	0.0000	0.7111	0.0000	0.0002	0.0001	0.0000	0.0002	0.0000	0.0006
20. H	0.7111	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
21. H	0.0000	0.0000	0.0000	0.7204	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0002	0.0000	0.7204	0.0000	0.7238	0.0000	0.0000	0.0000	0.0000
23. H	0.0001	0.0000	0.0006	0.7238	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7740	0.0007	0.0011
25. O	0.0002	0.0000	0.0000	0.0000	0.0000	0.7740	0.0000	0.6608	0.0233
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.6608	0.0000	0.0786
27. O	0.0006	0.0002	0.0000	0.0000	0.0000	0.0011	0.0233	0.0786	0.0000

28. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001	0.6527
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0001	0.7815
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
31. H	0.0000	0.0000	0.0001	0.0800	0.0001	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0000	0.0006	0.0239	0.0003	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0002	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0793	0.0001	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
38. O	0.0236	0.0008	0.0003	0.0115	0.0317	0.0000	0.0000	0.0000	0.0000
39. H	0.0010	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0001	0.0467	0.0000	0.0002
41. O	0.0127	0.0003	0.0000	0.0000	0.0000	0.0015	0.0158	0.0004	0.0003
42. H	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000	0.0001
43. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. C	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
48. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0000	0.0050	0.0000	0.0007	0.0000	0.0001	0.0019	0.0001
2. C	0.0000	0.0000	0.9144	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
3. H	0.0000	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
4. N	0.0000	0.0000	0.0116	0.0000	0.0003	0.0000	0.0003	0.0189	0.0004
5. H	0.0000	0.0000	0.0009	0.0000	0.0002	0.0000	0.0000	0.0489	0.0001
6. N	0.0001	0.0000	0.0039	0.0000	0.0004	0.0001	0.0001	0.0008	0.0001
7. H	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
9. N	0.0000	0.0000	0.0031	0.0002	0.0087	0.0009	0.0001	0.0024	0.0001
10. H	0.0000	0.0000	0.0000	0.0001	0.0200	0.0001	0.0000	0.0026	0.0001
11. H	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0002	0.0000
12. O	0.0040	0.0002	0.0000	0.0002	0.0003	0.0000	0.0000	0.0001	0.0000
13. O	0.0802	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14. C	0.0004	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15. C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0000	0.0000	0.0800	0.0239	0.0018	0.0000	0.0003	0.0001
23. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0005	0.0012	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.6527	0.7815	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

29. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.6659	0.0007	0.0000	0.0004	0.0001
32. O	0.0000	0.0000	0.0000	0.6659	0.0000	0.7743	0.0002	0.0093	0.0255
33. H	0.0000	0.0000	0.0000	0.0007	0.7743	0.0000	0.0000	0.0021	0.0001
34. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.7288	0.0006
35. O	0.0000	0.0000	0.0001	0.0004	0.0093	0.0021	0.7288	0.0000	0.7307
36. H	0.0000	0.0000	0.0000	0.0001	0.0255	0.0001	0.0006	0.7307	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000
38. O	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001	0.0267	0.0101	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000
40. H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0000	0.0001	0.0037	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. C	0.0000	0.0000	0.0025	0.0000	0.0000	0.0000	0.0000	0.0008	0.0001
44. H	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
45. H	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
46. H	0.0000	0.0000	0.0120	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
47. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0001	0.0002	0.0000	0.0000	0.0002	0.0000	0.0070	0.0001	0.0005
2. C	0.0000	0.0000	0.0000	0.0002	0.0025	0.0003	1.0324	0.0023	0.0031
3. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0029	0.0122	0.0014
4. N	0.0000	0.0003	0.0000	0.0001	0.0003	0.0000	0.0101	0.0018	0.0086
5. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0026	0.0005	0.0002
6. N	0.0000	0.0002	0.0000	0.0002	0.0007	0.0004	0.0010	0.0001	0.0001
7. H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. N	0.0001	0.0005	0.0002	0.0000	0.0002	0.0000	0.0007	0.0001	0.0003
10. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
12. O	0.0001	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
13. O	0.0001	0.0003	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
14. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0001	0.0009	0.0000	0.0001	0.0359	0.0001	0.0000	0.0000	0.0000
19. O	0.0793	0.0236	0.0010	0.0005	0.0127	0.0010	0.0000	0.0000	0.0000
20. H	0.0001	0.0008	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0004	0.0115	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. H	0.0001	0.0317	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0001	0.0015	0.0000	0.0000	0.0000	0.0000
25. O	0.0000	0.0000	0.0000	0.0467	0.0158	0.0007	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0000	0.0000	0.0002	0.0003	0.0001	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000

30. H	0.0000	0.0000	0.0000	0.0002	0.0037	0.0002	0.0025	0.0018	0.0009
31. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0001	0.0267	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. O	0.0005	0.0101	0.0010	0.0000	0.0000	0.0000	0.0008	0.0004	0.0001
36. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
37. H	0.0000	0.6595	0.0008	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
38. O	0.6595	0.0000	0.7773	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
39. H	0.0008	0.7773	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.7041	0.0007	0.0000	0.0000	0.0000
41. O	0.0001	0.0002	0.0000	0.7041	0.0000	0.7822	0.0002	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0007	0.7822	0.0000	0.0000	0.0000	0.0000
43. C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.9373	0.9420
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9373	0.0000	0.0007
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9420	0.0007	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.9410	0.0005	0.0007
47. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50
1. C	0.0001	0.0000	0.0000	0.0000	0.0000
2. C	0.0026	0.0000	0.0000	0.0000	0.0000
3. H	0.0017	0.0000	0.0000	0.0000	0.0000
4. N	0.0020	0.0000	0.0000	0.0000	0.0000
5. H	0.0001	0.0000	0.0000	0.0000	0.0000
6. N	0.0001	0.0001	0.0000	0.0000	0.0000
7. H	0.0000	0.0000	0.0000	0.0000	0.0000
8. H	0.0000	0.0002	0.0001	0.0000	0.0000
9. N	0.0002	0.0001	0.0000	0.0000	0.0000
10. H	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000
12. O	0.0000	0.0055	0.0020	0.0006	0.0007
13. O	0.0000	0.0099	0.0014	0.0005	0.0005
14. C	0.0000	0.0086	0.0093	0.0013	0.0014
15. C	0.0000	1.0299	0.0017	0.0022	0.0021
16. H	0.0000	0.0029	0.0015	0.0123	0.0012
17. H	0.0000	0.0028	0.0012	0.0013	0.0124
18. H	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0001	0.0000	0.0000	0.0000
20. H	0.0000	0.0001	0.0001	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0000	0.0001	0.0000	0.0001	0.0001
23. H	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000
27. O	0.0000	0.0001	0.0000	0.0000	0.0000
28. H	0.0000	0.0001	0.0000	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0120	0.0000	0.0000	0.0000	0.0000

31.	H	0.0000	0.0000	0.0000	0.0000	0.0000
32.	O	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000
35.	O	0.0001	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000
38.	O	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000
41.	O	0.0001	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000
43.	C	0.9410	0.0000	0.0000	0.0000	0.0000
44.	H	0.0005	0.0000	0.0000	0.0000	0.0000
45.	H	0.0007	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000
47.	C	0.0000	0.0000	0.9471	0.9420	0.9405
48.	H	0.0000	0.9471	0.0000	0.0005	0.0005
49.	H	0.0000	0.9420	0.0005	0.0000	0.0007
50.	H	0.0000	0.9405	0.0005	0.0007	0.0000

Table-9C-6-1: Wiberg index for salt bridge with 9 waters (bridge length=3.8 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0061	0.0107	0.0031	1.2328	0.0020	1.3104	0.0028	0.0029
2. H	0.0061	0.0000	0.9309	0.0010	0.0027	0.0021	0.0007	0.0000	0.0000
3. C	0.0107	0.9309	0.0000	0.9185	0.9611	0.0034	0.0036	0.0016	0.0002
4. H	0.0031	0.0010	0.9185	0.0000	0.0088	0.0041	0.0027	0.0015	0.0000
5. N	1.2328	0.0027	0.9611	0.0088	0.0000	0.7666	0.0799	0.0023	0.0081
6. H	0.0020	0.0021	0.0034	0.0041	0.7666	0.0000	0.0095	0.0003	0.0005
7. N	1.3104	0.0007	0.0036	0.0027	0.0799	0.0095	0.0000	0.7920	0.6959
8. H	0.0028	0.0000	0.0016	0.0015	0.0023	0.0003	0.7920	0.0000	0.0012
9. H	0.0029	0.0000	0.0002	0.0000	0.0081	0.0005	0.6959	0.0012	0.0000
10. N	1.3169	0.0003	0.0106	0.0018	0.0795	0.0014	0.0947	0.0104	0.0012
11. H	0.0025	0.0001	0.0003	0.0000	0.0016	0.0006	0.0096	0.0007	0.0001
12. H	0.0028	0.0002	0.0007	0.0000	0.0087	0.0001	0.0011	0.0001	0.0004
13. O	0.0020	0.0000	0.0003	0.0000	0.0018	0.0001	0.0024	0.0001	0.0012
14. O	0.0020	0.0001	0.0002	0.0000	0.0014	0.0004	0.0330	0.0005	0.0988
15. C	0.0004	0.0000	0.0000	0.0000	0.0003	0.0000	0.0031	0.0001	0.0016
16. C	0.0004	0.0000	0.0000	0.0000	0.0002	0.0000	0.0024	0.0001	0.0057
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0001	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000
22. O	0.0011	0.0000	0.0004	0.0001	0.0012	0.0001	0.0005	0.0001	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
25. O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0004	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. O	0.0005	0.0000	0.0001	0.0000	0.0016	0.0005	0.0002	0.0000	0.0000

31. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000
32. H	0.0001	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000
33. O	0.0007	0.0001	0.0027	0.0036	0.0005	0.0000	0.0076	0.0168	0.0001
34. H	0.0001	0.0000	0.0002	0.0001	0.0000	0.0000	0.0013	0.0001	0.0000
35. H	0.0000	0.0000	0.0002	0.0002	0.0001	0.0000	0.0004	0.0001	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
37. O	0.0003	0.0000	0.0002	0.0001	0.0001	0.0000	0.0012	0.0002	0.0003
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0001
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
40. O	0.0006	0.0000	0.0000	0.0000	0.0004	0.0003	0.0005	0.0001	0.0000
41. H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
42. O	0.0005	0.0005	0.0007	0.0001	0.0107	0.0248	0.0004	0.0000	0.0001
43. H	0.0001	0.0000	0.0001	0.0000	0.0010	0.0002	0.0001	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000
45. C	0.0059	0.0027	1.0224	0.0021	0.0183	0.0014	0.0040	0.0001	0.0001
46. H	0.0004	0.0117	0.0025	0.0014	0.0016	0.0000	0.0020	0.0000	0.0000
47. H	0.0009	0.0010	0.0034	0.0008	0.0106	0.0001	0.0002	0.0000	0.0000
48. H	0.0002	0.0017	0.0024	0.0116	0.0016	0.0001	0.0002	0.0001	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
50. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0002
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3169	0.0025	0.0028	0.0020	0.0020	0.0004	0.0004	0.0000	0.0000
2. H	0.0003	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
3. C	0.0106	0.0003	0.0007	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000
4. H	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0795	0.0016	0.0087	0.0018	0.0014	0.0003	0.0002	0.0000	0.0000
6. H	0.0014	0.0006	0.0001	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000
7. N	0.0947	0.0096	0.0011	0.0024	0.0330	0.0031	0.0024	0.0001	0.0000
8. H	0.0104	0.0007	0.0001	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000
9. H	0.0012	0.0001	0.0004	0.0012	0.0988	0.0016	0.0057	0.0001	0.0000
10. N	0.0000	0.7894	0.7070	0.0297	0.0027	0.0034	0.0019	0.0003	0.0000
11. H	0.7894	0.0000	0.0012	0.0008	0.0001	0.0001	0.0001	0.0000	0.0000
12. H	0.7070	0.0012	0.0000	0.0861	0.0010	0.0013	0.0044	0.0002	0.0000
13. O	0.0297	0.0008	0.0861	0.0000	0.1691	1.3504	0.0384	0.0086	0.0001
14. O	0.0027	0.0001	0.0010	0.1691	0.0000	1.4583	0.0343	0.0019	0.0000
15. C	0.0034	0.0001	0.0013	1.3504	1.4583	0.0000	0.9703	0.0029	0.0000
16. C	0.0019	0.0001	0.0044	0.0384	0.0343	0.9703	0.0000	0.9281	0.0000
17. H	0.0003	0.0000	0.0002	0.0086	0.0019	0.0029	0.9281	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0000	0.0000	0.0008	0.0003	0.0003	0.0002	0.0000	0.7737
20. H	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0001	0.0000	0.0007
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0003	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0008
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0002	0.0000	0.0001	0.0808	0.0044	0.0010	0.0006	0.0000	0.0000
25. O	0.0005	0.0000	0.0002	0.0215	0.0041	0.0067	0.0005	0.0001	0.0005
26. H	0.0001	0.0000	0.0000	0.0011	0.0002	0.0002	0.0001	0.0000	0.0000
27. H	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0015	0.0003	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000

29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. O	0.0003	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. O	0.0004	0.0001	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
34. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0002	0.0001	0.0000	0.0000
37. O	0.0001	0.0000	0.0000	0.0023	0.0095	0.0048	0.0004	0.0001	0.0011
38. H	0.0001	0.0000	0.0000	0.0021	0.0311	0.0008	0.0007	0.0000	0.0000
39. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. O	0.0095	0.0205	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. O	0.0005	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. C	0.0035	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
46. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0001	0.0000	0.0000	0.0049	0.0127	0.0057	0.9193	0.0006	0.0000
50. C	0.0002	0.0000	0.0001	0.0064	0.0116	0.0113	1.0226	0.0024	0.0000
51. H	0.0001	0.0000	0.0000	0.0015	0.0006	0.0016	0.0024	0.0123	0.0000
52. H	0.0001	0.0000	0.0001	0.0015	0.0013	0.0094	0.0018	0.0012	0.0000
53. H	0.0000	0.0000	0.0000	0.0004	0.0008	0.0011	0.0024	0.0015	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0001	0.0000	0.0001	0.0011	0.0000	0.0000	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
4. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0001	0.0000	0.0002	0.0012	0.0001	0.0000	0.0001	0.0000	0.0000
6. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. N	0.0001	0.0000	0.0001	0.0005	0.0000	0.0001	0.0001	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0001	0.0000	0.0001	0.0003	0.0000	0.0002	0.0005	0.0001	0.0002
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000
13. O	0.0008	0.0002	0.0000	0.0001	0.0000	0.0808	0.0215	0.0011	0.0002
14. O	0.0003	0.0001	0.0000	0.0001	0.0000	0.0044	0.0041	0.0002	0.0000
15. C	0.0003	0.0001	0.0000	0.0000	0.0000	0.0010	0.0067	0.0002	0.0000
16. C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0006	0.0005	0.0001	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
18. H	0.7737	0.0007	0.0000	0.0008	0.0000	0.0000	0.0005	0.0000	0.0000
19. O	0.0000	0.6891	0.0003	0.0107	0.0271	0.0003	0.0163	0.0009	0.0001
20. H	0.6891	0.0000	0.0000	0.0006	0.0001	0.0001	0.0517	0.0001	0.0000
21. H	0.0003	0.0000	0.0000	0.7328	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0107	0.0006	0.7328	0.0000	0.7334	0.0000	0.0002	0.0000	0.0000
23. H	0.0271	0.0001	0.0006	0.7334	0.0000	0.0000	0.0001	0.0000	0.0000
24. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.6496	0.0007	0.0001
25. O	0.0163	0.0517	0.0000	0.0002	0.0001	0.6496	0.0000	0.7722	0.0304
26. H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0007	0.7722	0.0000	0.0000

27. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0304	0.0000	0.0000
28. O	0.0002	0.0001	0.0000	0.0002	0.0000	0.0005	0.0118	0.0007	0.7238
29. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000	0.0007
30. O	0.0002	0.0000	0.0010	0.0135	0.0004	0.0000	0.0001	0.0000	0.0006
31. H	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0001	0.0000	0.0001	0.0411	0.0001	0.0000	0.0000	0.0000	0.0000
33. O	0.0002	0.0000	0.0233	0.0092	0.0003	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0001	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0001	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0271	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
37. O	0.0100	0.0005	0.0001	0.0006	0.0002	0.0001	0.0002	0.0000	0.0000
38. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
40. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0008
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. O	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
50. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0004	0.0000	0.0005	0.0000	0.0001	0.0007	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0027	0.0002	0.0002	0.0000
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0036	0.0001	0.0002	0.0000
5. N	0.0001	0.0000	0.0016	0.0004	0.0005	0.0005	0.0000	0.0001	0.0000
6. H	0.0001	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. N	0.0002	0.0000	0.0002	0.0001	0.0001	0.0076	0.0013	0.0004	0.0001
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0168	0.0001	0.0001	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
10. N	0.0015	0.0001	0.0003	0.0000	0.0000	0.0004	0.0002	0.0001	0.0000
11. H	0.0003	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
12. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
14. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0005
15. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0002	0.0000	0.0002	0.0000	0.0001	0.0002	0.0000	0.0001	0.0271
20. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
21. H	0.0000	0.0000	0.0010	0.0001	0.0001	0.0233	0.0001	0.0001	0.0000
22. O	0.0002	0.0001	0.0135	0.0004	0.0411	0.0092	0.0011	0.0005	0.0001
23. H	0.0000	0.0000	0.0004	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000
24. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

25. O	0.0118	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
26. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.7238	0.0007	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.6837	0.0190	0.0004	0.0005	0.0000	0.0000	0.0000	0.0000
29. H	0.6837	0.0000	0.0603	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
30. O	0.0190	0.0603	0.0000	0.7473	0.7052	0.0002	0.0000	0.0000	0.0000
31. H	0.0004	0.0001	0.7473	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000
32. H	0.0005	0.0001	0.7052	0.0006	0.0000	0.0002	0.0000	0.0000	0.0000
33. O	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.7782	0.6666	0.0005
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.7782	0.0000	0.0007	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.6666	0.0007	0.0000	0.0001
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000
37. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0243	0.0013	0.0807	0.7279
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0001	0.0006
39. H	0.1074	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. O	0.0303	0.0003	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0018	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. O	0.0003	0.0001	0.0075	0.0180	0.0003	0.0000	0.0000	0.0000	0.0000
43. H	0.0001	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0002	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0003	0.0000	0.0000	0.0006	0.0001	0.0005	0.0001	0.0000	0.0059
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000	0.0027
3. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0007	0.0001	0.0000	1.0224
4. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0021
5. N	0.0001	0.0000	0.0000	0.0004	0.0001	0.0107	0.0010	0.0002	0.0183
6. H	0.0000	0.0000	0.0000	0.0003	0.0000	0.0248	0.0002	0.0001	0.0014
7. N	0.0012	0.0003	0.0001	0.0005	0.0001	0.0004	0.0001	0.0001	0.0040
8. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
9. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001
10. N	0.0001	0.0001	0.0003	0.0095	0.0009	0.0005	0.0001	0.0001	0.0035
11. H	0.0000	0.0000	0.0001	0.0205	0.0001	0.0002	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0023	0.0021	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
14. O	0.0095	0.0311	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
15. C	0.0048	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0004	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0100	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0006	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001

23. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0002	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0001	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.0000	0.1074	0.0303	0.0018	0.0003	0.0001	0.0002	0.0000
29. H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
30. O	0.0000	0.0000	0.0002	0.0006	0.0002	0.0075	0.0011	0.0003	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0180	0.0000	0.0001	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
33. O	0.0243	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
34. H	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0807	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.7279	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. O	0.0000	0.7164	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. H	0.7164	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.6354	0.0007	0.0003	0.0000	0.0000	0.0000
40. O	0.0000	0.0000	0.6354	0.0000	0.7717	0.0175	0.0009	0.0546	0.0000
41. H	0.0000	0.0000	0.0007	0.7717	0.0000	0.0012	0.0000	0.0001	0.0000
42. O	0.0000	0.0000	0.0003	0.0175	0.0012	0.0000	0.7754	0.6912	0.0001
43. H	0.0000	0.0000	0.0000	0.0009	0.0000	0.7754	0.0000	0.0007	0.0000
44. H	0.0000	0.0000	0.0000	0.0546	0.0001	0.6912	0.0007	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9382
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9423
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9441
49. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50	51	52	53
1. C	0.0004	0.0009	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
2. H	0.0117	0.0010	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0025	0.0034	0.0024	0.0000	0.0000	0.0000	0.0000	0.0000
4. H	0.0014	0.0008	0.0116	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0016	0.0106	0.0016	0.0000	0.0000	0.0000	0.0000	0.0000
6. H	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. N	0.0020	0.0002	0.0002	0.0000	0.0004	0.0000	0.0001	0.0000
8. H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0002	0.0000
10. N	0.0004	0.0011	0.0001	0.0001	0.0002	0.0001	0.0001	0.0000
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
13. O	0.0000	0.0000	0.0000	0.0049	0.0064	0.0015	0.0015	0.0004
14. O	0.0000	0.0000	0.0000	0.0127	0.0116	0.0006	0.0013	0.0008
15. C	0.0000	0.0000	0.0000	0.0057	0.0113	0.0016	0.0094	0.0011
16. C	0.0000	0.0000	0.0000	0.9193	1.0226	0.0024	0.0018	0.0024
17. H	0.0000	0.0000	0.0000	0.0006	0.0024	0.0123	0.0012	0.0015
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
25.	O	0.0000	0.0000	0.0000	0.0003	0.0002	0.0001	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	O	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	O	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.9382	0.9423	0.9441	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0006	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0006	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0005	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0033	0.0012	0.0021	0.0126
50.	C	0.0000	0.0000	0.0000	0.0033	0.0000	0.9404	0.9454	0.9440
51.	H	0.0000	0.0000	0.0000	0.0012	0.9404	0.0000	0.0005	0.0006
52.	H	0.0000	0.0000	0.0000	0.0021	0.9454	0.0005	0.0000	0.0005
53.	H	0.0000	0.0000	0.0000	0.0126	0.9440	0.0006	0.0005	0.0000

Table-9C-6-2: Wiberg index for salt bridge with 9 waters (bridge length=4.0 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0060	0.0109	0.0032	1.2506	0.0022	1.2958	0.0027	0.0026
2. H	0.0060	0.0000	0.9313	0.0010	0.0027	0.0021	0.0006	0.0000	0.0000
3. C	0.0109	0.9313	0.0000	0.9194	0.9579	0.0034	0.0035	0.0013	0.0002
4. H	0.0032	0.0010	0.9194	0.0000	0.0084	0.0039	0.0025	0.0013	0.0000
5. N	1.2506	0.0027	0.9579	0.0084	0.0000	0.7587	0.0801	0.0021	0.0082
6. H	0.0022	0.0021	0.0034	0.0039	0.7587	0.0000	0.0097	0.0002	0.0005
7. N	1.2958	0.0006	0.0035	0.0025	0.0801	0.0097	0.0000	0.7901	0.7165
8. H	0.0027	0.0000	0.0013	0.0013	0.0021	0.0002	0.7901	0.0000	0.0010
9. H	0.0026	0.0000	0.0002	0.0000	0.0082	0.0005	0.7165	0.0010	0.0000
10. N	1.3146	0.0003	0.0106	0.0019	0.0826	0.0015	0.0903	0.0103	0.0013
11. H	0.0025	0.0001	0.0002	0.0000	0.0013	0.0006	0.0096	0.0007	0.0002
12. H	0.0025	0.0002	0.0008	0.0000	0.0085	0.0001	0.0011	0.0001	0.0006
13. O	0.0016	0.0000	0.0003	0.0000	0.0016	0.0000	0.0021	0.0001	0.0015
14. O	0.0016	0.0000	0.0002	0.0000	0.0012	0.0003	0.0254	0.0004	0.0738
15. C	0.0003	0.0000	0.0000	0.0000	0.0002	0.0000	0.0022	0.0001	0.0015
16. C	0.0002	0.0000	0.0000	0.0000	0.0002	0.0000	0.0021	0.0001	0.0054
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001

18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
20. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0001	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000
22. O	0.0012	0.0000	0.0004	0.0001	0.0011	0.0001	0.0005	0.0001	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0003	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000
29. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. O	0.0006	0.0000	0.0001	0.0000	0.0015	0.0005	0.0002	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000
32. H	0.0001	0.0000	0.0000	0.0000	0.0004	0.0000	0.0001	0.0000	0.0000
33. O	0.0007	0.0001	0.0024	0.0032	0.0005	0.0000	0.0080	0.0179	0.0001
34. H	0.0001	0.0000	0.0002	0.0001	0.0000	0.0000	0.0014	0.0001	0.0000
35. H	0.0000	0.0000	0.0002	0.0002	0.0001	0.0000	0.0004	0.0001	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
37. O	0.0003	0.0000	0.0002	0.0001	0.0001	0.0000	0.0012	0.0002	0.0004
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0001
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
40. O	0.0006	0.0000	0.0000	0.0000	0.0004	0.0003	0.0005	0.0001	0.0000
41. H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
42. O	0.0005	0.0006	0.0007	0.0002	0.0120	0.0285	0.0005	0.0000	0.0001
43. H	0.0001	0.0000	0.0001	0.0000	0.0010	0.0002	0.0001	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000
45. C	0.0061	0.0027	1.0229	0.0022	0.0177	0.0014	0.0039	0.0001	0.0001
46. H	0.0004	0.0117	0.0024	0.0014	0.0016	0.0000	0.0019	0.0000	0.0000
47. H	0.0009	0.0011	0.0033	0.0008	0.0106	0.0001	0.0002	0.0000	0.0000
48. H	0.0002	0.0017	0.0024	0.0116	0.0017	0.0001	0.0002	0.0001	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
50. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3146	0.0025	0.0025	0.0016	0.0016	0.0003	0.0002	0.0000	0.0000
2. H	0.0003	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0106	0.0002	0.0008	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000
4. H	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0826	0.0013	0.0085	0.0016	0.0012	0.0002	0.0002	0.0000	0.0000
6. H	0.0015	0.0006	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
7. N	0.0903	0.0096	0.0011	0.0021	0.0254	0.0022	0.0021	0.0001	0.0000
8. H	0.0103	0.0007	0.0001	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000
9. H	0.0013	0.0002	0.0006	0.0015	0.0738	0.0015	0.0054	0.0001	0.0000
10. N	0.0000	0.7859	0.7230	0.0235	0.0022	0.0023	0.0017	0.0002	0.0000
11. H	0.7859	0.0000	0.0010	0.0006	0.0001	0.0001	0.0001	0.0000	0.0000
12. H	0.7230	0.0010	0.0000	0.0659	0.0011	0.0012	0.0043	0.0002	0.0000
13. O	0.0235	0.0006	0.0659	0.0000	0.1706	1.3500	0.0381	0.0088	0.0001
14. O	0.0022	0.0001	0.0011	0.1706	0.0000	1.4639	0.0349	0.0020	0.0000
15. C	0.0023	0.0001	0.0012	1.3500	1.4639	0.0000	0.9720	0.0030	0.0000

16.	C	0.0017	0.0001	0.0043	0.0381	0.0349	0.9720	0.0000	0.9276	0.0000
17.	H	0.0002	0.0000	0.0002	0.0088	0.0020	0.0030	0.9276	0.0000	0.0000
18.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
19.	O	0.0001	0.0000	0.0000	0.0008	0.0003	0.0003	0.0001	0.0000	0.7741
20.	H	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0001	0.0000	0.0007
21.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0003	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0009
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0002	0.0000	0.0001	0.0851	0.0046	0.0011	0.0007	0.0000	0.0000
25.	O	0.0006	0.0000	0.0002	0.0222	0.0042	0.0068	0.0005	0.0001	0.0006
26.	H	0.0001	0.0000	0.0000	0.0011	0.0002	0.0002	0.0001	0.0000	0.0000
27.	H	0.0002	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
28.	O	0.0016	0.0003	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000
29.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	O	0.0003	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	O	0.0004	0.0001	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
34.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0002	0.0001	0.0000	0.0000
37.	O	0.0001	0.0000	0.0000	0.0024	0.0100	0.0049	0.0004	0.0001	0.0011
38.	H	0.0001	0.0000	0.0000	0.0022	0.0337	0.0009	0.0007	0.0000	0.0000
39.	H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	O	0.0101	0.0220	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	O	0.0006	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.0036	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
46.	H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0001	0.0000	0.0000	0.0049	0.0128	0.0056	0.9192	0.0006	0.0000
50.	C	0.0001	0.0000	0.0001	0.0065	0.0120	0.0117	1.0215	0.0024	0.0000
51.	H	0.0001	0.0000	0.0000	0.0015	0.0006	0.0016	0.0024	0.0122	0.0000
52.	H	0.0000	0.0000	0.0001	0.0016	0.0013	0.0092	0.0017	0.0012	0.0000
53.	H	0.0000	0.0000	0.0000	0.0004	0.0008	0.0010	0.0024	0.0015	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0001	0.0000	0.0001	0.0012	0.0000	0.0000	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
4. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0001	0.0000	0.0002	0.0011	0.0001	0.0000	0.0001	0.0000	0.0000
6. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. N	0.0001	0.0000	0.0001	0.0005	0.0000	0.0000	0.0001	0.0000	0.0000
8. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0001	0.0000	0.0001	0.0003	0.0000	0.0002	0.0006	0.0001	0.0002
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000
13. O	0.0008	0.0002	0.0000	0.0001	0.0000	0.0851	0.0222	0.0011	0.0002

14. O	0.0003	0.0001	0.0000	0.0001	0.0000	0.0046	0.0042	0.0002	0.0001
15. C	0.0003	0.0001	0.0000	0.0000	0.0000	0.0011	0.0068	0.0002	0.0000
16. C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0007	0.0005	0.0001	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
18. H	0.7741	0.0007	0.0000	0.0009	0.0000	0.0000	0.0006	0.0000	0.0000
19. O	0.0000	0.6878	0.0004	0.0109	0.0277	0.0003	0.0166	0.0008	0.0001
20. H	0.6878	0.0000	0.0000	0.0006	0.0001	0.0001	0.0527	0.0001	0.0000
21. H	0.0004	0.0000	0.0000	0.7326	0.0006	0.0000	0.0000	0.0000	0.0000
22. O	0.0109	0.0006	0.7326	0.0000	0.7319	0.0000	0.0002	0.0000	0.0000
23. H	0.0277	0.0001	0.0006	0.7319	0.0000	0.0000	0.0001	0.0000	0.0000
24. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.6436	0.0007	0.0001
25. O	0.0166	0.0527	0.0000	0.0002	0.0001	0.6436	0.0000	0.7730	0.0308
26. H	0.0008	0.0001	0.0000	0.0000	0.0000	0.0007	0.7730	0.0000	0.0000
27. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0308	0.0000	0.0000
28. O	0.0002	0.0001	0.0000	0.0002	0.0000	0.0005	0.0119	0.0007	0.7225
29. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000	0.0007
30. O	0.0002	0.0000	0.0011	0.0135	0.0004	0.0000	0.0001	0.0000	0.0006
31. H	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0001	0.0000	0.0001	0.0414	0.0001	0.0000	0.0000	0.0000	0.0000
33. O	0.0002	0.0000	0.0236	0.0093	0.0003	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0001	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0001	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0263	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
37. O	0.0098	0.0005	0.0001	0.0006	0.0002	0.0001	0.0002	0.0000	0.0000
38. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
40. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0008
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. O	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
50. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0003	0.0000	0.0006	0.0000	0.0001	0.0007	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0024	0.0002	0.0002	0.0000
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0032	0.0001	0.0002	0.0000
5. N	0.0001	0.0000	0.0015	0.0003	0.0004	0.0005	0.0000	0.0001	0.0000
6. H	0.0001	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. N	0.0001	0.0000	0.0002	0.0001	0.0001	0.0080	0.0014	0.0004	0.0001
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0179	0.0001	0.0001	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
10. N	0.0016	0.0001	0.0003	0.0000	0.0000	0.0004	0.0002	0.0001	0.0000
11. H	0.0003	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000

12. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
14. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0005
15. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0002	0.0000	0.0002	0.0000	0.0001	0.0002	0.0000	0.0001	0.0263
20. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
21. H	0.0000	0.0000	0.0011	0.0001	0.0001	0.0236	0.0001	0.0001	0.0000
22. O	0.0002	0.0001	0.0135	0.0004	0.0414	0.0093	0.0011	0.0005	0.0001
23. H	0.0000	0.0000	0.0004	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000
24. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0119	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
26. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.7225	0.0007	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.6850	0.0187	0.0004	0.0005	0.0000	0.0000	0.0000	0.0000
29. H	0.6850	0.0000	0.0591	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
30. O	0.0187	0.0591	0.0000	0.7491	0.7051	0.0002	0.0000	0.0000	0.0000
31. H	0.0004	0.0001	0.7491	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000
32. H	0.0005	0.0001	0.7051	0.0006	0.0000	0.0002	0.0000	0.0000	0.0000
33. O	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.7777	0.6646	0.0005
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.7777	0.0000	0.0007	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.6646	0.0007	0.0000	0.0001
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000
37. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0245	0.0014	0.0819	0.7289
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0001	0.0006
39. H	0.1088	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. O	0.0305	0.0003	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0018	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. O	0.0003	0.0001	0.0073	0.0172	0.0003	0.0000	0.0000	0.0000	0.0000
43. H	0.0001	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0003	0.0000	0.0000	0.0006	0.0001	0.0005	0.0001	0.0000	0.0061
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000	0.0027
3. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0007	0.0001	0.0000	1.0229
4. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0022
5. N	0.0001	0.0000	0.0000	0.0004	0.0001	0.0120	0.0010	0.0002	0.0177
6. H	0.0000	0.0000	0.0000	0.0003	0.0000	0.0285	0.0002	0.0001	0.0014
7. N	0.0012	0.0003	0.0001	0.0005	0.0001	0.0005	0.0001	0.0001	0.0039
8. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
9. H	0.0004	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001

10. N	0.0001	0.0001	0.0003	0.0101	0.0009	0.0006	0.0001	0.0001	0.0036
11. H	0.0000	0.0000	0.0001	0.0220	0.0001	0.0002	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0024	0.0022	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
14. O	0.0100	0.0337	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
15. C	0.0049	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0004	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0098	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0006	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001
23. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0002	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0001	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.0000	0.1088	0.0305	0.0018	0.0003	0.0001	0.0002	0.0000
29. H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
30. O	0.0000	0.0000	0.0002	0.0006	0.0002	0.0073	0.0011	0.0003	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0172	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
33. O	0.0245	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
34. H	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0819	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.7289	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. O	0.0000	0.7108	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. H	0.7108	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.6336	0.0007	0.0003	0.0000	0.0000	0.0000
40. O	0.0000	0.0000	0.6336	0.0000	0.7707	0.0177	0.0009	0.0555	0.0000
41. H	0.0000	0.0000	0.0007	0.7707	0.0000	0.0012	0.0000	0.0001	0.0000
42. O	0.0000	0.0000	0.0003	0.0177	0.0012	0.0000	0.7744	0.6892	0.0002
43. H	0.0000	0.0000	0.0000	0.0009	0.0000	0.7744	0.0000	0.0007	0.0000
44. H	0.0000	0.0000	0.0000	0.0555	0.0001	0.6892	0.0007	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9380
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9419
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9440
49. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50	51	52	53
1. C	0.0004	0.0009	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
2. H	0.0117	0.0011	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0024	0.0033	0.0024	0.0000	0.0000	0.0000	0.0000	0.0000
4. H	0.0014	0.0008	0.0116	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0016	0.0106	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
6. H	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. N	0.0019	0.0002	0.0002	0.0000	0.0003	0.0000	0.0001	0.0000

8.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0002	0.0000
10.	N	0.0004	0.0011	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
13.	O	0.0000	0.0000	0.0000	0.0049	0.0065	0.0015	0.0016	0.0004
14.	O	0.0000	0.0000	0.0000	0.0128	0.0120	0.0006	0.0013	0.0008
15.	C	0.0000	0.0000	0.0000	0.0056	0.0117	0.0016	0.0092	0.0010
16.	C	0.0000	0.0000	0.0000	0.9192	1.0215	0.0024	0.0017	0.0024
17.	H	0.0000	0.0000	0.0000	0.0006	0.0024	0.0122	0.0012	0.0015
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
25.	O	0.0000	0.0000	0.0000	0.0003	0.0002	0.0001	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	O	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	O	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.9380	0.9419	0.9440	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0006	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0006	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0005	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0033	0.0012	0.0021	0.0125
50.	C	0.0000	0.0000	0.0000	0.0033	0.0000	0.9401	0.9460	0.9443
51.	H	0.0000	0.0000	0.0000	0.0012	0.9401	0.0000	0.0005	0.0006
52.	H	0.0000	0.0000	0.0000	0.0021	0.9460	0.0005	0.0000	0.0005
53.	H	0.0000	0.0000	0.0000	0.0125	0.9443	0.0006	0.0005	0.0000

Table-9C-6-3: Wiberg index for salt bridge with 9 waters (bridge length=4.2 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0059	0.0111	0.0033	1.2624	0.0023	1.2884	0.0026	0.0023
2. H	0.0059	0.0000	0.9312	0.0009	0.0026	0.0020	0.0005	0.0000	0.0000
3. C	0.0111	0.9312	0.0000	0.9201	0.9555	0.0033	0.0034	0.0012	0.0003
4. H	0.0033	0.0009	0.9201	0.0000	0.0082	0.0037	0.0025	0.0012	0.0000

5.	N	1.2624	0.0026	0.9555	0.0082	0.0000	0.7513	0.0805	0.0020	0.0083
6.	H	0.0023	0.0020	0.0033	0.0037	0.7513	0.0000	0.0097	0.0001	0.0005
7.	N	1.2884	0.0005	0.0034	0.0025	0.0805	0.0097	0.0000	0.7873	0.7387
8.	H	0.0026	0.0000	0.0012	0.0012	0.0020	0.0001	0.7873	0.0000	0.0008
9.	H	0.0023	0.0000	0.0003	0.0000	0.0083	0.0005	0.7387	0.0008	0.0000
10.	N	1.3112	0.0003	0.0105	0.0019	0.0841	0.0015	0.0874	0.0102	0.0015
11.	H	0.0024	0.0000	0.0002	0.0000	0.0011	0.0005	0.0095	0.0007	0.0002
12.	H	0.0023	0.0002	0.0008	0.0000	0.0085	0.0002	0.0012	0.0002	0.0006
13.	O	0.0012	0.0000	0.0002	0.0000	0.0013	0.0000	0.0018	0.0001	0.0016
14.	O	0.0012	0.0000	0.0001	0.0000	0.0009	0.0002	0.0176	0.0003	0.0491
15.	C	0.0003	0.0000	0.0000	0.0000	0.0002	0.0000	0.0015	0.0001	0.0014
16.	C	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0017	0.0000	0.0047
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0001	0.0000	0.0001	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000
22.	O	0.0012	0.0000	0.0004	0.0001	0.0011	0.0001	0.0006	0.0001	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	O	0.0003	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	O	0.0006	0.0000	0.0001	0.0000	0.0014	0.0005	0.0002	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000
32.	H	0.0001	0.0000	0.0000	0.0000	0.0004	0.0000	0.0001	0.0000	0.0000
33.	O	0.0007	0.0001	0.0022	0.0027	0.0005	0.0000	0.0082	0.0186	0.0001
34.	H	0.0001	0.0000	0.0001	0.0001	0.0001	0.0000	0.0014	0.0001	0.0000
35.	H	0.0000	0.0000	0.0002	0.0002	0.0001	0.0000	0.0004	0.0001	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
37.	O	0.0003	0.0000	0.0002	0.0001	0.0001	0.0000	0.0012	0.0002	0.0004
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
40.	O	0.0006	0.0000	0.0000	0.0000	0.0004	0.0003	0.0005	0.0001	0.0000
41.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
42.	O	0.0006	0.0006	0.0007	0.0002	0.0135	0.0329	0.0005	0.0000	0.0001
43.	H	0.0001	0.0000	0.0001	0.0000	0.0010	0.0001	0.0001	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000
45.	C	0.0063	0.0028	1.0237	0.0023	0.0172	0.0014	0.0039	0.0001	0.0001
46.	H	0.0004	0.0118	0.0024	0.0014	0.0016	0.0000	0.0018	0.0000	0.0000
47.	H	0.0009	0.0010	0.0033	0.0008	0.0107	0.0001	0.0002	0.0000	0.0000
48.	H	0.0002	0.0017	0.0023	0.0117	0.0017	0.0001	0.0002	0.0001	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
50.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3112	0.0024	0.0023	0.0012	0.0012	0.0003	0.0002	0.0000	0.0000
2. H	0.0003	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

3. C	0.0105	0.0002	0.0008	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
4. H	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0841	0.0011	0.0085	0.0013	0.0009	0.0002	0.0001	0.0000	0.0000
6. H	0.0015	0.0005	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
7. N	0.0874	0.0095	0.0012	0.0018	0.0176	0.0015	0.0017	0.0001	0.0000
8. H	0.0102	0.0007	0.0002	0.0001	0.0003	0.0001	0.0000	0.0000	0.0000
9. H	0.0015	0.0002	0.0006	0.0016	0.0491	0.0014	0.0047	0.0000	0.0000
10. N	0.0000	0.7826	0.7415	0.0169	0.0018	0.0015	0.0015	0.0002	0.0000
11. H	0.7826	0.0000	0.0008	0.0005	0.0001	0.0001	0.0001	0.0000	0.0000
12. H	0.7415	0.0008	0.0000	0.0449	0.0012	0.0011	0.0038	0.0002	0.0000
13. O	0.0169	0.0005	0.0449	0.0000	0.1733	1.3524	0.0386	0.0090	0.0001
14. O	0.0018	0.0001	0.0012	0.1733	0.0000	1.4704	0.0361	0.0021	0.0000
15. C	0.0015	0.0001	0.0011	1.3524	1.4704	0.0000	0.9712	0.0030	0.0000
16. C	0.0015	0.0001	0.0038	0.0386	0.0361	0.9712	0.0000	0.9277	0.0000
17. H	0.0002	0.0000	0.0002	0.0090	0.0021	0.0030	0.9277	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0001	0.0000	0.0000	0.0007	0.0003	0.0003	0.0001	0.0000	0.7746
20. H	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0001	0.0000	0.0007
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0003	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0009
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0002	0.0000	0.0001	0.0870	0.0046	0.0012	0.0009	0.0000	0.0000
25. O	0.0006	0.0000	0.0002	0.0224	0.0042	0.0068	0.0005	0.0001	0.0006
26. H	0.0001	0.0000	0.0000	0.0011	0.0002	0.0002	0.0001	0.0000	0.0000
27. H	0.0002	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
28. O	0.0016	0.0003	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000
29. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. O	0.0004	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. O	0.0004	0.0001	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
34. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0002	0.0001	0.0000	0.0000
37. O	0.0001	0.0000	0.0000	0.0024	0.0103	0.0048	0.0004	0.0001	0.0011
38. H	0.0000	0.0000	0.0000	0.0022	0.0355	0.0009	0.0009	0.0000	0.0000
39. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. O	0.0106	0.0233	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. O	0.0006	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. C	0.0036	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
46. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0050	0.0128	0.0055	0.9194	0.0006	0.0000
50. C	0.0001	0.0000	0.0001	0.0065	0.0122	0.0115	1.0218	0.0024	0.0000
51. H	0.0001	0.0000	0.0000	0.0016	0.0006	0.0016	0.0025	0.0122	0.0000
52. H	0.0000	0.0000	0.0001	0.0017	0.0014	0.0092	0.0017	0.0012	0.0000
53. H	0.0000	0.0000	0.0000	0.0004	0.0008	0.0010	0.0024	0.0016	0.0000

Atom	19	20	21	22	23	24	25	26	27

1.	C	0.0001	0.0000	0.0001	0.0012	0.0000	0.0000	0.0001	0.0000	0.0000
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
4.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
5.	N	0.0001	0.0000	0.0002	0.0011	0.0001	0.0000	0.0001	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	N	0.0001	0.0000	0.0001	0.0006	0.0000	0.0000	0.0001	0.0000	0.0000
8.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	N	0.0001	0.0000	0.0001	0.0003	0.0000	0.0002	0.0006	0.0001	0.0002
11.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000
13.	O	0.0007	0.0002	0.0000	0.0001	0.0000	0.0870	0.0224	0.0011	0.0002
14.	O	0.0003	0.0001	0.0000	0.0001	0.0000	0.0046	0.0042	0.0002	0.0001
15.	C	0.0003	0.0001	0.0000	0.0000	0.0000	0.0012	0.0068	0.0002	0.0000
16.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0009	0.0005	0.0001	0.0000
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
18.	H	0.7746	0.0007	0.0000	0.0009	0.0000	0.0000	0.0006	0.0000	0.0000
19.	O	0.0000	0.6864	0.0004	0.0110	0.0282	0.0003	0.0169	0.0008	0.0001
20.	H	0.6864	0.0000	0.0000	0.0006	0.0001	0.0001	0.0540	0.0001	0.0000
21.	H	0.0004	0.0000	0.0000	0.7330	0.0006	0.0000	0.0000	0.0000	0.0000
22.	O	0.0110	0.0006	0.7330	0.0000	0.7304	0.0000	0.0002	0.0000	0.0000
23.	H	0.0282	0.0001	0.0006	0.7304	0.0000	0.0000	0.0001	0.0000	0.0000
24.	H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.6389	0.0007	0.0001
25.	O	0.0169	0.0540	0.0000	0.0002	0.0001	0.6389	0.0000	0.7730	0.0320
26.	H	0.0008	0.0001	0.0000	0.0000	0.0000	0.0007	0.7730	0.0000	0.0000
27.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0320	0.0000	0.0000
28.	O	0.0002	0.0001	0.0000	0.0002	0.0000	0.0005	0.0122	0.0007	0.7201
29.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000	0.0007
30.	O	0.0002	0.0000	0.0011	0.0134	0.0004	0.0000	0.0001	0.0000	0.0006
31.	H	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0001	0.0000	0.0001	0.0411	0.0001	0.0000	0.0000	0.0000	0.0000
33.	O	0.0002	0.0000	0.0235	0.0093	0.0003	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0001	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0257	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
37.	O	0.0096	0.0004	0.0001	0.0006	0.0002	0.0001	0.0002	0.0000	0.0000
38.	H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
40.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0008
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	O	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
50.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0003	0.0000	0.0006	0.0000	0.0001	0.0007	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0022	0.0001	0.0002	0.0000
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0027	0.0001	0.0002	0.0000
5. N	0.0001	0.0000	0.0014	0.0003	0.0004	0.0005	0.0001	0.0001	0.0000
6. H	0.0001	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7. N	0.0001	0.0000	0.0002	0.0001	0.0001	0.0082	0.0014	0.0004	0.0001
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0186	0.0001	0.0001	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
10. N	0.0016	0.0001	0.0004	0.0000	0.0000	0.0004	0.0002	0.0001	0.0000
11. H	0.0003	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
12. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
14. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0005
15. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0002	0.0000	0.0002	0.0000	0.0001	0.0002	0.0000	0.0001	0.0257
20. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
21. H	0.0000	0.0000	0.0011	0.0001	0.0001	0.0235	0.0000	0.0001	0.0000
22. O	0.0002	0.0001	0.0134	0.0004	0.0411	0.0093	0.0010	0.0005	0.0001
23. H	0.0000	0.0000	0.0004	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000
24. H	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0122	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
26. H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.7201	0.0007	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.6865	0.0183	0.0004	0.0005	0.0000	0.0000	0.0000	0.0000
29. H	0.6865	0.0000	0.0576	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
30. O	0.0183	0.0576	0.0000	0.7508	0.7053	0.0002	0.0000	0.0000	0.0000
31. H	0.0004	0.0001	0.7508	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000
32. H	0.0005	0.0001	0.7053	0.0006	0.0000	0.0002	0.0000	0.0000	0.0000
33. O	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.7775	0.6623	0.0005
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.7775	0.0000	0.0007	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.6623	0.0007	0.0000	0.0001
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000
37. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0247	0.0014	0.0830	0.7296
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0001	0.0006
39. H	0.1102	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. O	0.0307	0.0003	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. H	0.0018	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. O	0.0003	0.0001	0.0071	0.0165	0.0003	0.0000	0.0000	0.0000	0.0000
43. H	0.0001	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
49. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Atom	37	38	39	40	41	42	43	44	45
1. C	0.0003	0.0000	0.0000	0.0006	0.0001	0.0006	0.0001	0.0000	0.0063
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000	0.0028
3. C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0007	0.0001	0.0000	1.0237
4. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0023
5. N	0.0001	0.0000	0.0000	0.0004	0.0000	0.0135	0.0010	0.0002	0.0172
6. H	0.0000	0.0000	0.0000	0.0003	0.0000	0.0329	0.0001	0.0001	0.0014
7. N	0.0012	0.0002	0.0001	0.0005	0.0001	0.0005	0.0001	0.0001	0.0039
8. H	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
9. H	0.0004	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001
10. N	0.0001	0.0000	0.0003	0.0106	0.0009	0.0006	0.0001	0.0001	0.0036
11. H	0.0000	0.0000	0.0001	0.0233	0.0001	0.0003	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0024	0.0022	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
14. O	0.0103	0.0355	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
15. C	0.0048	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0004	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. O	0.0096	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. O	0.0006	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001
23. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. O	0.0002	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0001	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000
28. O	0.0000	0.0000	0.1102	0.0307	0.0018	0.0003	0.0001	0.0002	0.0000
29. H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
30. O	0.0000	0.0000	0.0002	0.0006	0.0002	0.0071	0.0010	0.0003	0.0000
31. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0165	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
33. O	0.0247	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
34. H	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0830	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.7296	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. O	0.0000	0.7058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. H	0.7058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.6309	0.0007	0.0003	0.0000	0.0000	0.0000
40. O	0.0000	0.0000	0.6309	0.0000	0.7696	0.0181	0.0009	0.0574	0.0000
41. H	0.0000	0.0000	0.0007	0.7696	0.0000	0.0013	0.0000	0.0001	0.0000
42. O	0.0000	0.0000	0.0003	0.0181	0.0013	0.0000	0.7736	0.6860	0.0002
43. H	0.0000	0.0000	0.0000	0.0009	0.0000	0.7736	0.0000	0.0007	0.0000
44. H	0.0000	0.0000	0.0000	0.0574	0.0001	0.6860	0.0007	0.0000	0.0000
45. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9378
47. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9413
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9436
49. H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

50.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		46	47	48	49	50	51	52	53
1.	C	0.0004	0.0009	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0118	0.0010	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0024	0.0033	0.0023	0.0000	0.0000	0.0000	0.0000	0.0000
4.	H	0.0014	0.0008	0.0117	0.0000	0.0000	0.0000	0.0000	0.0000
5.	N	0.0016	0.0107	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	N	0.0018	0.0002	0.0002	0.0000	0.0002	0.0000	0.0001	0.0000
8.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0001	0.0000
10.	N	0.0004	0.0011	0.0001	0.0000	0.0001	0.0001	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
13.	O	0.0000	0.0000	0.0000	0.0050	0.0065	0.0016	0.0017	0.0004
14.	O	0.0000	0.0000	0.0000	0.0128	0.0122	0.0006	0.0014	0.0008
15.	C	0.0000	0.0000	0.0000	0.0055	0.0115	0.0016	0.0092	0.0010
16.	C	0.0000	0.0000	0.0000	0.9194	1.0218	0.0025	0.0017	0.0024
17.	H	0.0000	0.0000	0.0000	0.0006	0.0024	0.0122	0.0012	0.0016
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
25.	O	0.0000	0.0000	0.0000	0.0002	0.0002	0.0001	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	O	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	O	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.9378	0.9413	0.9436	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0006	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0006	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000

48. H	0.0005	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
49. H	0.0000	0.0000	0.0000	0.0000	0.0032	0.0011	0.0020	0.0125	
50. C	0.0000	0.0000	0.0000	0.0032	0.0000	0.9399	0.9465	0.9446	
51. H	0.0000	0.0000	0.0000	0.0011	0.9399	0.0000	0.0005	0.0006	
52. H	0.0000	0.0000	0.0000	0.0020	0.9465	0.0005	0.0000	0.0005	
53. H	0.0000	0.0000	0.0000	0.0125	0.9446	0.0006	0.0005	0.0000	

Table-9C-7-1: Wiberg index for salt bridge with 10 waters (bridge length=3.8 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0064	0.0111	0.0026	1.2526	0.0022	1.3114	0.0026	0.0028
2. H	0.0064	0.0000	0.9281	0.0011	0.0033	0.0020	0.0006	0.0000	0.0000
3. C	0.0111	0.9281	0.0000	0.9201	0.9596	0.0036	0.0036	0.0017	0.0002
4. H	0.0026	0.0011	0.9201	0.0000	0.0069	0.0048	0.0029	0.0017	0.0000
5. N	1.2526	0.0033	0.9596	0.0069	0.0000	0.7566	0.0842	0.0019	0.0083
6. H	0.0022	0.0020	0.0036	0.0048	0.7566	0.0000	0.0093	0.0002	0.0004
7. N	1.3114	0.0006	0.0036	0.0029	0.0842	0.0093	0.0000	0.7935	0.7117
8. H	0.0026	0.0000	0.0017	0.0017	0.0019	0.0002	0.7935	0.0000	0.0011
9. H	0.0028	0.0000	0.0002	0.0000	0.0083	0.0004	0.7117	0.0011	0.0000
10. N	1.2956	0.0006	0.0106	0.0014	0.0784	0.0017	0.0903	0.0096	0.0013
11. H	0.0024	0.0001	0.0003	0.0000	0.0016	0.0006	0.0091	0.0008	0.0001
12. H	0.0026	0.0002	0.0008	0.0000	0.0088	0.0001	0.0012	0.0001	0.0003
13. O	0.0022	0.0000	0.0003	0.0000	0.0015	0.0001	0.0027	0.0001	0.0016
14. O	0.0020	0.0001	0.0002	0.0000	0.0012	0.0003	0.0260	0.0005	0.0798
15. C	0.0004	0.0000	0.0001	0.0000	0.0005	0.0000	0.0044	0.0001	0.0017
16. C	0.0004	0.0000	0.0000	0.0000	0.0002	0.0000	0.0017	0.0001	0.0045
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
23. O	0.0006	0.0000	0.0005	0.0001	0.0009	0.0001	0.0003	0.0001	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
26. O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0001
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0004	0.0000	0.0000	0.0000	0.0002	0.0001	0.0002	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
31. O	0.0005	0.0001	0.0004	0.0000	0.0017	0.0005	0.0002	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
34. O	0.0001	0.0001	0.0016	0.0025	0.0002	0.0000	0.0002	0.0000	0.0000
35. H	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
36. H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
38. O	0.0003	0.0000	0.0001	0.0001	0.0001	0.0000	0.0013	0.0002	0.0004
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
41. O	0.0007	0.0000	0.0001	0.0000	0.0005	0.0003	0.0005	0.0001	0.0000
42. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
43. O	0.0006	0.0007	0.0009	0.0002	0.0129	0.0312	0.0005	0.0000	0.0001
44. H	0.0001	0.0000	0.0001	0.0000	0.0011	0.0002	0.0002	0.0000	0.0000

45. H	0.0000	0.0000	0.0001	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000
46. H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0007	0.0001	0.0000
47. O	0.0007	0.0000	0.0009	0.0009	0.0003	0.0000	0.0071	0.0139	0.0001
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
49. C	0.0068	0.0025	1.0222	0.0022	0.0181	0.0009	0.0034	0.0002	0.0000
50. H	0.0004	0.0119	0.0025	0.0015	0.0013	0.0000	0.0011	0.0000	0.0000
51. H	0.0008	0.0011	0.0033	0.0007	0.0107	0.0001	0.0003	0.0000	0.0000
52. H	0.0001	0.0016	0.0024	0.0117	0.0018	0.0002	0.0002	0.0001	0.0000
53. C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0003
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.2956	0.0024	0.0026	0.0022	0.0020	0.0004	0.0004	0.0000	0.0000
2. H	0.0006	0.0001	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
3. C	0.0106	0.0003	0.0008	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000
4. H	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0784	0.0016	0.0088	0.0015	0.0012	0.0005	0.0002	0.0000	0.0000
6. H	0.0017	0.0006	0.0001	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
7. N	0.0903	0.0091	0.0012	0.0027	0.0260	0.0044	0.0017	0.0001	0.0001
8. H	0.0096	0.0008	0.0001	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000
9. H	0.0013	0.0001	0.0003	0.0016	0.0798	0.0017	0.0045	0.0000	0.0000
10. N	0.0000	0.7882	0.7264	0.0234	0.0032	0.0051	0.0011	0.0002	0.0003
11. H	0.7882	0.0000	0.0010	0.0005	0.0001	0.0001	0.0001	0.0000	0.0000
12. H	0.7264	0.0010	0.0000	0.0690	0.0016	0.0016	0.0029	0.0001	0.0001
13. O	0.0234	0.0005	0.0690	0.0000	0.1704	1.3552	0.0395	0.0073	0.0089
14. O	0.0032	0.0001	0.0016	0.1704	0.0000	1.4509	0.0370	0.0124	0.0020
15. C	0.0051	0.0001	0.0016	1.3552	1.4509	0.0000	0.9725	0.0077	0.0031
16. C	0.0011	0.0001	0.0029	0.0395	0.0370	0.9725	0.0000	0.9115	0.9271
17. H	0.0002	0.0000	0.0001	0.0073	0.0124	0.0077	0.9115	0.0000	0.0008
18. H	0.0003	0.0000	0.0001	0.0089	0.0020	0.0031	0.9271	0.0008	0.0000
19. H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
20. O	0.0000	0.0000	0.0000	0.0006	0.0003	0.0002	0.0001	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0002	0.0000	0.0001	0.0798	0.0026	0.0012	0.0024	0.0001	0.0001
26. O	0.0005	0.0000	0.0002	0.0215	0.0032	0.0063	0.0010	0.0003	0.0001
27. H	0.0001	0.0000	0.0000	0.0010	0.0001	0.0001	0.0002	0.0000	0.0000
28. H	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0014	0.0003	0.0001	0.0006	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. O	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000
38. O	0.0001	0.0000	0.0001	0.0020	0.0106	0.0041	0.0006	0.0003	0.0001
39. H	0.0001	0.0000	0.0000	0.0015	0.0343	0.0009	0.0015	0.0001	0.0000

40. H	0.0004	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0099	0.0216	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0008	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0005	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
47. O	0.0004	0.0001	0.0000	0.0001	0.0004	0.0001	0.0000	0.0000	0.0000
48. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
49. C	0.0038	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
50. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0003	0.0000	0.0001	0.0056	0.0111	0.0095	1.0261	0.0032	0.0024
54. H	0.0001	0.0000	0.0000	0.0016	0.0006	0.0016	0.0024	0.0011	0.0123
55. H	0.0000	0.0000	0.0001	0.0014	0.0014	0.0092	0.0017	0.0021	0.0010
56. H	0.0001	0.0000	0.0000	0.0004	0.0007	0.0011	0.0024	0.0125	0.0015

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0000	0.0001	0.0000	0.0000	0.0006	0.0000	0.0000	0.0001	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
4. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
5. N	0.0000	0.0000	0.0000	0.0001	0.0009	0.0000	0.0000	0.0001	0.0000
6. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
7. N	0.0000	0.0002	0.0000	0.0000	0.0003	0.0000	0.0001	0.0001	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
10. N	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0005	0.0001
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
13. O	0.0001	0.0006	0.0002	0.0000	0.0001	0.0000	0.0798	0.0215	0.0010
14. O	0.0001	0.0003	0.0001	0.0000	0.0000	0.0000	0.0026	0.0032	0.0001
15. C	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0012	0.0063	0.0001
16. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0024	0.0010	0.0002
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000
19. H	0.0000	0.7757	0.0007	0.0000	0.0008	0.0000	0.0000	0.0006	0.0000
20. O	0.7757	0.0000	0.6862	0.0004	0.0099	0.0242	0.0003	0.0173	0.0008
21. H	0.0007	0.6862	0.0000	0.0000	0.0004	0.0001	0.0001	0.0548	0.0001
22. H	0.0000	0.0004	0.0000	0.0000	0.7145	0.0006	0.0000	0.0000	0.0000
23. O	0.0008	0.0099	0.0004	0.7145	0.0000	0.7350	0.0000	0.0003	0.0000
24. H	0.0000	0.0242	0.0001	0.0006	0.7350	0.0000	0.0000	0.0001	0.0000
25. H	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.6483	0.0007
26. O	0.0006	0.0173	0.0548	0.0000	0.0003	0.0001	0.6483	0.0000	0.7733
27. H	0.0000	0.0008	0.0001	0.0000	0.0000	0.0000	0.0007	0.7733	0.0000
28. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0291	0.0000
29. O	0.0000	0.0002	0.0001	0.0000	0.0002	0.0000	0.0004	0.0113	0.0005
30. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000
31. O	0.0000	0.0001	0.0000	0.0008	0.0159	0.0008	0.0000	0.0002	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0001	0.0489	0.0001	0.0000	0.0000	0.0000
34. O	0.0000	0.0001	0.0000	0.0372	0.0135	0.0004	0.0000	0.0000	0.0000

35. H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0345	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
38. O	0.0009	0.0126	0.0005	0.0000	0.0002	0.0000	0.0000	0.0002	0.0000
39. H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
41. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
47. O	0.0000	0.0002	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0004	0.0000	0.0005	0.0000	0.0000	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
3. C	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0016	0.0003	0.0001
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025	0.0002	0.0002
5. N	0.0000	0.0002	0.0000	0.0017	0.0005	0.0004	0.0002	0.0000	0.0000
6. H	0.0000	0.0001	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
7. N	0.0000	0.0002	0.0001	0.0002	0.0001	0.0000	0.0002	0.0001	0.0001
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0002	0.0014	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
11. H	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0002	0.0006	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
14. O	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0002	0.0000	0.0001	0.0000	0.0001	0.0001	0.0000	0.0000
21. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0008	0.0000	0.0001	0.0372	0.0000	0.0001
23. O	0.0000	0.0002	0.0001	0.0159	0.0005	0.0489	0.0135	0.0010	0.0005
24. H	0.0000	0.0000	0.0000	0.0008	0.0000	0.0001	0.0004	0.0000	0.0000
25. H	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0291	0.0113	0.0004	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.7255	0.0007	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.7255	0.0000	0.6776	0.0208	0.0004	0.0005	0.0000	0.0000	0.0000

30. H	0.0007	0.6776	0.0000	0.0669	0.0001	0.0001	0.0000	0.0000	0.0000
31. O	0.0006	0.0208	0.0669	0.0000	0.7551	0.6945	0.0002	0.0000	0.0000
32. H	0.0000	0.0004	0.0001	0.7551	0.0000	0.0006	0.0000	0.0000	0.0000
33. H	0.0000	0.0005	0.0001	0.6945	0.0006	0.0000	0.0002	0.0000	0.0000
34. O	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.7847	0.6986
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7847	0.0000	0.0008
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6986	0.0008	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
38. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0001	0.1082	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0009	0.0304	0.0003	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0019	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0004	0.0001	0.0058	0.0127	0.0003	0.0000	0.0000	0.0000
44. H	0.0000	0.0001	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0000	0.0001
47. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0179	0.0006	0.0532
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001
49. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0000	0.0003	0.0000	0.0000	0.0007	0.0001	0.0006	0.0001	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000
3. C	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0009	0.0001	0.0001
4. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
5. N	0.0000	0.0001	0.0000	0.0000	0.0005	0.0000	0.0129	0.0011	0.0002
6. H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0312	0.0002	0.0001
7. N	0.0001	0.0013	0.0003	0.0001	0.0005	0.0001	0.0005	0.0002	0.0001
8. H	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0004	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
10. N	0.0000	0.0001	0.0001	0.0004	0.0099	0.0008	0.0005	0.0001	0.0001
11. H	0.0000	0.0000	0.0000	0.0001	0.0216	0.0001	0.0002	0.0000	0.0000
12. H	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
13. O	0.0001	0.0020	0.0015	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
14. O	0.0005	0.0106	0.0343	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0001	0.0041	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0001	0.0006	0.0015	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0345	0.0126	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0001	0.0002	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0001	0.0009	0.0000	0.0000	0.0000	0.0000
29. O	0.0000	0.0000	0.0000	0.1082	0.0304	0.0019	0.0004	0.0001	0.0002
30. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000
31. O	0.0000	0.0000	0.0000	0.0002	0.0005	0.0001	0.0058	0.0009	0.0002
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0127	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
34. O	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.7176	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.7176	0.0000	0.7093	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0006	0.7093	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.6335	0.0007	0.0003	0.0000	0.0000
41. O	0.0000	0.0000	0.0000	0.6335	0.0000	0.7712	0.0172	0.0009	0.0540
42. H	0.0000	0.0000	0.0000	0.0007	0.7712	0.0000	0.0012	0.0000	0.0001
43. O	0.0000	0.0000	0.0000	0.0003	0.0172	0.0012	0.0000	0.7747	0.6907
44. H	0.0000	0.0000	0.0000	0.0000	0.0009	0.0000	0.7747	0.0000	0.0007
45. H	0.0000	0.0000	0.0000	0.0000	0.0540	0.0001	0.6907	0.0007	0.0000
46. H	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. O	0.0007	0.0273	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0001	0.0949	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50	51	52	53	54
1. C	0.0001	0.0007	0.0000	0.0068	0.0004	0.0008	0.0001	0.0001	0.0000
2. H	0.0000	0.0000	0.0000	0.0025	0.0119	0.0011	0.0016	0.0000	0.0000
3. C	0.0001	0.0009	0.0000	1.0222	0.0025	0.0033	0.0024	0.0000	0.0000
4. H	0.0000	0.0009	0.0000	0.0022	0.0015	0.0007	0.0117	0.0000	0.0000
5. N	0.0000	0.0003	0.0000	0.0181	0.0013	0.0107	0.0018	0.0000	0.0000
6. H	0.0000	0.0000	0.0000	0.0009	0.0000	0.0001	0.0002	0.0000	0.0000
7. N	0.0007	0.0071	0.0003	0.0034	0.0011	0.0003	0.0002	0.0005	0.0000
8. H	0.0001	0.0139	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
9. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
10. N	0.0001	0.0004	0.0000	0.0038	0.0004	0.0011	0.0001	0.0003	0.0001
11. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
13. O	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0056	0.0016
14. O	0.0001	0.0004	0.0002	0.0001	0.0000	0.0000	0.0000	0.0111	0.0006
15. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0095	0.0016
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0261	0.0024
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0032	0.0011
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0024	0.0123
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

20. O	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. O	0.0009	0.0179	0.0005	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
35. H	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0532	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0007	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.0013	0.0273	0.0949	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.7756	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. O	0.7756	0.0000	0.6477	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0007	0.6477	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0001	0.0000	0.0000	0.9411	0.9415	0.9439	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.9411	0.0000	0.0006	0.0005	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.9415	0.0006	0.0000	0.0006	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.9439	0.0005	0.0006	0.0000	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9389
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9389	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9464	0.0005
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9451	0.0006

Atom	55	56
1. C	0.0000	0.0000
2. H	0.0000	0.0000
3. C	0.0000	0.0000
4. H	0.0000	0.0000
5. N	0.0000	0.0000
6. H	0.0000	0.0000
7. N	0.0001	0.0000
8. H	0.0000	0.0000
9. H	0.0001	0.0000
10. N	0.0000	0.0001
11. H	0.0000	0.0000
12. H	0.0001	0.0000
13. O	0.0014	0.0004
14. O	0.0014	0.0007

15.	C	0.0092	0.0011
16.	C	0.0017	0.0024
17.	H	0.0021	0.0125
18.	H	0.0010	0.0015
19.	H	0.0000	0.0000
20.	O	0.0000	0.0000
21.	H	0.0000	0.0000
22.	H	0.0000	0.0000
23.	O	0.0000	0.0000
24.	H	0.0000	0.0000
25.	H	0.0000	0.0000
26.	O	0.0000	0.0000
27.	H	0.0000	0.0000
28.	H	0.0000	0.0000
29.	O	0.0000	0.0000
30.	H	0.0000	0.0000
31.	O	0.0000	0.0000
32.	H	0.0000	0.0000
33.	H	0.0000	0.0000
34.	O	0.0000	0.0000
35.	H	0.0000	0.0000
36.	H	0.0000	0.0000
37.	H	0.0000	0.0000
38.	O	0.0000	0.0000
39.	H	0.0000	0.0000
40.	H	0.0000	0.0000
41.	O	0.0000	0.0000
42.	H	0.0000	0.0000
43.	O	0.0000	0.0000
44.	H	0.0000	0.0000
45.	H	0.0000	0.0000
46.	H	0.0000	0.0000
47.	O	0.0000	0.0000
48.	H	0.0000	0.0000
49.	C	0.0000	0.0000
50.	H	0.0000	0.0000
51.	H	0.0000	0.0000
52.	H	0.0000	0.0000
53.	C	0.9464	0.9451
54.	H	0.0005	0.0006
55.	H	0.0000	0.0005
56.	H	0.0005	0.0000

Table-9C-7-2: Wiberg index for salt bridge with 10 waters (bridge length=4.0 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0058	0.0111	0.0034	1.2507	0.0021	1.3016	0.0025	0.0026
2. H	0.0058	0.0000	0.9306	0.0011	0.0025	0.0022	0.0006	0.0000	0.0000
3. C	0.0111	0.9306	0.0000	0.9152	0.9578	0.0032	0.0029	0.0014	0.0002
4. H	0.0034	0.0011	0.9152	0.0000	0.0091	0.0031	0.0033	0.0011	0.0000
5. N	1.2507	0.0025	0.9578	0.0091	0.0000	0.7592	0.0811	0.0019	0.0081
6. H	0.0021	0.0022	0.0032	0.0031	0.7592	0.0000	0.0096	0.0002	0.0005
7. N	1.3016	0.0006	0.0029	0.0033	0.0811	0.0096	0.0000	0.7939	0.7164
8. H	0.0025	0.0000	0.0014	0.0011	0.0019	0.0002	0.7939	0.0000	0.0010

9.	H	0.0026	0.0000	0.0002	0.0000	0.0081	0.0005	0.7164	0.0010	0.0000
10.	N	1.3100	0.0002	0.0101	0.0020	0.0815	0.0016	0.0914	0.0096	0.0012
11.	H	0.0024	0.0001	0.0003	0.0000	0.0013	0.0006	0.0092	0.0007	0.0002
12.	H	0.0025	0.0002	0.0008	0.0000	0.0080	0.0002	0.0010	0.0002	0.0006
13.	O	0.0015	0.0000	0.0003	0.0000	0.0015	0.0000	0.0020	0.0001	0.0014
14.	O	0.0013	0.0000	0.0002	0.0000	0.0011	0.0003	0.0249	0.0005	0.0723
15.	C	0.0003	0.0000	0.0000	0.0000	0.0002	0.0000	0.0020	0.0001	0.0015
16.	C	0.0002	0.0000	0.0000	0.0000	0.0002	0.0000	0.0021	0.0001	0.0054
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
20.	O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
23.	O	0.0011	0.0000	0.0006	0.0002	0.0012	0.0001	0.0005	0.0001	0.0000
24.	H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
26.	O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	O	0.0003	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	O	0.0004	0.0000	0.0001	0.0000	0.0010	0.0004	0.0002	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000
34.	O	0.0001	0.0001	0.0025	0.0043	0.0002	0.0000	0.0003	0.0001	0.0000
35.	H	0.0000	0.0000	0.0005	0.0004	0.0000	0.0000	0.0001	0.0000	0.0000
36.	H	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
38.	O	0.0003	0.0000	0.0001	0.0001	0.0001	0.0000	0.0015	0.0002	0.0005
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
41.	O	0.0006	0.0000	0.0000	0.0000	0.0004	0.0002	0.0005	0.0001	0.0000
42.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
43.	O	0.0005	0.0006	0.0007	0.0001	0.0118	0.0279	0.0005	0.0000	0.0001
44.	H	0.0001	0.0000	0.0001	0.0000	0.0009	0.0001	0.0001	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000
46.	H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0007	0.0001	0.0000
47.	O	0.0007	0.0000	0.0006	0.0006	0.0003	0.0000	0.0071	0.0139	0.0001
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000
49.	C	0.0057	0.0026	1.0235	0.0020	0.0173	0.0019	0.0037	0.0002	0.0001
50.	H	0.0003	0.0118	0.0025	0.0015	0.0014	0.0000	0.0018	0.0001	0.0000
51.	H	0.0008	0.0012	0.0033	0.0007	0.0105	0.0001	0.0001	0.0000	0.0000
52.	H	0.0002	0.0017	0.0025	0.0116	0.0018	0.0001	0.0002	0.0001	0.0000
53.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	C	1.3100	0.0024	0.0025	0.0015	0.0013	0.0003	0.0002	0.0000	0.0000
2.	H	0.0002	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0101	0.0003	0.0008	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000

4. H	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0815	0.0013	0.0080	0.0015	0.0011	0.0002	0.0002	0.0000	0.0000
6. H	0.0016	0.0006	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
7. N	0.0914	0.0092	0.0010	0.0020	0.0249	0.0020	0.0021	0.0000	0.0001
8. H	0.0096	0.0007	0.0002	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000
9. H	0.0012	0.0002	0.0006	0.0014	0.0723	0.0015	0.0054	0.0001	0.0001
10. N	0.0000	0.7869	0.7221	0.0243	0.0022	0.0024	0.0017	0.0001	0.0003
11. H	0.7869	0.0000	0.0011	0.0006	0.0001	0.0001	0.0001	0.0000	0.0000
12. H	0.7221	0.0011	0.0000	0.0683	0.0011	0.0012	0.0043	0.0000	0.0002
13. O	0.0243	0.0006	0.0683	0.0000	0.1700	1.3517	0.0382	0.0053	0.0089
14. O	0.0022	0.0001	0.0011	0.1700	0.0000	1.4601	0.0351	0.0128	0.0020
15. C	0.0024	0.0001	0.0012	1.3517	1.4601	0.0000	0.9723	0.0061	0.0029
16. C	0.0017	0.0001	0.0043	0.0382	0.0351	0.9723	0.0000	0.9177	0.9281
17. H	0.0001	0.0000	0.0000	0.0053	0.0128	0.0061	0.9177	0.0000	0.0006
18. H	0.0003	0.0000	0.0002	0.0089	0.0020	0.0029	0.9281	0.0006	0.0000
19. H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0000	0.0000	0.0007	0.0004	0.0003	0.0001	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0001	0.0000	0.0000
22. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0003	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0002	0.0000	0.0001	0.0852	0.0043	0.0012	0.0010	0.0001	0.0000
26. O	0.0008	0.0000	0.0002	0.0220	0.0042	0.0072	0.0006	0.0003	0.0001
27. H	0.0002	0.0000	0.0000	0.0011	0.0001	0.0002	0.0001	0.0000	0.0000
28. H	0.0003	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0016	0.0003	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. O	0.0003	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000
38. O	0.0001	0.0000	0.0000	0.0025	0.0108	0.0052	0.0004	0.0003	0.0001
39. H	0.0001	0.0000	0.0000	0.0024	0.0365	0.0008	0.0006	0.0001	0.0000
40. H	0.0003	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0097	0.0210	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0006	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
47. O	0.0004	0.0001	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000
48. H	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
49. C	0.0034	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
50. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0001	0.0000	0.0000	0.0064	0.0119	0.0114	1.0221	0.0033	0.0024
54. H	0.0001	0.0000	0.0000	0.0016	0.0006	0.0017	0.0023	0.0010	0.0121
55. H	0.0000	0.0000	0.0001	0.0016	0.0013	0.0092	0.0017	0.0022	0.0010
56. H	0.0000	0.0000	0.0000	0.0004	0.0007	0.0010	0.0023	0.0124	0.0016

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0000	0.0001	0.0000	0.0000	0.0011	0.0001	0.0000	0.0001	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000
4. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
5. N	0.0000	0.0001	0.0000	0.0002	0.0012	0.0001	0.0000	0.0001	0.0000
6. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
7. N	0.0001	0.0003	0.0000	0.0000	0.0005	0.0001	0.0001	0.0001	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0000	0.0001	0.0000	0.0001	0.0003	0.0000	0.0002	0.0008	0.0002
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
13. O	0.0001	0.0007	0.0002	0.0000	0.0001	0.0000	0.0852	0.0220	0.0011
14. O	0.0001	0.0004	0.0001	0.0000	0.0001	0.0000	0.0043	0.0042	0.0001
15. C	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0012	0.0072	0.0002
16. C	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0010	0.0006	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
19. H	0.0000	0.7760	0.0007	0.0000	0.0006	0.0000	0.0000	0.0005	0.0000
20. O	0.7760	0.0000	0.6883	0.0005	0.0109	0.0272	0.0003	0.0166	0.0008
21. H	0.0007	0.6883	0.0000	0.0000	0.0005	0.0001	0.0001	0.0525	0.0001
22. H	0.0000	0.0005	0.0000	0.0000	0.7165	0.0006	0.0000	0.0000	0.0000
23. O	0.0006	0.0109	0.0005	0.7165	0.0000	0.7327	0.0000	0.0002	0.0000
24. H	0.0000	0.0272	0.0001	0.0006	0.7327	0.0000	0.0000	0.0001	0.0000
25. H	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.6455	0.0007
26. O	0.0005	0.0166	0.0525	0.0000	0.0002	0.0001	0.6455	0.0000	0.7738
27. H	0.0000	0.0008	0.0001	0.0000	0.0000	0.0000	0.0007	0.7738	0.0000
28. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0297	0.0000
29. O	0.0000	0.0002	0.0001	0.0000	0.0002	0.0000	0.0005	0.0116	0.0006
30. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000
31. O	0.0000	0.0002	0.0000	0.0012	0.0145	0.0006	0.0000	0.0002	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0001	0.0443	0.0001	0.0000	0.0000	0.0000
34. O	0.0000	0.0001	0.0000	0.0337	0.0124	0.0003	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0283	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
38. O	0.0009	0.0105	0.0005	0.0000	0.0002	0.0000	0.0001	0.0002	0.0000
39. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
41. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. O	0.0000	0.0002	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0003	0.0000	0.0004	0.0000	0.0000	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
3. C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0025	0.0005	0.0002
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043	0.0004	0.0002
5. N	0.0000	0.0001	0.0000	0.0010	0.0002	0.0003	0.0002	0.0000	0.0000
6. H	0.0000	0.0001	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000
7. N	0.0000	0.0002	0.0000	0.0002	0.0001	0.0001	0.0003	0.0001	0.0001
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0003	0.0016	0.0001	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000
11. H	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0002	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
14. O	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0002	0.0000	0.0002	0.0000	0.0001	0.0001	0.0000	0.0000
21. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0012	0.0000	0.0001	0.0337	0.0000	0.0001
23. O	0.0000	0.0002	0.0001	0.0145	0.0004	0.0443	0.0124	0.0010	0.0005
24. H	0.0000	0.0000	0.0000	0.0006	0.0000	0.0001	0.0003	0.0000	0.0000
25. H	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0297	0.0116	0.0004	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.7244	0.0007	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.7244	0.0000	0.6820	0.0197	0.0004	0.0005	0.0000	0.0000	0.0000
30. H	0.0007	0.6820	0.0000	0.0627	0.0001	0.0001	0.0000	0.0000	0.0000
31. O	0.0006	0.0197	0.0627	0.0000	0.7495	0.7003	0.0002	0.0000	0.0000
32. H	0.0000	0.0004	0.0001	0.7495	0.0000	0.0006	0.0000	0.0000	0.0000
33. H	0.0000	0.0005	0.0001	0.7003	0.0006	0.0000	0.0002	0.0000	0.0000
34. O	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.7828	0.7005
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7828	0.0000	0.0007
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7005	0.0007	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
38. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0001	0.1083	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0008	0.0304	0.0003	0.0006	0.0001	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0019	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0003	0.0001	0.0076	0.0177	0.0003	0.0000	0.0000	0.0000
44. H	0.0000	0.0001	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0002	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0001

47. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0166	0.0007	0.0494
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001
49. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0000	0.0003	0.0000	0.0000	0.0006	0.0001	0.0005	0.0001	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000
3. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0007	0.0001	0.0000
4. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
5. N	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000	0.0118	0.0009	0.0002
6. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0279	0.0001	0.0001
7. N	0.0002	0.0015	0.0002	0.0001	0.0005	0.0001	0.0005	0.0001	0.0001
8. H	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
10. N	0.0000	0.0001	0.0001	0.0003	0.0097	0.0009	0.0006	0.0001	0.0001
11. H	0.0000	0.0000	0.0000	0.0001	0.0210	0.0001	0.0003	0.0000	0.0001
12. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
13. O	0.0001	0.0025	0.0024	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
14. O	0.0005	0.0108	0.0365	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0001	0.0052	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0001	0.0004	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0283	0.0105	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0001	0.0002	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0001	0.0008	0.0000	0.0000	0.0000	0.0000
29. O	0.0000	0.0000	0.0000	0.1083	0.0304	0.0019	0.0003	0.0001	0.0002
30. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000
31. O	0.0000	0.0000	0.0000	0.0003	0.0006	0.0002	0.0076	0.0011	0.0003
32. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0177	0.0000	0.0001
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
34. O	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.7236	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.7236	0.0000	0.7074	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0007	0.7074	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.6339	0.0007	0.0003	0.0000	0.0000
41. O	0.0000	0.0000	0.0000	0.6339	0.0000	0.7707	0.0179	0.0009	0.0562

42. H	0.0000	0.0000	0.0000	0.0007	0.7707	0.0000	0.0012	0.0000	0.0001
43. O	0.0000	0.0000	0.0000	0.0003	0.0179	0.0012	0.0000	0.7757	0.6889
44. H	0.0000	0.0000	0.0000	0.0000	0.0009	0.0000	0.7757	0.0000	0.0007
45. H	0.0000	0.0000	0.0000	0.0000	0.0562	0.0001	0.6889	0.0007	0.0000
46. H	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. O	0.0006	0.0266	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0001	0.0922	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50	51	52	53	54
1. C	0.0000	0.0007	0.0000	0.0057	0.0003	0.0008	0.0002	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0026	0.0118	0.0012	0.0017	0.0000	0.0000
3. C	0.0001	0.0006	0.0000	1.0235	0.0025	0.0033	0.0025	0.0000	0.0000
4. H	0.0000	0.0006	0.0000	0.0020	0.0015	0.0007	0.0116	0.0000	0.0000
5. N	0.0001	0.0003	0.0000	0.0173	0.0014	0.0105	0.0018	0.0000	0.0000
6. H	0.0000	0.0000	0.0000	0.0019	0.0000	0.0001	0.0001	0.0000	0.0000
7. N	0.0007	0.0071	0.0003	0.0037	0.0018	0.0001	0.0002	0.0003	0.0000
8. H	0.0001	0.0139	0.0001	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000
9. H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
10. N	0.0001	0.0004	0.0001	0.0034	0.0004	0.0011	0.0002	0.0001	0.0001
11. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0064	0.0016
14. O	0.0001	0.0004	0.0002	0.0001	0.0000	0.0000	0.0000	0.0119	0.0006
15. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0114	0.0017
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0221	0.0023
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0033	0.0010
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0024	0.0121
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
26. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. O	0.0010	0.0166	0.0005	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
35. H	0.0000	0.0007	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0001	0.0494	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

37. H	0.0000	0.0006	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.0013	0.0266	0.0922	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
39. H	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.7752	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. O	0.7752	0.0000	0.6505	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0007	0.6505	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0001	0.0000	0.0000	0.9398	0.9418	0.9438	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.9398	0.0000	0.0006	0.0005	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.9418	0.0006	0.0000	0.0006	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.9438	0.0005	0.0006	0.0000	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9391
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9391	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9462	0.0005
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9446	0.0006

Atom	55	56
1. C	0.0000	0.0000
2. H	0.0000	0.0000
3. C	0.0000	0.0000
4. H	0.0000	0.0000
5. N	0.0000	0.0000
6. H	0.0000	0.0000
7. N	0.0001	0.0000
8. H	0.0000	0.0000
9. H	0.0002	0.0000
10. N	0.0000	0.0000
11. H	0.0000	0.0000
12. H	0.0001	0.0000
13. O	0.0016	0.0004
14. O	0.0013	0.0007
15. C	0.0092	0.0010
16. C	0.0017	0.0023
17. H	0.0022	0.0124
18. H	0.0010	0.0016
19. H	0.0000	0.0000
20. O	0.0000	0.0000
21. H	0.0000	0.0000
22. H	0.0000	0.0000
23. O	0.0000	0.0000
24. H	0.0000	0.0000
25. H	0.0000	0.0000
26. O	0.0000	0.0000
27. H	0.0000	0.0000
28. H	0.0000	0.0000
29. O	0.0000	0.0000
30. H	0.0000	0.0000
31. O	0.0000	0.0000

32.	H	0.0000	0.0000
33.	H	0.0000	0.0000
34.	O	0.0000	0.0000
35.	H	0.0000	0.0000
36.	H	0.0000	0.0000
37.	H	0.0000	0.0000
38.	O	0.0000	0.0000
39.	H	0.0000	0.0000
40.	H	0.0000	0.0000
41.	O	0.0000	0.0000
42.	H	0.0000	0.0000
43.	O	0.0000	0.0000
44.	H	0.0000	0.0000
45.	H	0.0000	0.0000
46.	H	0.0000	0.0000
47.	O	0.0000	0.0000
48.	H	0.0000	0.0000
49.	C	0.0000	0.0000
50.	H	0.0000	0.0000
51.	H	0.0000	0.0000
52.	H	0.0000	0.0000
53.	C	0.9462	0.9446
54.	H	0.0005	0.0006
55.	H	0.0000	0.0005
56.	H	0.0005	0.0000

Table-9C-7-3: Wiberg index for salt bridge with 10 waters (bridge length=4.2 angstroms)

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.0057	0.0113	0.0035	1.2667	0.0022	1.2916	0.0024	0.0023
2. H	0.0057	0.0000	0.9308	0.0011	0.0025	0.0022	0.0005	0.0000	0.0000
3. C	0.0113	0.9308	0.0000	0.9148	0.9544	0.0032	0.0029	0.0012	0.0002
4. H	0.0035	0.0011	0.9148	0.0000	0.0087	0.0030	0.0032	0.0010	0.0000
5. N	1.2667	0.0025	0.9544	0.0087	0.0000	0.7517	0.0820	0.0017	0.0081
6. H	0.0022	0.0022	0.0032	0.0030	0.7517	0.0000	0.0097	0.0001	0.0005
7. N	1.2916	0.0005	0.0029	0.0032	0.0820	0.0097	0.0000	0.7925	0.7379
8. H	0.0024	0.0000	0.0012	0.0010	0.0017	0.0001	0.7925	0.0000	0.0008
9. H	0.0023	0.0000	0.0002	0.0000	0.0081	0.0005	0.7379	0.0008	0.0000
10. N	1.3049	0.0003	0.0102	0.0020	0.0835	0.0017	0.0876	0.0095	0.0014
11. H	0.0024	0.0000	0.0002	0.0000	0.0011	0.0005	0.0091	0.0008	0.0002
12. H	0.0023	0.0002	0.0009	0.0000	0.0079	0.0002	0.0011	0.0002	0.0006
13. O	0.0011	0.0000	0.0002	0.0000	0.0013	0.0000	0.0017	0.0001	0.0016
14. O	0.0010	0.0000	0.0001	0.0000	0.0009	0.0002	0.0175	0.0004	0.0488
15. C	0.0003	0.0000	0.0000	0.0000	0.0002	0.0000	0.0014	0.0001	0.0013
16. C	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0017	0.0001	0.0047
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
20. O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000
21. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000
23. O	0.0012	0.0000	0.0005	0.0001	0.0012	0.0001	0.0006	0.0001	0.0000
24. H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
25. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

26. O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0003	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000
30. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. O	0.0005	0.0000	0.0001	0.0000	0.0010	0.0002	0.0002	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000
33. H	0.0001	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
34. O	0.0001	0.0001	0.0026	0.0043	0.0002	0.0000	0.0003	0.0001	0.0000
35. H	0.0000	0.0000	0.0005	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000
36. H	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
38. O	0.0003	0.0000	0.0001	0.0001	0.0001	0.0000	0.0014	0.0002	0.0005
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
41. O	0.0006	0.0000	0.0000	0.0000	0.0004	0.0002	0.0005	0.0001	0.0000
42. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
43. O	0.0006	0.0006	0.0007	0.0002	0.0132	0.0316	0.0006	0.0000	0.0001
44. H	0.0001	0.0000	0.0001	0.0000	0.0010	0.0001	0.0001	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000
46. H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0007	0.0001	0.0000
47. O	0.0007	0.0000	0.0005	0.0005	0.0003	0.0000	0.0071	0.0140	0.0001
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
49. C	0.0058	0.0027	1.0242	0.0021	0.0167	0.0019	0.0037	0.0002	0.0001
50. H	0.0003	0.0118	0.0025	0.0014	0.0015	0.0000	0.0017	0.0001	0.0000
51. H	0.0008	0.0012	0.0034	0.0007	0.0105	0.0001	0.0001	0.0000	0.0000
52. H	0.0002	0.0017	0.0025	0.0116	0.0018	0.0001	0.0002	0.0001	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. C	1.3049	0.0024	0.0023	0.0011	0.0010	0.0003	0.0002	0.0000	0.0000
2. H	0.0003	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0102	0.0002	0.0009	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
4. H	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5. N	0.0835	0.0011	0.0079	0.0013	0.0009	0.0002	0.0001	0.0000	0.0000
6. H	0.0017	0.0005	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
7. N	0.0876	0.0091	0.0011	0.0017	0.0175	0.0014	0.0017	0.0000	0.0000
8. H	0.0095	0.0008	0.0002	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000
9. H	0.0014	0.0002	0.0006	0.0016	0.0488	0.0013	0.0047	0.0001	0.0000
10. N	0.0000	0.7836	0.7404	0.0178	0.0018	0.0016	0.0015	0.0001	0.0002
11. H	0.7836	0.0000	0.0009	0.0005	0.0001	0.0001	0.0001	0.0000	0.0000
12. H	0.7404	0.0009	0.0000	0.0477	0.0012	0.0011	0.0039	0.0000	0.0002
13. O	0.0178	0.0005	0.0477	0.0000	0.1725	1.3545	0.0386	0.0054	0.0091
14. O	0.0018	0.0001	0.0012	0.1725	0.0000	1.4655	0.0361	0.0130	0.0021
15. C	0.0016	0.0001	0.0011	1.3545	1.4655	0.0000	0.9722	0.0060	0.0030
16. C	0.0015	0.0001	0.0039	0.0386	0.0361	0.9722	0.0000	0.9180	0.9280
17. H	0.0001	0.0000	0.0000	0.0054	0.0130	0.0060	0.9180	0.0000	0.0006
18. H	0.0002	0.0000	0.0002	0.0091	0.0021	0.0030	0.9280	0.0006	0.0000
19. H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0000	0.0000	0.0006	0.0004	0.0003	0.0001	0.0000	0.0000

21. H	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0001	0.0000	0.0000
22. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0002	0.0000	0.0001	0.0886	0.0043	0.0014	0.0012	0.0001	0.0000
26. O	0.0008	0.0000	0.0002	0.0226	0.0043	0.0072	0.0006	0.0003	0.0001
27. H	0.0002	0.0000	0.0000	0.0011	0.0001	0.0002	0.0001	0.0000	0.0000
28. H	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.0016	0.0003	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000
30. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31. O	0.0004	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0001	0.0001	0.0000	0.0000
38. O	0.0001	0.0000	0.0000	0.0025	0.0111	0.0051	0.0004	0.0003	0.0001
39. H	0.0000	0.0000	0.0000	0.0024	0.0386	0.0009	0.0008	0.0001	0.0000
40. H	0.0003	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0102	0.0224	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
42. H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0008	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
47. O	0.0004	0.0001	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000
48. H	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
49. C	0.0034	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
50. H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0001	0.0000	0.0001	0.0065	0.0122	0.0114	1.0219	0.0033	0.0024
54. H	0.0001	0.0000	0.0000	0.0017	0.0007	0.0017	0.0024	0.0010	0.0121
55. H	0.0000	0.0000	0.0001	0.0016	0.0014	0.0091	0.0017	0.0022	0.0010
56. H	0.0000	0.0000	0.0000	0.0004	0.0007	0.0010	0.0024	0.0124	0.0016

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0000	0.0001	0.0000	0.0000	0.0012	0.0001	0.0000	0.0001	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
4. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
5. N	0.0000	0.0001	0.0000	0.0002	0.0012	0.0001	0.0000	0.0001	0.0000
6. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
7. N	0.0001	0.0003	0.0000	0.0001	0.0006	0.0001	0.0000	0.0001	0.0000
8. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0000	0.0001	0.0000	0.0001	0.0003	0.0000	0.0002	0.0008	0.0002
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
13. O	0.0001	0.0006	0.0002	0.0000	0.0001	0.0000	0.0886	0.0226	0.0011
14. O	0.0001	0.0004	0.0001	0.0000	0.0000	0.0000	0.0043	0.0043	0.0001
15. C	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0014	0.0072	0.0002

16. C	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0012	0.0006	0.0001
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
19. H	0.0000	0.7763	0.0007	0.0000	0.0006	0.0000	0.0000	0.0005	0.0000
20. O	0.7763	0.0000	0.6878	0.0005	0.0111	0.0278	0.0003	0.0167	0.0007
21. H	0.0007	0.6878	0.0000	0.0000	0.0005	0.0001	0.0001	0.0527	0.0001
22. H	0.0000	0.0005	0.0000	0.0000	0.7167	0.0006	0.0000	0.0000	0.0000
23. O	0.0006	0.0111	0.0005	0.7167	0.0000	0.7313	0.0000	0.0002	0.0000
24. H	0.0000	0.0278	0.0001	0.0006	0.7313	0.0000	0.0000	0.0001	0.0000
25. H	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.6402	0.0007
26. O	0.0005	0.0167	0.0527	0.0000	0.0002	0.0001	0.6402	0.0000	0.7744
27. H	0.0000	0.0007	0.0001	0.0000	0.0000	0.0000	0.0007	0.7744	0.0000
28. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0302	0.0000
29. O	0.0000	0.0002	0.0001	0.0000	0.0002	0.0000	0.0005	0.0117	0.0006
30. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000
31. O	0.0000	0.0002	0.0000	0.0012	0.0146	0.0006	0.0000	0.0001	0.0000
32. H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
33. H	0.0000	0.0001	0.0000	0.0001	0.0445	0.0001	0.0000	0.0000	0.0000
34. O	0.0000	0.0001	0.0000	0.0336	0.0124	0.0003	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.0275	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
38. O	0.0009	0.0103	0.0005	0.0000	0.0002	0.0000	0.0001	0.0002	0.0000
39. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
41. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
44. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. O	0.0000	0.0002	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
48. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	28	29	30	31	32	33	34	35	36
1. C	0.0000	0.0003	0.0000	0.0005	0.0000	0.0001	0.0001	0.0000	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
3. C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0026	0.0005	0.0002
4. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043	0.0003	0.0002
5. N	0.0000	0.0001	0.0000	0.0010	0.0002	0.0003	0.0002	0.0000	0.0000
6. H	0.0000	0.0001	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
7. N	0.0000	0.0001	0.0000	0.0002	0.0001	0.0000	0.0003	0.0001	0.0001
8. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10. N	0.0002	0.0016	0.0001	0.0004	0.0000	0.0000	0.0001	0.0000	0.0000

11. H	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. O	0.0002	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
14. O	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0001	0.0002	0.0000	0.0002	0.0000	0.0001	0.0001	0.0000	0.0000
21. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0012	0.0000	0.0001	0.0336	0.0000	0.0001
23. O	0.0000	0.0002	0.0001	0.0146	0.0004	0.0445	0.0124	0.0010	0.0005
24. H	0.0000	0.0000	0.0000	0.0006	0.0000	0.0001	0.0003	0.0000	0.0000
25. H	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0302	0.0117	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.7224	0.0007	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000
29. O	0.7224	0.0000	0.6830	0.0194	0.0004	0.0005	0.0000	0.0000	0.0000
30. H	0.0007	0.6830	0.0000	0.0617	0.0001	0.0001	0.0000	0.0000	0.0000
31. O	0.0006	0.0194	0.0617	0.0000	0.7512	0.7001	0.0002	0.0000	0.0000
32. H	0.0000	0.0004	0.0001	0.7512	0.0000	0.0007	0.0000	0.0000	0.0000
33. H	0.0000	0.0005	0.0001	0.7001	0.0007	0.0000	0.0002	0.0000	0.0000
34. O	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.7827	0.6994
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7827	0.0000	0.0007
36. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6994	0.0007	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
38. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0001	0.1107	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
41. O	0.0008	0.0309	0.0003	0.0006	0.0001	0.0000	0.0000	0.0000	0.0000
42. H	0.0000	0.0019	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
43. O	0.0000	0.0003	0.0001	0.0075	0.0171	0.0003	0.0000	0.0000	0.0000
44. H	0.0000	0.0001	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
45. H	0.0000	0.0002	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
46. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0001
47. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0169	0.0007	0.0504
48. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001
49. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
53. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	37	38	39	40	41	42	43	44	45
1. C	0.0000	0.0003	0.0000	0.0000	0.0006	0.0001	0.0006	0.0001	0.0000
2. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000
3. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0007	0.0001	0.0000
4. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
5. N	0.0000	0.0001	0.0000	0.0000	0.0004	0.0000	0.0132	0.0010	0.0003

6. H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0316	0.0001	0.0001
7. N	0.0001	0.0014	0.0002	0.0001	0.0005	0.0001	0.0006	0.0001	0.0001
8. H	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9. H	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
10. N	0.0000	0.0001	0.0000	0.0003	0.0102	0.0009	0.0008	0.0001	0.0001
11. H	0.0000	0.0000	0.0000	0.0001	0.0224	0.0001	0.0004	0.0000	0.0001
12. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
13. O	0.0001	0.0025	0.0024	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
14. O	0.0005	0.0111	0.0386	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15. C	0.0001	0.0051	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16. C	0.0001	0.0004	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17. H	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. O	0.0275	0.0103	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0001	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. O	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26. O	0.0001	0.0002	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28. H	0.0000	0.0000	0.0000	0.0001	0.0008	0.0000	0.0000	0.0000	0.0000
29. O	0.0000	0.0000	0.0000	0.1107	0.0309	0.0019	0.0003	0.0001	0.0002
30. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000
31. O	0.0000	0.0000	0.0000	0.0003	0.0006	0.0002	0.0075	0.0010	0.0003
32. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0171	0.0000	0.0001
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
34. O	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37. H	0.0000	0.7246	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. O	0.7246	0.0000	0.7020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0006	0.7020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.6309	0.0007	0.0004	0.0000	0.0000
41. O	0.0000	0.0000	0.0000	0.6309	0.0000	0.7696	0.0182	0.0009	0.0576
42. H	0.0000	0.0000	0.0000	0.0007	0.7696	0.0000	0.0013	0.0000	0.0001
43. O	0.0000	0.0000	0.0000	0.0004	0.0182	0.0013	0.0000	0.7747	0.6863
44. H	0.0000	0.0000	0.0000	0.0000	0.0009	0.0000	0.7747	0.0000	0.0007
45. H	0.0000	0.0000	0.0000	0.0000	0.0576	0.0001	0.6863	0.0007	0.0000
46. H	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47. O	0.0006	0.0271	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48. H	0.0001	0.0946	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
50. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53. C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Atom	46	47	48	49	50	51	52	53	54

1.	C	0.0000	0.0007	0.0000	0.0058	0.0003	0.0008	0.0002	0.0000	0.0000
2.	H	0.0000	0.0000	0.0000	0.0027	0.0118	0.0012	0.0017	0.0000	0.0000
3.	C	0.0001	0.0005	0.0000	1.0242	0.0025	0.0034	0.0025	0.0000	0.0000
4.	H	0.0000	0.0005	0.0000	0.0021	0.0014	0.0007	0.0116	0.0000	0.0000
5.	N	0.0001	0.0003	0.0000	0.0167	0.0015	0.0105	0.0018	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0019	0.0000	0.0001	0.0001	0.0000	0.0000
7.	N	0.0007	0.0071	0.0003	0.0037	0.0017	0.0001	0.0002	0.0002	0.0000
8.	H	0.0001	0.0140	0.0000	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000
9.	H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
10.	N	0.0001	0.0004	0.0001	0.0034	0.0004	0.0011	0.0002	0.0001	0.0001
11.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
13.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0065	0.0017
14.	O	0.0001	0.0004	0.0002	0.0001	0.0000	0.0000	0.0000	0.0122	0.0007
15.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0114	0.0017
16.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0219	0.0024
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0033	0.0010
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0024	0.0121
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	O	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	O	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
26.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	O	0.0010	0.0169	0.0005	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000
35.	H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0001	0.0504	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0006	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	O	0.0013	0.0271	0.0946	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
39.	H	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	O	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.7749	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	O	0.7749	0.0000	0.6473	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0007	0.6473	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	C	0.0000	0.0001	0.0000	0.0000	0.9397	0.9413	0.9436	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.9397	0.0000	0.0006	0.0005	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.9413	0.0006	0.0000	0.0006	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.9436	0.0005	0.0006	0.0000	0.0000	0.0000
53.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9389

54. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9389	0.0000
55. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9467	0.0005
56. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9449	0.0006

Atom	55	56
1. C	0.0000	0.0000
2. H	0.0000	0.0000
3. C	0.0000	0.0000
4. H	0.0000	0.0000
5. N	0.0000	0.0000
6. H	0.0000	0.0000
7. N	0.0001	0.0000
8. H	0.0000	0.0000
9. H	0.0001	0.0000
10. N	0.0000	0.0000
11. H	0.0000	0.0000
12. H	0.0001	0.0000
13. O	0.0016	0.0004
14. O	0.0014	0.0007
15. C	0.0091	0.0010
16. C	0.0017	0.0024
17. H	0.0022	0.0124
18. H	0.0010	0.0016
19. H	0.0000	0.0000
20. O	0.0000	0.0000
21. H	0.0000	0.0000
22. H	0.0000	0.0000
23. O	0.0000	0.0000
24. H	0.0000	0.0000
25. H	0.0000	0.0000
26. O	0.0000	0.0000
27. H	0.0000	0.0000
28. H	0.0000	0.0000
29. O	0.0000	0.0000
30. H	0.0000	0.0000
31. O	0.0000	0.0000
32. H	0.0000	0.0000
33. H	0.0000	0.0000
34. O	0.0000	0.0000
35. H	0.0000	0.0000
36. H	0.0000	0.0000
37. H	0.0000	0.0000
38. O	0.0000	0.0000
39. H	0.0000	0.0000
40. H	0.0000	0.0000
41. O	0.0000	0.0000
42. H	0.0000	0.0000
43. O	0.0000	0.0000
44. H	0.0000	0.0000
45. H	0.0000	0.0000
46. H	0.0000	0.0000
47. O	0.0000	0.0000
48. H	0.0000	0.0000

49. C 0.0000 0.0000
50. H 0.0000 0.0000
51. H 0.0000 0.0000
52. H 0.0000 0.0000
53. C 0.9467 0.9449
54. H 0.0005 0.0006
55. H 0.0000 0.0005
56. H 0.0005 0.0000

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