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COMPUTER GENERATION OF SUBDUCTION FREQUENCIES FOR 2ND ORDER PHASE TRANSITIONS IN 2-DIMENSIONS

by

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Abstract

COMPUTER GENERATION OF SUBDUSTION FREQUENCIES FOR 2ND ORDER PHASE TRANSITIONS IN 2 - DIMENSIONS

by

Samaroo Deonarine

Adviser : Professor Joseph L. Birman

The Landau theory of 2nd order phase transitions and Group theory Criteria are used to predict which subgroups $G \subseteq G_o$ can occur in transitions for 2-D systems (plane-group to plane-group and diperiodic to diperiodic) . Previous work [1] on the 17 plane space groups has been based on the tables of Coxeter & Moser [2] and the International Tables of X-ray Crystallography (ITXRC,1965) [3] . These tables do not exhaust all the possible subgroups of a space group [4] . Since such explicit tables are non-existent for other families of space groups we have developed algorithms that make a systematic search of the parent unit cell of G_o to locate the origin and orientation of all its subgroups G ,$G \subseteq G_o$.

We have written a RATFOR/FORTRAN program for the VAX 11-780 which will generate the subduction frequencies n : $n\,\Gamma_G^{1+} \in (D_{G_o}^{j,k} \downarrow G)$ for allowed second order phase transitions in 2- dimensional systems that are describable by the 80 diperiodic Groups G_o and G [5] .

Our program gives a complete tabulation(Origin,new Translation Sublattice, Subduction Frequency , Subgroup and its Generators) of the allowed continuous or second order phase transitions from a parent diperiodic group G_o to a another diperiodic subgroup G .

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DEDICATED TO MY PARENTS

WHO ARE SO FAR AWAY

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INTRODUCTION

Two dimensional systems are being widely studied at the present time [6 - 9] . Improvements in technology have made it possible to realise and analyse quasi - 2 dimensional systems such as admolecule arrays , submonolayers , Graphite Intercalation Compounds (*GIC's*) [10] and 2-D magnets [11] . Information on surface reconstruction and catalytic activity have important industrial applications . In addition these systems allow us to test exactly solvable quantum mechanical models and to study the role of fluctuations in low dimensions *'D'* ($D < 3$) [12,13].

One aspect of phase transitions in 2-D that has received comparatively little attention is concerned with the symmetry change from an initial phase describable by a 2-D crystallographic group G_0 to a another phase of lower symmetry with crystallographic space group symmetry G , $G \subseteq G_0$. The valid space groups are the 80 diperiodic groups which describe the symmetry of a layer or 2-sided plane [14] . This thesis deals with symmetry changes from such systems.

Previous work on surfaces [15] has lead to a listing of all the universality classes for transitions based on the 17 plane space groups and the magnetic space groups [16] . This would serve as a basis for studies on their critical hehaviour using renormalization group methods [6,12] .

Studies on continuous or second order phase transitions rely heavily on the traditional Landau theory [17,18]. However important extensions and deeper insight into the nature of the symmetry change have been made by subsequent workers . These include various group theory criteria that simplify and serve as an alternative to the traditional hand calculations , which can be quite lengthy and tedious for multi-component order parameters (*Liubarskii*,[18]). In order to fully utilise these selection rules reliable and complete listings of Group - Subgroup relations , such as those recently published hy *Billiet et al* . [4] only for the 17 plane space groups are absolutely essential .

Even so the usual hand calculation would be too time consuming and prone to human error . The use of a computer in Group theory applications overcomes many of these obstacles.Accordingly we have written a RATFOR - FORTRAN program for the VAX 11-780 which will generate the subduction frequencies ' n ' for allowed 2nd order phase transitions in 2-D systems at points **k** of high symmetry in the 2-D Brillouin Zones ($\mathbf{k} \neq 0$) . The program can be easily adapted for the $\mathbf{k}= 0$ (trivial) case .

The chain subduction criteria [19-21] are used to determine which subgroups can result from such transitions and to eliminate those which cannot be derived from a parent phase G_o . Using the algorithms we have developed , the parent unit cell of G_0 is explored for all possible origins that may site the origin of the subgroup G . We thereby overcome the handicap of not having tables on group-subgroup relations for the 80 diperiodic groups .

Work on the subduction frequencies for the 17 plane space groups has already been done us [1] and others [22]. However additional *fine structure* details for this family that show the distinct members of an allowed subgroup class **G** were not included with the subduction frequencies *n*. Preliminary results for **P4** were presented by us earlier [23]. Complete results of the latter type has been generated by our programs for the 17 plane space groups (APPENDIX III).

Chapter 1
LANDAU THEORY

1.1 The Landau theory of second order phase transitions

The Landau theory is based on a thermodynamic potential Φ and a density function $\rho(\vec{r})$ [17,18] . The order parameters **C** may be taken as bases $\{C_\alpha^j\}$ for a single irreducible representation *(irrep)* $D_{G_o}^j$ of G_o [21].
The free energy $\Phi(C)$ is a scalar or invariant function of the $\{C_\alpha^j\}$ i.e. for every matrix transformation $D_{G_o}^j(g)$ with g taken as some element $\{\phi|t\}$ in the space-group G_o , we have

$$\Phi(D_{G_o}^j(g)\{C_\alpha^j\}) = \Phi(\{C_\alpha^j\}) \tag{1.1}$$

The density function $\rho(\vec{r})$ is expressed as

$$\rho(\vec{r}) = \rho_o(\vec{r})+\delta\rho(\vec{r}) \tag{1.2}$$

where

$$\rho_o(\vec{r}) = \rho_o(g^{-1}\vec{r}) \tag{1.3}$$

is invariant under all the transformations 'g' of G_o .

The symmetry breaking density $\delta\rho(\vec{r})$ is invariant only under a subset of operations $\bar{g}$;

$$\delta\rho(\vec{r}) = \delta\rho(\bar{g}^{-1}\vec{r}) \tag{1.4}$$

By the group-theoretical completeness theorem any function on the group G_o may be expanded in a complete set consisting of basis functions from all the irreducible representations of G_o [21].

Thus

$$\delta\rho(\vec{r}) = \sum_j\sum_\alpha C_\alpha^j\,\psi_\alpha^j(\vec{r}) \tag{1.5}$$

where the $\{\psi_\alpha^j(\vec{r})\}, \alpha=1,...l_j$ are bases for *irreps* $D^j_{G_o}$:

$$\psi^j_\alpha(\bar{g}^{-1}\vec{r}) = \sum_\beta [D^j_{G_o}(g)]_{\beta\alpha}\psi^j_\beta(\vec{r}) \quad (1.6)$$

We assume that the order parameters which are bases for a single *irrep* $D^j_{G_o}$ *drive* the transition . This is consistent with standard group-theoretical arguments of treating each *irrep* separately [21] . The broken symmetry density is then

$$\delta\rho(\vec{r}) = \sum_{\alpha=1}^{l_j} C^j_\alpha \psi^j_\alpha(\vec{r}) \quad (1.7)$$

In an expansion such as Eq. (1.7) we may equally well take $\{C^j_\alpha\}$ to be bases for $D^j_{G_o}$; thus we use the same set in Φ as in $\delta\rho(\vec{r})$. Different broken-symmetry densities can arise from different sets of coefficients : $\{C^j_1, C^j_2, \cdots, C^j_{l_j}\}$. We call such a set $\{\bar{C}^j_\alpha\}$; it may arise from solving an extremum problem [18] for $\Phi(\{C^j_\alpha\})$.

$$\delta\bar{\rho}(\vec{r}) = \sum_{\alpha=1}^{l_j} \bar{C}^j_\alpha \psi^j_\alpha(\vec{r}) \quad (1.8)$$

with

$$\bar{g}\,\delta\bar{\rho}(\vec{r}) = \delta\bar{\rho}(\bar{g}^{-1}\vec{r}) = \delta\bar{\rho}(\vec{r}) \quad (1.9)$$

The subset $\{\bar{g}\}$ defined by Eq.(1.9) determines the broken - symmetry subgroup $\bar{G}$ and the transition $G_o \to \bar{G}$ occurs via $D^j_{G_o}$. Φ is expanded in a series of homogenous $D^j_{G_o}$ invariant polynomials in the order parameters $\{C^j_1, C^j_2, \cdots, C^j_{l_j}\}$. Since the transformation is homogenous , terms of any given degree are transformed among themselves by $D^j_{G_o}$. It is usual to take each term itself to be $D^j_{G_o}$ invariant .

$$\Phi = \Phi_o + af^{\,2} + \sum_\sigma b^4_\sigma f^{\,4}_\sigma + \sum_\rho b^6_\rho f^{\,6}_\rho + \ldots\ldots \quad (1.10)$$

where $f^{s}_{\sigma}(\{C^{j}_{\alpha}\})$ is a homogenous polynomial of s^{th} degree which is $D^{j}_{G_o}$ invariant .

$$f^{s}_{\sigma}(\{\lambda C^{j}_{\alpha}\}) = \lambda^{s} f^{s}_{\sigma}(\{C^{j}_{\alpha}\})$$

$$f^{s}_{\sigma}(D^{j}_{G_o}(g)\{C^{j}_{\alpha}\}) = f^{s}_{\sigma}(\{C^{j}_{\alpha}\}) \qquad (1.11)$$

the sum in Eq. (1.10) is over all linearly independent f^{s}_{σ} of degree s .

Φ is then extremized by solving the equations resulting from

$$\vec{\nabla}_{\{C^{j}_{\alpha}\}}\Phi = 0 \qquad (1.12)$$

or

$$\left|\frac{\partial\Phi}{\partial C^{j}_{\beta}}\right|_{\{\bar{C}\}} = 0\ ; \qquad \beta = 1,...l_j \qquad (1.13)$$

This step produces l_j homogenous algebraic equations (not all of which are independent) each of degree N - 1 , where N is the degree of the highest polynomial f^{N}_{σ} retained in Eq. (1.10) . Let $\{\bar{C}^{j}_{\alpha}\}$ be an extremezing set of solutions . Further let the eigenvalues ω_γ of the Hessian matrix of Φ evaluated at $\{\bar{C}^{j}_{\alpha}\}$ all be positive , so that Φ is a minimum at $\{\bar{C}^{j}_{\alpha}\}$.

$$diag\left|\left|H_{\alpha\beta}\right|\right| \equiv diag\left|\left|\frac{\partial^2\Phi}{\partial C^{j}_{\alpha}\partial C^{j}_{\beta}}\right|_{\{\bar{C}\}}\right| \qquad (1.14)$$

$$\omega_\gamma > 0\ ;\ \gamma = 1,...l_j$$

Among all mimima , let $\{\bar{C}^{j}_{\alpha}\}$ be an absolute minima . Then $\Phi(\{\bar{C}^{j}_{\alpha}\})$ is a stable value of the Landau free energy , and the set of order parameters $\{\bar{C}^{j}_{\alpha}\}$ corresponds to a stable miminum of the free energy Φ. The broken-symmetry density for this equilibrium is :

$$\delta\bar{\rho}(\vec{r}) = \sum_{\alpha=1}^{l_j} \bar{C}^{j}_{\alpha}\psi^{j}_{\alpha}(\vec{r}) \qquad (1.8)$$

The group $\overline{G}$ is the invariance or isotrophy group of this $\delta\overline{\rho}(\vec{r})$. The second order transition $G_o \rightarrow \overline{G}$ is permitted . Renormalization - scaling theories [12,24] are usually based on a $D^j_{G_o}$ invariant Landau-Ginzburg-Wilson (LGW) Hamiltonian truncated at the 4^{th} degree :

$$H(\{\psi^j_\alpha\}) = af^{\,2}(\{\psi^j_\alpha\}) + rf^{\,2}(\{\vec{\nabla}\psi^j_\alpha\}) + \sum_\sigma u_\sigma f^{\,4}_\sigma(\{\psi^j_\alpha\}) + \cdots \quad (1.15)$$

The renormalization program results in a step by step scaling of the coupling parameters $(a, r, u_1, \ldots) \rightarrow (a', r', u'_1, \ldots) \rightarrow \ \ldots.$
If this process converges to a stable fixed point

$$\ldots\ldots \rightarrow (a^*, r^*, u^*, \cdots)$$

the resulting Hamiltonian or free energy

$$H^* = a^* f^{\,2}(\{\psi^j_\alpha\}) + r^* f^{\,2}(\{\vec{\nabla}\psi^j_\alpha\}) + \sum_\sigma u^*_\sigma f^{\,4}_\sigma(\{\psi^j_\alpha\}) + \cdots \quad (1.16)$$

corresponds to an allowed transition . The stable parameters $(a^*, r^*, u^* \cdots)$ give a set of coefficients $\overline{C}^j_\alpha(a^*, r^*, u^*_\sigma, \cdots)$ and a density $\delta\overline{\rho}$

$$\delta\overline{\rho}(\vec{r}) = \sum_\alpha \overline{C}^j_\alpha(a^*, r^*, u^*_\sigma, \cdots)\psi^j_\alpha(\vec{r}) \quad (1.17)$$

As before $\overline{G}$ is the isotrophy group of Eq. (1.17) .

The particular form of the Landau-Lifshitz series expansion as in Eq. (1.10) leads to certain selection rules . The transition temperature for $G_o \rightarrow \overline{G}$ is determined by the vanishing of the coefficient of the quadratic term i.e. $a(T) = 0$. For the transition to be simple only one such quadratic term should be present ; thus only one *irrep* $D^j_{G_o}$ drives a simple transition .

For Φ to be stable at the origin where all $C_\alpha^j = 0$, we require that the cubic term be absent in Eq.(1.10) or in Eq. (1.15) . Hence the symmetrized cube of the *irrep* $D_{G_o}^j$ should not contain the trivial representation $\Gamma_{G_o}^{1+}$

$$\Gamma_{G_o}^{1+} \notin \left[D_{G_o}^j\right]^3 \qquad (\mathrm{I})$$

In order that the free energy should correspond to homogenous phase transitions, the *Lifshitz invariant* $C_\alpha^j \frac{\partial \Phi}{\partial C_\beta^j} - C_\beta^j \frac{\partial \Phi}{\partial C_\alpha^j}$ should be absent . This implies that the anti-symmetrized square of $D_{G_o}^j$ should not contain a representation in common with the polar-vector representation $D_{G_o}^v$:

$$\Gamma_{G_o}^{1+} \notin \left\{D_{G_o}^j\right\}^2 \otimes D_{G_o}^v \qquad (\mathrm{II})$$

A *physically* irreducible representation that satisfies the Landau and Lifshitz conditions I and II respectively is said to be both Landau and Lifshitz *active*.

1.2 Group Theory Criteria

The direct determination of allowed second-order(continuous) symmetry changing phase transitions in solids and other systems has been a challenging topic of continuing interest [25] . A particular objective of such work [26] is the derivation of selection rules that predict whether a transition may occur from group G_o (given here as a higher symmetry group) to group $\bar{G}$, as a simple second order phase transition driven by a specified set of order parameters . We have denoted the latter $\{C^j_\alpha\}$, with j fixed and $\alpha = 1,\dots\ l_j$.

It is usual to discuss this question in the general framework of the *Landau Theory* of second order phase transitions . In the present work *direct determination* means the use of group-theoretically derived [27] criteria to give explicit predictions of allowed/forbidden group-subgroup transitions . The standard implementation of Landau's program requires the explicit algebraic extremization and then minimization of a 4^{th} or higher degree polymonial (Eq. 1.10) . It is this step which one wishes to bypass by use of direct methods to determine symmetry change .

The general statements just given already result in some restrictions on allowable transitions determined group theoretically i.e. selection rules without need for algebraic calculations . Evidently $\bar{G}$ must be a subgroup of G_o :

$$\bar{G} \subseteq G_o \qquad\qquad (A)$$

This selection rule was already known to Landau [28] . If $\{C^j_\alpha\}$ is a basis for $D^j_{G_o}$ and some subset of the $\{C^j_\alpha\}$ is a basis for the trivial (scalar) representation $\Gamma^{1+}_{\bar{G}}$, it follows that the restriction of $D^j_{G_o}$

to the subgroup $\bar{G}$ must contain $\Gamma_{\bar{G}}^{1+}$ at least once. This is the simple subduction criterion [29] :

$$\textit{If } \Gamma_{\bar{G}}^{1+} \in (D_{G_o}^{j} \downarrow \bar{G}) \quad \text{then the transition } G_o \rightarrow \bar{G} \textit{ may occur.} \qquad (B)$$

The subduction criterion is a necessary condition which must be satisfied if representation $D_{G_o}^{j}$, which is used in expanding the broken-symmetry density $\delta\bar{\rho}(\vec{r})$ (Eq. 1.8) is to be consistent with invariance under $\bar{G}$. This criterion can be applied to any *irrep* $D_{G_o}^{j}$ and tests the possibility of a transition $G_o \rightarrow \bar{G}$ to any subgroup $\bar{G}$.

However the simple sybduction criterion is not sufficiently restrictive. If the subgroup $\bar{G}$, satisfies (B) $\bar{G} \subseteq G_o$ so will every subgroup $\bar{\bar{G}}$ of $\bar{G}$. A broken symmetry density $\delta\bar{\rho}(\vec{r})$ invariant under the group $\bar{G}$ is also invariant under any subgroup of $\bar{G}$. The actual symmetry group of $\delta\bar{\rho}(\vec{r})$ is the maximal subgroup of a sequence of subgroups .

A criterion can be formulated in order to examine a chain of subgroups . Let

$$G_o \supseteq \bar{G} \supseteq \bar{\bar{G}} \qquad (C1)$$

be a three chain of maximal subgroups . Let the *irrep* $D_{G_o}^{j}$ satisfy

$$\Gamma_{\bar{G}}^{1+} \in (D_{G_o}^{j} \downarrow \bar{G}) \quad \text{and} \quad \Gamma_{\bar{\bar{G}}}^{1+} \in (D_{G_o}^{j} \downarrow \bar{\bar{G}}) \qquad (C2)$$

Here subduction ($\downarrow$) onto each of $\bar{G}$ and $\bar{\bar{G}}$ contains the trivial *irreps* $\Gamma_{\bar{G}}^{1+}$ and $\Gamma_{\bar{\bar{G}}}^{1+}$ each once . Then the chain subduction criterion [19] states that the transition

$$G_o \rightarrow \bar{G} \textit{ may occur but } G_o \rightarrow \bar{\bar{G}} \textit{ does not occur} \qquad (C3)$$

In a similar way we include multiplicity [20] .

Again considering the three chain (C1) , let

$$p\,\Gamma^{1+}_{\bar{G}} \in \ (D^{j}_{G_o} \downarrow \bar{G}) \quad \text{and} \quad q\,\Gamma^{1+}_{\bar{\bar{G}}} \in \ (D^{j}_{G_o} \downarrow \bar{\bar{G}}) \qquad \text{(C4)}$$

where *p,q are integers* . If $p = q$ then each of the trivial *irreps* $\Gamma^{1+}_{\bar{G}}$ maps onto one counterpart $\Gamma^{1+}_{\bar{\bar{G}}}$ without exception and we obtain the chain subduction criterion with equal multiplicity :

$$G_o \rightarrow \bar{G} \ \textit{may occur, but} \ G_o \rightarrow \bar{\bar{G}} \ \textit{does not occur} \qquad \text{(C5)}$$

A further extension was recently formulated [26] in case $p < q$. In this cae as we descend down the chain of maximal subgroups , a break occcurs at $\bar{\bar{G}}$. The p $\Gamma^{1+}_{\bar{G}}$ that are contained in $(D^{j}_{G_o} \downarrow \bar{G})$ each map onto a counterpart $\Gamma^{1+}_{\bar{\bar{G}}}$. In addition $(q - p)$ new trivial *irreps* $\Gamma^{1+}_{\bar{\bar{G}}}$ arise at the step $\bar{G} \rightarrow \bar{\bar{G}}$. Some *irrep* $D^{i}_{\bar{G}}$ of $\bar{G}$ restricted to $\bar{\bar{G}}$, produce additional *irreps* $\Gamma^{1+}_{\bar{\bar{G}}}$:

$$p\,\Gamma^{1+}_{\bar{G}} + D^{i}_{\bar{G}} + \cdots \quad \in (D^{j}_{G_o} \downarrow \bar{G}) \qquad \text{(1.2.1)}$$

and

$$(q-p)\,\Gamma^{1+}_{\bar{\bar{G}}} + \cdots \quad \in (D^{j}_{G_o} \downarrow \bar{\bar{G}}) \qquad \text{(1.2.2)}$$

Increasing multiplicity as we descend the chain appears to give rise to higher order critical transitions . Hence a chain subduction criterion with increasing multiplicity was proposed :

If $p < q$, $G_o \rightarrow \bar{G}$ *may occur as a simple second order transition and* $G_o \rightarrow G$ *may occur as a higher order critical transition* (C6)

These necessary selection rules appear to exhaust the presently available direct group-theoretically derived tools for analysing the possible occurence of transitions from group G_o to any subgroup G via *irrep* $D^{j}_{G_o}$, without algebraic computations (including in the latter , renormalization- scaling calculations) based on a power series expanded free energy (Eq. 1.10).

1.3.1 Comments on the test for Landau Activity

The actual test for Landau activitity (Rule (I) , page 5) can be quite intricate at points k $\neq 0$ in the Brillouin Zone for non-symmorphic space groups . A formula (see Eq. 1.3.5 below) recently given by Koscinski [30] is based on the use of multiplier irreps of G_{k_o} which is the point group of the wave-vector group G_k { the little group method } . We show below that this formula holds only in special cases . Alternative tests for Landau activity are based on work of P. Gard [31] ; these were utilized by Cracknell Davies Miller and Love { CDML } in their Kronecker Product Tables - Vol. I of 4 Volumes [32] .

Following Liubarski [18] , the symmetrized cube of $D^{j}_{G_o}$, $\left[\chi(g)\right]^3$ is given by

$$\left[\chi(g)\right]^3 = \frac{1}{3}\chi(g^3) + \frac{1}{2}\chi(g^2)\chi(g) + \frac{1}{6}\chi^3(g) \qquad (1.3.1)$$

where $\chi(g)$ is the character of the element g in $D^{j}_{G_o}$ ..

A similar formula has been given by Koscinski :

$$\left[\chi(D_k)\right]^3(g) = \frac{1}{3}\chi(D_k(g^3)) + \frac{1}{2}\chi(D_k(g^2))\chi(D_k(g)) + \frac{1}{6}(\chi(D_k(g)))^3 \qquad (1.3.2)$$

where $g = \{R \mid \vec{\tau}\}$ and

$$\chi(D_k(g)) = e^{-i\vec{k}\cdot\vec{\tau}}\chi(\Gamma_k(R)) \qquad (1.3.3)$$

Γ_k is the multiplier *irrep* of G_{k_o} and $\chi(\Gamma_k(R))$ is the character of R in G_{k_o} ; let $|F|$ be the order of G_{k_o}. Then Koscinski's test for *Landau activity* is

$$\frac{\sigma}{|F|}\sum_{R\in G_{k_o}}\left|\chi(D_k)\right|^3(g) = 0 \qquad (1.3.4)$$

σ is number of vectors (arms) in *star* k (*k).

Using $\chi(D_k(g^3)) = e^{-i\vec{k}\cdot(\vec{\tau} + R\vec{\tau} + R^2\vec{\tau})}\chi(\Gamma_k(R^3))$

and $\chi(D_k(g^2)) = e^{-i\vec{k}\cdot(\vec{\tau} + R\vec{\tau})}\chi(\Gamma_k(R^2))$

this test for Landau activity becomes

$$\frac{\sigma}{|F|}\sum_{R\in G_{k_o}}\frac{1}{3}e^{-i\vec{k}\cdot(\vec{\tau} + R\vec{\tau} + R^2\vec{\tau})}\chi(\Gamma_k(R^3)) + \frac{1}{2}e^{-i\vec{k}\cdot(2\vec{\tau} + R\vec{\tau})}\chi(\Gamma_k(R^2))\chi(\Gamma_k(R)) + \frac{1}{6}e^{-3i\vec{k}\cdot\vec{\tau}}\chi(\Gamma_k(R))^3 = 0 \qquad (1.3.5)$$

Since tables of the multiplier *irreps* of all 230 3-D space groups have been tabulated (*Kovalev*) [33] it would appear that this test is a straightfoward and simple one . We will now show that Koscinski's formula Eq. 1.3.5 is a special case of the more general formula also based on the *little group method* .

Let *k $= (k^1, k^2, \ldots . k^n)$ with $k = k^1$ as its representative arm . If G_k is the group of this wave-vector then the coset decomposition of G_k with respect to G_o is [34] :

$$G_o = g^1G_k + g^2G_k + \ldots + g^nG_k \qquad (1.3.6)$$

Here $g^l = \{R^l\,|\,\vec{\tau}'^l\}$ is the l^{th} coset representative and $k^l = R^l k$ is the l^{th} arm of *k ; $g^1 = E$ is the identity element .

Let $\chi_k^j(g)$ be the character of the element $g = (R \mid \vec{\tau})$ in the induced representation $D_{G_o}^{j,k}$ of G_o. G_k^j is the j^{th} *irrep* of G_k.

$$\chi_k^j(g) = \chi(G_k^j(g) \uparrow G_o) \qquad (1.3.7)$$

We then have [ ]

$$\chi_k^j(g) = \sum_{l=1}^{n} e^{-i\vec{k}^l\cdot(\vec{\tau} + R\vec{\tau}^l - \vec{\tau}^l)} \chi^j(\Gamma_k\{(R^l)^{-1}RR^l\})\delta_{Rk^l,k^l} \qquad (1.3.8)$$

$$\chi_k^j(g^2) = \sum_{l=1}^{n} e^{-i\vec{k}^l\cdot(\vec{\tau} + R\tau + R\vec{\tau}^l - \vec{\tau}^l)} \chi^j(\Gamma_k\{(R^l)^{-1}R^2R^l\})\delta_{R^2k^l,k^l} \qquad (1.3.9)$$

$$\chi_k^j(g^3) = \sum_{l=1}^{n} e^{-i\vec{k}^l\cdot(\vec{\tau} + R\tau + R^2\vec{\tau} + R\vec{\tau}^l - \vec{\tau}^l)} \chi^j(\Gamma_k\{(R^l)^{-1}R^3R^l\})\delta_{R^3k^l,k^l} \qquad (1.3.10)$$

$$(\chi_k^j(g))^3 = \sum_{l=1}^{n}\sum_{l'=1}^{n}\sum_{l''=1}^{n} e^{-i(\vec{k}^l + \vec{k}^{l'} + \vec{k}^{l''})\cdot\vec{\tau}} e^{-i\vec{k}^l\cdot(\vec{\tau}^l + R^{l'}\vec{\tau}^{l'} + R^{l''}\vec{\tau}^{l''})}$$
$$e^{-iR^{-1}(\vec{k}^l\cdot\vec{\tau}^l + \vec{k}^{l'}\cdot\vec{\tau}^l + \vec{k}^{l}\cdot\vec{\tau}^l)} \chi^j(\Gamma_k\{(R^l)^{-1}RR^l\})\delta_{Rk^l,k^l}$$
$$\chi^j(\Gamma_k\{(R^{l'})^{-1}RR^{l'}\})\delta_{Rk^{l'},k^{l'}} \chi^j(\Gamma_k\{(R^{l''})^{-1}RR^{l''}\})\delta_{Rk^{l''},k^{l''}} \qquad (1.3.11)$$

Comparing Eq. 1.3.8 - Eq. 1.3.11 with the corresponding terms in Eq. 1.3.5 we will find Eq. 1.3.5 to be true : -

(i) only if the coset reps are chosen so that they are purely rotational , i.e. $\vec{\tau}^l = 0$, for all l

(ii) all the arms in *k contribute equally to $\chi_k^j(g)$

(iii) $l = l' = l''$ or if $l = 1$

Koscinski's formula is obviously true for symmorphic space groups and for the Γ point $\mathbf{k} = 0$.

1.3.2 Comments on the Selection Rules

The Group theory Criteria (A - C6) are all necessary conditions for symmetry breaking in continuous phase transitions . Their sufficiency has not yet been established . While the subduction criterion may correspond to the algebraic step

$$\frac{\partial \Phi}{\partial C_{\alpha}^{j}} = 0$$

there is no selection rule for the next one

$$\frac{\partial^2 \Phi}{\partial C_{\alpha}^{j} \partial C_{\beta}^{j}} > 0$$

Work , both geometric and group theoretical , is in progress on this aspect of the theory . The continuous rotational symmetry of order parameter space under SU_N transformations and the analytic properties of the free energy $\Phi(C)$ are being investigated by us [35] .

According to the *Landau theory* only *active* representations can produce second order phase transitions . This selection rule limits the $D_{G_o}^{j}$ which may be considered . It limits the allowable *physical* order parameters for continuous transitions to those which transform according to *one* active $D_{G_o}^{j}$.

Series expansions [1.10] also give rise to two very general *Landau index theorems* [17,36] .

A transition $G_o \rightarrow \bar{G}$ *is permitted if* $\left| G_o / \bar{G} \right| = 2$ (III)

A transition $G_o \rightarrow \bar{G}$ *is prohibited if* $\left| G_o / \bar{G} \right| = 3$ (IV)

An additional *selection rule* , of a different type has been proposed based on the renormalization program [37] .

A continuous transition occurs if H has a non-trivial fixed point (V)

This is not a group-theoretically based rule but one originating in the renormalization calculations . Recent work on fluctuation - driven transitions has resulted in some clarification of rule (V) . Going back to the *LGW* Hamiltonian for an *active irrep* $D^j_{G_o}$, a stability region can be defined . It is a region in the $\{u_\sigma\}$ space where the 4^{th} degree term in Eq. 1.10 will be positive definite for all values of the basis functions $\{\psi^j_\alpha\}$; the remainder of the $\{u_\sigma\}$ space will be an instability region .

If some *bare* starting values (a , r , u_σ , $\cdots$) are now assumed , it may be that under the renormalization transformation the Hamiltonian will *flow* towards an unstable region , away from a stable fixed point . Thus not only is it necessary to determine whether or not the Hamiltonian has stable fixed points , but also whether the flow of H carries it to such a point i.e. whether the transition is second order . If not it is first order [37] . An added modification is to take into account in H the extra *symmetry - breaking* field . By decreasing the effective number of order parameters (splitting $D^j_{G_o}$ into subrepresentations) the order of the transition can be changed back again - the stable fixed point may become accessible .

In order to predict symmetry changes directly , the subduction criteria (C1-C6) will be utilized in our work . These selection rules could be applied to any $D^j_{G_o}$ irrespective of its Landau and/or Lifshitz activity . The group theory criteria are based on the existence of G_o and $\overline{G}$ and the invariance of $\delta\rho$ in the vector space of $D^j_{G_o}$.

Both the selection rules for deciding the *activity* of $D^j_{G_o}$ are necessary in 3 - dimensions . However for 2 - dimensional systems microscopic models have been developed (e.g. 3-state and 4-state Potts models) for which the order parameter violates the Landau condition , yet the transition is continuous [13] . While the original Landau argument based on the stability of the transition seems to have a validity independent of dimensionality , in this thesis we have used the *irreps* irrespective of their Landau or Lifshitz activity . Future computer programming by us to test for the activity of an *irrep* will serve to further distinguish them in this fashion .

CHAPTER 2

THE 80 DIPERIODIC GROUPS

2.1 The Nature of the Diperiodic Groups

A proper analysis of 2-D systems such as Graphite Intercalation Compounds [10], layered dichalcogenides [14] and 2-D magnets [11] requires the use of the 80 diperiodic groups. These have been tabulated in the standard notation by Wood [5].

The ordinary 17 plane space groups [3] describe the symmetry of a one-sided plane or crystal surface. Here all symmetry axes and mirror planes are normal to the surface. While there is 2-D periodicity parallel to the planar surface there is none perpendicular to the surface. In order to describe the symmetry of layered systems that have a finite thickness we must use the diperiodic groups. These groups are intermediate between the 17 2-D space groups and the 230 3-D crystallographic groups {ITXRC} [3]. Some 3 - Dimensional symmetry operations absent in the former are now allowed for the diperiodic groups. These are screw axes parallel to the layer and glide - mirror planes in the layer.

Experimental evidence for a 2nd-order phase transition has been obtained for the Tungsten (100) crystal surface [38]. This is consistent with a symmetry change $G_o = P4mm \rightarrow P2gg = \bar{G}$ at the (rectangular) Brillouin Zone boundary point k = 1/2 , 1/2 [1]. However surface phase transitions are not confined entirely to the surface in a real crystal. Surface activity decays exponentially with depth into the bulk of a crystal and involves a finite layer, even though it is a few atomic planes thick.

In spite of the asymmetry of the crystal layer - vacuum on one side and the bulk of the crystal on the other side - its symmetry is higher than that described by any one of the 17 plane groups. An example of a diperiodic system is the layered dichalcogenide(s) As_2S_3 and $As_s Se_3$ whose $\mathbf{k} = 0$ optical phonon properties were investigated recently by *Zallen et al*. [14] using far-infrared reflectivity and transmission measurements. In interpreting the observed spectra they found it imperative to analyze group-theoretically the *diperiodic* layer symmetry $G_o = Pnm2_1$ (DG 32) as well as the triperiodic crystal symmetry $G_o = P2_1/n$ (C_{2h}^5 – in Schoenflies notation).
They found that the two symmetries lead to distinctly different photon - phonon selection rules. The experiments demonstrated the dominance of layer symmetry in predicting lattice-optical properties.

On the theoretical side *Ipatova et al.* [39] have studied the breaking of translational symmetry in 2nd-order phase changes for clean crystal surfaces based on the 80 diperiodic groups. In APPENDIX III we list the 80 diperiodic groups and their subgroups in a *Zellengleich - Klassengleich* form [40,41]. All *Zellengleich* (Z) subgroups have the same translational symmetry while all *Klassengleich* (K) subgroups belong to the same crystal class. A similar classification given by *Holser* [40] is based on a notation and orientation that is not consistent with the standard setting of these space groups. In our listing we have reset the subgroups in the current notation of Wood's tables [5].

We used the new International Tables {ITC} [3] to obtain the standard setting and also to double-check the entries of Holser's tables . Each entry in APPENDIX III is a class symbol for a family of space groups . For example we list a space group as **Cam2** , (DG 36) . Holser's entry for this space-group is **Cb2m** . In Wood's notation Cam2 is the label for a Body - Centered Rectangular (Orthorhombic) space-group Γ_b^o with a , 2 as *generators* of the factor group G_o / T_o . In the z,x,y notation these are :

$\{m_z \mid \frac{1}{2},0\} \equiv a$, $\{C2y \mid 0,0\} \equiv 2$

The setting for Cb2m has b , 2 as *generators*

$\{m_z \mid 0,\frac{1}{2}\} \equiv b$, $\{C2x \mid 0,0\} \equiv 2$

In APPENDIX III use the *generic* symbol *Cam2* to represent the variety of 2-Dimensional setting for this space-group.

This Z - K outline is based on Hermann's Group - Subgroup Theorem [41] :-

Every subgroup can be considered to be a Klassengleich subgroup of another subgroup which itself is a Zellengleich subgroup of some third group .

The recursive use of this theorem and the ITC allows us to set up group - subgroup family trees prior to the application of the Chain Subduction Criteria (C1 - C6) in eliminating subgroups $\bar{G}$ which can result via a second-order phase transition . We will discuss this theorem further in Section 3 .

2.2 Bravais Lattices and Brillouin Zones

Since the 2-D periodicity parallel to a surface or layer is unchanged in systems describable by the 17 plane space groups or the 80 diperiodic groups, the Bravais lattices and Brillouin zones remain unchanged. Even though a layer has a finite thickness 't' and is truly tri-periodic, one could argue that the Brillouin Zones should be all 3-Dimensional for the diperiodic groups. However the 3^{rd} dimension of the Brillouin Zone is related to $\frac{1}{t}$. As $t \rightarrow 0$, this 3^{rd} layer in reciprocal space is at ifinitity. The Brillouin Zones of the diperiodic groups are effectively 2-Dimensional.

We follow the notation of Cracknell [42] for the 17 plane - space groups and the notation of Bradley and Cracknell [34] for the space group operators in this section. In Tables I & II we summarize the properties of the 5 Bravais nets and the 5 Brillouin Zones respectively.

Table I

Basic Vectors of the 2-D Bravais Lattices

		$\vec{t}_1$	$\vec{t}_2$
Oblique	p	(a , 0)	(bcosθ , bsinθ)
Rectangular	p	(a , 0)	(0 , b)
Rectangular	c	(a/2 , b/2)	(-a/2 , b/2)
Square	p	(a , 0)	(0 , a)
Hexagonal	p	(0 , -a)	($\sqrt{3}$a/2 , a/2)

Table II

Basic Vectors of the 2-D Reciprocal Lattices

		$\vec{g}_1$	$\vec{g}_2$
Oblique	p	$2\pi/a(1 , -\cot\theta)$	$2\pi/a(0 , \operatorname{cosec}\theta)$
Rectangular	p	$2\pi/a(1 , 0)$	$2\pi/b(0 , 1)$
Rectangular	c	$2\pi/a(1/a , 1/b)$	$2\pi/b(-1/a , 1/b)$
Square	p	$2\pi/a(1 , 0)$	$2\pi/a(0 , 1)$
Hexagonal	p	$2\pi/a(1/\sqrt{3} , -1)$	$2\pi/a(2/\sqrt{3} , 0)$

The Brillouin Zones of the above lattices are shown in Figure 1 . In our work we concentrate on points of high symmetry $\mathbf{k} \neq 0$ on the boundary of the Brillouin Zones . We do not consider transitions associated with $\mathbf{k} = 0$ since these may be trivially obtained from the point group tables.

Figure 1

Brillouin Zones for the five planar nets

Oblique p

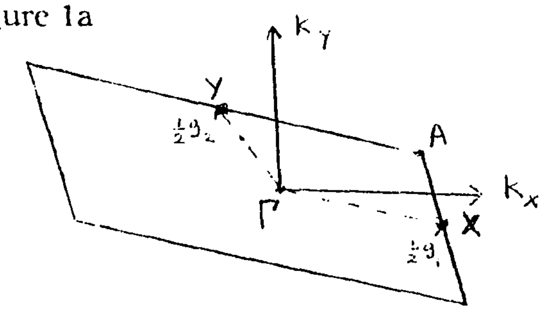
$\Gamma(0 , 0)$

$X(1/2 , 0)$

$Y(0 , 1/2)$

$A(1/2 , 1/2)$

Figure 1a



Rectangular p

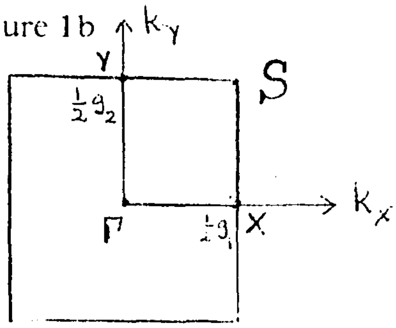
$\Gamma(0 , 0)$

$X(1/2 , 0)$

$Y(0 , 1/2)$

$S(1/2 , 1/2)$

Figure 1b



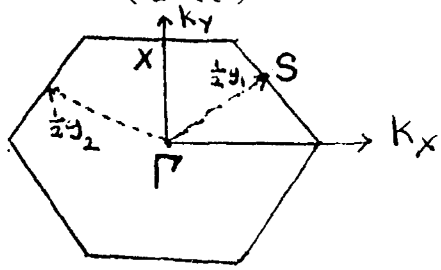
Rectangular c

Γ (0 , 0)

S (1/2 , 0)

X (1/2 , 1/2)

Figure 1c
(a < c)



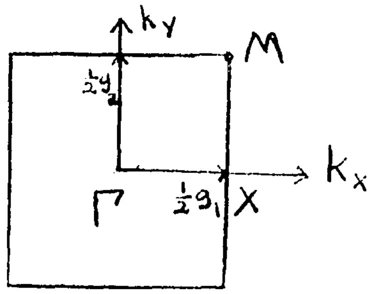
Square p

Γ (0 , 0)

X (1/2 , 0)

M (1/2 , 1/2)

Figure 1d



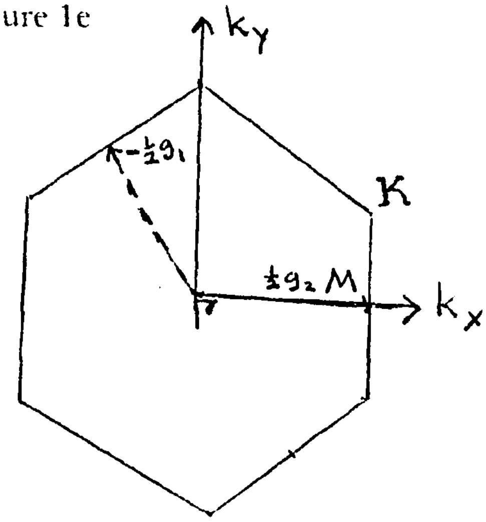
Hexagonal p

Γ (0 , 0)

M (0 , 1/2)

K (-1/3 , 2/3)

Figure 1e



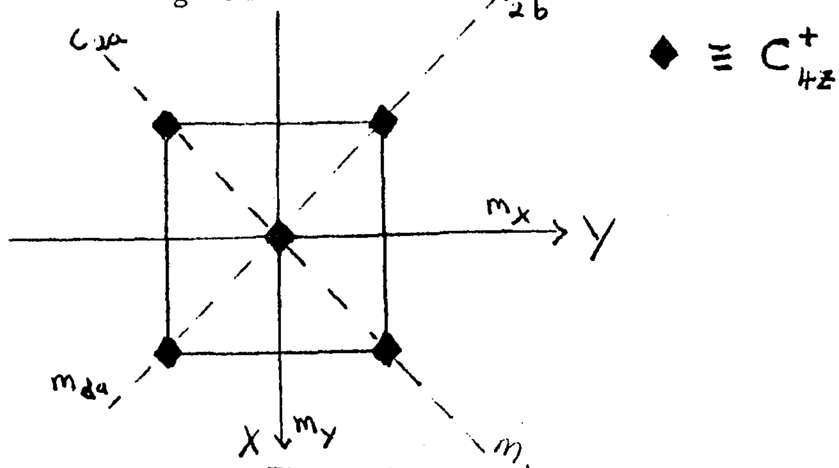
In Figures 2a, 2b we indicate the orientation of the symmetry operations of the Square and Hexagonal Lattices. These also determine the operations for the lattices of lower symmetry .

Figure 2

Symmetry Operations

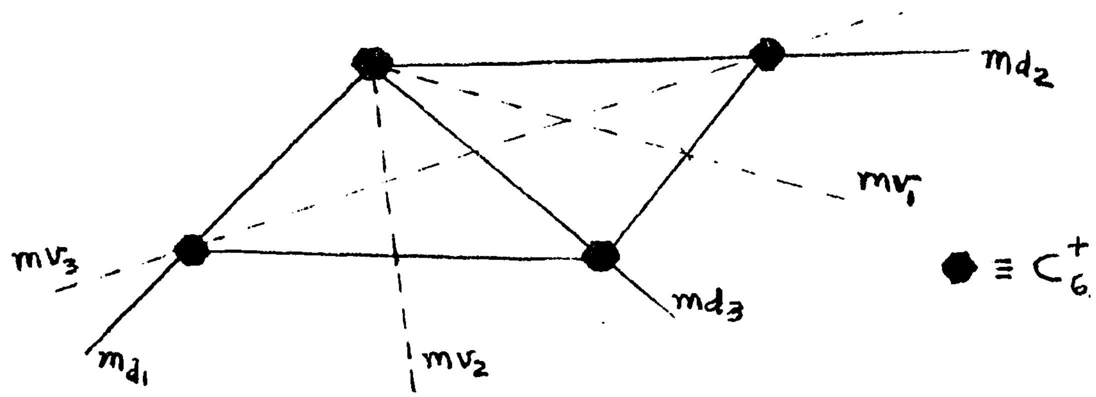
Square Lattice

Figure 2a



Hexagonal Lattice

Figure 2b



In Tables III & IV we give the effect of the point symmetry operations on a general point (x , y , z) in the Jones faithful representation symbols (Bradley & Cracknell) [34] .

Table III

Square Symmetry Operations

E	(x,y,z)	I	(-x,-y,-z)
C2x	(x,-y,-z)	mx	(-x,y,z)
C2y	(-x,y,-z)	my	(x,-y,z)
C2z	(-x,-y,z)	mz	(x,y,-z)
C4z+	(-y,x,z)	S4z-	(y,-x,-z)
C4z-	(y,-x,z)	S4z+	(-y,x,-z)
C2a	(y,x,-z)	mda	(-y,-x,z)
C2b	(-y,-x,-z)	mdb	(y,x,z)

Table IV

Hexagonal Symmetry Operations

E	(x,y,z)	I	(-x,-y,-z)
C6+	(x-y,x,z)	S3-	(-x+y,x,z)
C3+	(-y,x-y,z)	S3-	(y,-x+y,-z)
C2z	(-x,-y,z)	mz	(x,y,-z)
C3-	(-x+y,-x,z)	S3-	(x-y,x,-z)
C6-	(y,-x+y,z)	S3+	(-y,x-y,z)
C21′	(-x+y,y,-z)	md1	(x-y,-y,z)
C22′	(x,x-y,-z)	md2	(-x-x+y,z)
C23′	(-y,-x,-z)	md3	(y,x,z)
C21″	(x-y,-y,-z)	mv1	(-x+y,y,z)
C22″	(-x,-x+y,-z)	mv2	(x,x-y,z)
C23″	(y,x,-z)	mv3	(-y,-x,z)

The *point* symmetry operations of the Square and Hexagonal lattices 4/mmm (C_{4h}) and 6/mmm (D_{6h}) respectively determine the 31 point subgroups of a layer . We must remove the 5 cubic point groups from the 32 (3-D) crystallographic point groups . In *z* , *x* , *y* notation the point groups **2 , m , 2/m and mm2** can be written as *211 , m11 , 2/m11 and 2mm*

There are alternate orientations of these 4 crystallographic point groups :- *121(or 112) , 1m1(or 11m) , 12/m1(or 112/m) and m2m(or mm2)* [40]. Hence we must add also 4 extra point groups . These 31 *point* group families when combined with space group translations , screw axes and glide planes (in the layer) produce the 80 diperiodic groups .

2.3 Determination of the Character Tables for the Diperiodic Groups

There are extensive tables for the irreps of the 17 plane space groups (*Cracknell*) [42] and for the 230 3-D space groups (*Cracknell, Davies, Miller & Love*) { CDML }[32] . These tables list the irreps of G_k , - *the Group of the wave-vector at arbitrary points in the Brillouin Zones of the space group* G_o ; $G_o \supseteq G_k$. *By induction from an irrep* of G_k *viz.* $D^j_{G_k}$

$$D^j_{G_k}(g) \uparrow G_o$$

a full group irrep of G_o *may be obtained* (*Bradley & Cracknell*) [34] . Alternative tables based on the multiplier irreps Γ_k of G_{k_o} , the point group of the wave-vector group G_k , have been derived by *Kovalev* [33] . The relation between the *irreps* of G_k and those of G_{k_o} is (Eq. 1.3.3)

$$\chi(D_k(g)) = e^{-i\vec{k}\cdot\vec{\tau}}\chi(\Gamma_k(R)) \qquad ; \quad g = \{R \mid \vec{\tau}\} \qquad (2.3.1)$$

It would appear then that their should be no need for separate tables of the diperiodic groups . However the orientations of the 2-D space groups often differ from those of the 3-D space groups . Use of the following method allows one to obtain the multiplier *irreps* $\Gamma_k(R)$ of the diperiodic groups from the related *irreps* $D^j_{G_k}$ of a corresponding 3-D space group . Consider the non-symmorphic space group **Pbb2** (DG 27). This space group can be derived from its parent space group **Pcc2** . Its orientation with respect to the 3-D setting of **Pcc2** (#27 Triperiodic ,ITC) is $a\bar{c}b \equiv C4x+$ as listed on page 2 of Wood's tables [5] .

From the ITC the generators of **Pcc2** are : -

E { x,y,z } C2z{ -x,-y, z} mx{-x, y, z | 0,0,1/2} my{ x,-y, z | 0,0,1/2}

To go from the 3-D setting to its Diperiodic orientation we perform the unitary transformation $C4x+ \equiv x\bar{z}y$ on the above generators of **Pcc2** .

C4x+ E C4x-	=	E
C4x+ C2z C4x-	=	C2y
C4x+ {mx|0,0,1/2} C4x-	=	{mx|0,1/2,0}
C4x+ {my|0,0,1/2} C4x-	=	{mz|0,1/2,0}

The elements in the last column are the generators of **Pbb2** (DG 27) in Wood's notation . In Volume I of CDML the irreps of G_k for the 3-D space group **Pcc2** (#27 ITC) can be found . To find the irreps of **Pbb2** we perform the same unitary transformation C4x+ on the k-vectors of the 3-D Brillouin Zone in order to project out the corresponding vectors of the 2-D Brillouin Zone appropriate for the diperiodic setting **Pbb2** . At the points of high symmetry in 3-D the following correspondence between k - vectors in 3-D and 2-D for this space group exists :

3-D	2-D
Γ(0,0,0)	Γ(0,0,0)
X(1/2,0,0)	X′(1/2,0,0)
Y(0,1/2,0)	Y′(0,0,1/2)
Z(0,0,1/2)	Z′(0,1/2,0)
S(1/2,1/2,0)	S′(1/2,0,1/2)
T(0,1/2,1/2)	T′(0,1/2,1/2)
U(1/2,0,1/2)	U′(1/2,1/2,0)
R(1/2,1/2,1/2)	R′(1/2,1/2,1/2)

Hence the following equivalence between the k-vectors in 3-D and 2-D : -

3-D	2-D
Γ(0,0,0)	Γ(0,0,0)
X(1/2,0,0)	X(1/2,0,0)
Z(1/2,0,0)	Y(1/2,0,0)
U(1/2,0,0)	M(1/2,0,0)

We look up in CDML the irreps of X(1/2,0,0) , Z(0,0,1/2) and U(1/2,0,1/2), and relabel these points X(1/2,0,0) , Y(0,1/2,0) and M(1/2,1/2,0).

X(1/2,0,0)

R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

Y(0,1/2,0)

M(1/2,1/2)

R1	1	1	1	1
R2	1	1	-1	-1
R3	i	-i	i	-i
R4	i	-i	-i	i

These however are the irreps of G_k . We need the irreps $\bar{\Gamma}_k$ of G_{k_o} . Using (Eq. 2.3.1) we obtain the Γ_k at * k = 1/2,0 ; * k = 0,1/2 ; * k = 1/2, 1/2 for **Pbb2** as in APPENDIX II.

27 Pbb2 * k = 1/2 ,0 ; * k = 0, 1/2 ; * k = 1/2 ; 1/2

Γ_k	E	C2y	mx	my
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

An explicit calculation using the definition of the multiplier μ [43]

$$\mu = e^{-i(\vec{k}^* - R_p{}^{-1}\vec{k}^* \cdot \tau_q)}\{R_p \mid \tau_p\}\{R_q \mid \tau_q\} \equiv \{R_r \mid \tau_r\} \qquad (2.3.2)$$

gives the following table for the multipliers μ

TABLE V

Table of Multipliers μ for Pbb2 at
* k = 1/2 ,0 ; * k = 0, 1/2 ; * k = 1/2 ; 1/2

μ	E	C2y	mx	my
R1	1	1	1	1
R2	1	1	1	1
R3	1	1	1	1
R4	1	1	1	1

Since the multipliers μ are all + 1 the ordinary point group table for *mm2 or 2mm* may be used as the table of multiplier *irreps* $\Gamma_k(R)$. All the multiplier reps for the nonsymmorphic space groups were obtained by projection from 3-D , based on the orientational setting given in Wood's tables . The character tables for all the 80 diperiodic groups are listed in APPENDIX II .

CHAPTER 3
COMPUTER PROGRAMMING

3.1 Development of the Computer programs

In the practical implementation of the Selection rules (A - C6) one needs easily accessible and manipulatable tables of the crystallographic space groups . In particular there is need for tables of the kind published by *Billiet et al.* [4] for the 17 plane space groups - a complete listing , for each parent space group , all its subgroups with explicit mention of their origin and orientation in the unit cell of the parent space group . For this information to be useful some ordering is essential . Hermann's space group decomposition therom , recently discussed by Senechal [44] gives us the rationale for preparing a family-tree of group - subgroup lattices for each parent space group G_o . Hermann [41] first demonstrated that any subgroup $\bar{G}$ of a space group G_o is a class-equivalent (*Klassengleich*) subgroup of a translation-equivalent (*Zellengleich*) subgroup of G_o .

A class-equivalent (K) subgroup of a space group G is a space subgroup (of G) whose factor group is isomorphic to the factor group of G . A translation-equivalent (Z) subgroup of a space group is a space subgroup with the same translation group as G . Let G_o be a 3 -D space group with translation subgroup T_o . The factor group of G_o with respect to T_o is

$$P_o \equiv G_o / T_o \qquad (3.1.1)$$

Let $\bar{P}$ be a subgroup of P_o with index ν .

$$\nu = \left| \frac{P_o}{\bar{P}} \right| \qquad (3.1.2)$$

A Z-subgroup of G_o say G_z , is a spacegroup also having translation subgroup T_o .

$$\bar{P} \equiv G_z / T_o \qquad (3.1.3)$$

Let $\bar{T}$ be a subgroup of G_o with index Δ .

$$\Delta = \left| \frac{T_o}{\bar{T}} \right| \qquad (3.1.4)$$

A K-subgroup of G_z , say G_k , is a space group with translation subgroup $\bar{T}$ and factor group $\bar{P}$

$$\bar{P} \equiv G_k / \bar{T} \qquad (3.1.5)$$

The chain of space subgroups in Hermann's theorem is thus

$$G_o \supseteq G_z \supseteq G_k \equiv \bar{G} \qquad (3.1.6)$$

where G_z is isomorphic to $\bar{G}$. If the index of $\bar{G}$ in G_o is λ

$$\lambda = \left| \frac{G_o}{\bar{G}} \right| \qquad (3.1.7)$$

then

$$\left| \frac{G_o}{\bar{G}} \right| = \left| \frac{P_o}{\bar{P}} \right| \left| \frac{T_o}{\bar{T}} \right| \qquad (3.1.8)$$

or

$$\lambda \equiv \nu \Delta \qquad (3.1.9)$$

For a Z-subgroup $\Delta = 1$; for a K-subgroup $\nu = 1$. A general subgroup G of G_o breaks both rotational and translational symmetry ; it may be considered to descend from G_o *via* a two-step sequence according to Hermann's theorem . First rotational (Z - step) and then translational (K - step) symmetry elements are discarded .

Let G_o be a parent space group with translational symmetry subgroup T_o . Also let G' be a subgroup of G_o , $G' \subseteq G_o$ and T' be its translational subgroup ; the factor grouup $F' = G'/T'$ has $g' = \{R'|\vec{r}''\}$ as a general symmetry element . If $D_{G_o}^{j,k}$ is an *irrep* of G_o , then the subduction frequency n of the representation $D_{G'}^{\Gamma_1}$ of G' in $D_{G_o}^{j,k}$ is given by

$$n = \frac{1}{|F'|} \sum_{g' \in F'} \chi_k^j(g') \chi_{G'}^{\Gamma_1}(g')$$

$$= \frac{1}{|F'|} \sum_{g' \in F'} \chi_k^j(g') \qquad (3.1.10)$$

$\chi_k^j(g')$ is the character of element $g' \in G'$ with matrix representative $(D_{G_k}^j(g') \uparrow G_o)$. $D_{G_k}^j$ is the j^{th} matrix irreducible representation of G_k - the wave-vector group at **k** .

The element g' is common to both G' and G_o . However it is generally expressed differently under G' and G_o in the standard entries of space groups in the International Tables (ITC) .

$$g' = \{R'|\vec{r}''\} \equiv \{R|r + \vec{t}_o\} = g \in G_o$$

In general $R' \neq R$ and $\vec{r}'' \neq \vec{r}$. While R' and R are connected by a unitary transformation , the relation between the non-primitive translations $\vec{r}''$ and $\vec{r}$ is , *Bradley & Cracknell* [34]

$$\vec{r} + \vec{t}_o = \vec{r}'' + \vec{s} - R\vec{s} \qquad (3.1.11)$$

where $\vec{s}$ is the *shift* vector needed to take origin O' of G' back to the parent origin O of G_o and $\vec{t}_o$ is a primitive lattice vector of T_o that does not belong to T'.

The character of g', $\chi_k^j(g')$ is obtained *via* a joint induction ($\uparrow$) - subduction ($\downarrow$) process :-

$$\chi_k^j(g') = \chi[(D_{G_k}^j(g') \uparrow G_o) \downarrow G']$$

A compact formula for $\chi_k^j(g')$ has been given by *Lavrencic & Shigenari* [45]

$$\chi_k^j(g') = \sum_i{}' e^{-ik^{(i)}\cdot(t_o' + \vec{r} + R'\vec{r}_1^{(i)} - \vec{r}_1^{(i)})} \chi^j(\Gamma_k\{R_1^{(i)-1} R R_1^{(i)}\}) \quad (3.1.12)$$

where $g_1^{(i)} \equiv \{R_1^{(i)} | \vec{r}_1^{(i)}\}$ is the i^{th} coset representative of G_o with respect to $G_{k^{(1)}}$, i.e. $G_o = \sum_i g_1^{(i)} G_{k^{(1)}}$.

$k^{(1)}$ is the representative arm of ${}^*k$: ${}^*k = \{k^{(1)}, k^{(2)}, \ldots k^{(\omega)}\}$ and the i^{th} arm is defined as $k^{(i)} = R_1^{(i)} k^{(1)}$.

The $\sum_i{}'$ is only over those arms $k^{(i)}$ in ${}^*k$ that satisfies the condition for translation invariance T' :

$$e^{-ik^{(i)}\cdot\vec{t}'} = +1 \quad (3.1.13)$$

The *Kronecker* δ in Eq. (3.1.12) implies that the character for χ vanishes unless R' leaves *these* $\vec{k}^{(i)}$ invariant .

If $\vec{t}'$ and $\vec{t}$ are the primitive translations of the new lattice T' and the old lattice T_o respectively , *viz.*

$$\vec{t}'_j = m_1'\vec{a}_1' + m_2'\vec{a}_2' + m_3'\vec{a}_3' \quad ; m_i' = 0, \pm1, \pm2, \ldots$$
$$j = 1, 2, 3 .$$
$$\vec{t}_j = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3 \quad ; m_i = 0, \pm1, \pm2, \ldots$$

then symmetry operation $R \neq R'$ in general because of the difference in the basic sets $\{\vec{a}'\}$ and $\{\vec{a}\}$. However some operation U_o in G_o connects them *via* a unitary transformation $R' \equiv U_o\ R\ U_o^{-1}$.

The arms of $^*k$ that satisfy Eq. (3.1.13) form the sub-star $^*k_s$

$$^*k_s = \{ \; k^{(1)}, k^{(2)}, \; .. \; k^{(\omega')} \; \} \qquad ; \quad \omega < \omega'$$

Formula 3.1.12 is the key equation to be programmed as the calculation of the subduction frequency *n or sf* is a finite sum over the elements of a factor group F' of order $|F'|$. The identification of R' is easy and can be done by inspection for 2-D stsyems .

Since no tables of the kind published by *Billiet et al.* [4] exists for the diperiodic groups we have developed new algorithms based on Eq. 3.1.11

$$\vec{t_o} = \vec{r''} - \vec{r'} + \vec{s} - R\vec{s'} \qquad (3.1.14)$$

We explored all possible values of O' lying on a planar grid at the points

$$X = 0 , \frac{1}{4} , \frac{1}{3} , \frac{1}{2} , \frac{2}{3} , \frac{3}{4} , 1$$

$$y = 0 , \frac{1}{4} , \frac{1}{3} , \frac{1}{2} , \frac{2}{3} , \frac{3}{4} , 1$$

in the parent unit cell of G_o . These are points of high site symmetry and are the likely origins O' of all planar subgroups .

We now summarize the main steps of the algorithms :-

(i) For each value of $\vec{s}$ all values of R' and all values of $\vec{r''}$ were tested to see if Eq. (3.1.11) was satisfied , i.e. *if* $\vec{t_o}$ *is an integer lattice vector in the parent lattice* . Only if this condition is satisfied will the calculations outlined in the *flowchart* Figure 3 proceed . If we do obtain an integer lattice vector for some $\vec{s}$ in the grid above , then that $\vec{s}$ is stored as a probable origin O' of G' .

(ii) The new basic vectors of the translation lattice T' must satisy translation invariance , Eq. (3.1.13) :- $e^{-i\,\vec{k}_s\cdot\vec{t}'} = +1$. For 2-D these are $\vec{t}_1'$ and $\vec{t}_2'$:

$$\vec{t}_1' = n_{11}\vec{t}' + n_{12}'$$
$$\vec{t}_2' = n_{21}\vec{t}' + n_{22}'$$

To avoid some redundancy we have restricted the elements of the *2 X 2 matrix* N :

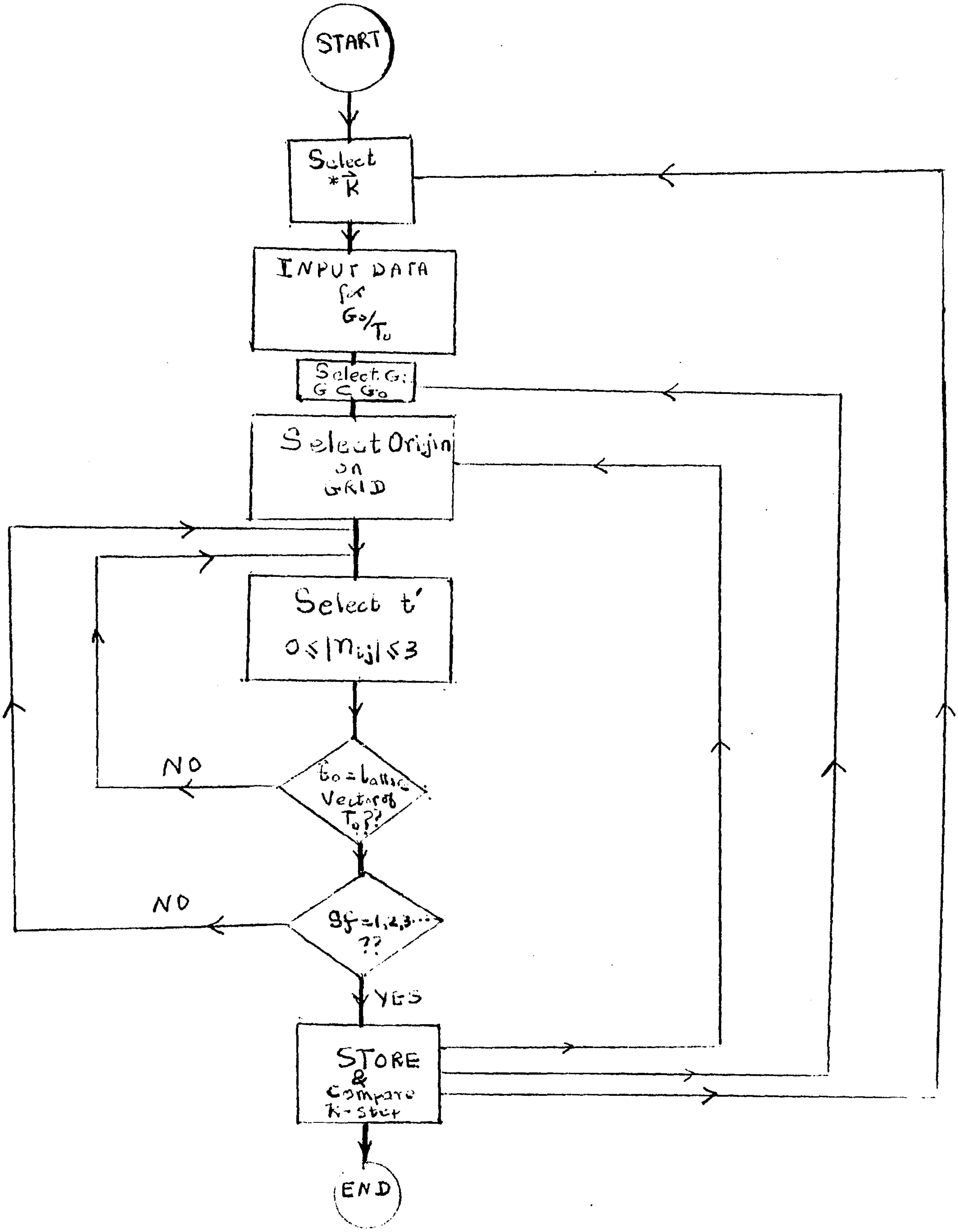
$$N = \begin{vmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{vmatrix} \quad ; \quad 0 \leqslant | n_{ij} | \leqslant 3$$

This range was found to be sufficient to generate the new Bravais lattices . New cells of larger size with the same subduction frequency (sf) will be eliminated by the *Chain Subduction Criteria* at the K-Step .

(iii) Of all values of $k^{(i)} \in {}^*k$ only those arms that satisfy $e^{-i\vec{k}^{(i)}\cdot\vec{t}} = +1$ and thus form the sub-star $*k_s$ [46] were retained . At least one arm of $^*k$ must satisfy this condition . If this condition is not met a new cycle is initiated (*see Flowchart*) .

(iv) For each parent space group G_o , the input data consisted of the characters $\chi(\Gamma_k^j(R))$ of the multiplier *irrep* ,Γ_k the distinct stars $^*k$ on the Brillouin Zone boundary , the elements of F' and the parent factor group $F_o = G_o / T_o$. Multiplication tables needed to calculate $R^{(i)-1}RR^{(i)}$ were wriiten into a special subroutine .

Figure 3 (FLOWCHART)



(v) Each distinct G' (*name & orientation*) was built into a separate subroutine . Various tests were made to reduce redundancy . Even in the first quadrant identical information was produced at various sites O' in the unit cell of index $\eta = \vec{t}_1 \times \vec{t}_2$ - e.g. at $O' \equiv (0,0)$, (0,1) , (1,1) especially for the lower symmetry space groups .

Additional *fine structure* in space group notation were obtained and stored for the 17-plane groups [4] . We explored all 4 - quadrants and our data for the allowed transitions are listed in Section 4.2 for this family of surface groups . As can be expected , computing time quadrupled in exploring the whole unit cell . A compromise on the time factor when tackling the 80 diperiodic groups resulted in the minimum information *viz.* spacegroup **type** allowed and subduction frequency ,**not** generators , being collected and displayed in Section 4.1 .

The program units were written in RATFOR - *A Rational Fortran* (*Kernighan*) [47] . Because of the many tests and loops in the main program ordinary FORTRAN would have been unwieldy in trying to read or modify the program for $\mathbf{k} = 0$. Debugging the program's would also have proven to be a nightmare what with the many GO TO'S and STATEMENT NUMBERS . The ratfor flow logic made a complex program tractable and a preprocessor gave the option of converting *.r to *.f (machine fortran) . This and its converse using the *struct* package (UNIX) gave greater flexibility in program building . Even so , use of a higher level language such as the *C - Language* would have made the implementation of checks to avoid redundancy easier .

3.2 Computer Generation of the Subduction Frequencies

Our program is basically a bottom-up approach in predicting second -order phase transitions . Given a G_o and all its $\bar{G}$ we proceed to test each $\bar{G} \subseteq G_o$ to find whether it has a non-zero subduction frequency (sf) in D_{G_o} . The flowchart , Figure 3 gives an outline of the method and a copy of the program for $G_o = P1g1$, PL4 in the family of 17-plane space groups or DG 12 , $G_o = P11a$ as a member of the Diperiodic family , is listed in APPENDIX I . While shorter (in terms of memory space) and more elegant programs could have been displayed we deferred in order to retain the mnemonics and readability . A sample of the printout for the non-symmorphic planar space group P1g1 is shown overleaf .

The 3 k vectors (also k-stars) on the Zone boundary are :-
star 1 , k = 1/2 , 0 ; star 2 , k = 0 , 1/2 ; star 3 , k = 1/2 , 1/2
The 1st line gives the parent G_o and some of the elements in a planar factor group . This *heading* was changed as we modified the program and its printout for higher symmetry groups . The elements of the multiplier irrep Γ_k that have non-zero characters can be easily identified from the 2nd line . The 3rd line is a heading indicating space subgroup (sg) , angle between the $\vec{t}$ ',θ , cell size (η) ,new translations t_1,t_2 , shift in origin $\vec{s}$ via $x_o y_o$ and a blank space . Under this *blank* the *generators* of the subgroup $\bar{G}$ indicated by a number-identifier *(n)* . The entry 0. (5) 0. indicates that the 5th element of the 2nd line*viz.* m_x is the symmetry operator of the factor group F' . On either side of the "(5)" is the integer translation $\vec{t}_o$ in component form .

COMPUTER PRINTOUT FOR G_o = P1g1

elem $\Gamma_k : G_o$ = P1g1 e c2z c4z- c4z+ mx my da db
star 1 ,characters 1 0 0 0 1 0 0 0 : for k = 1/2,0

sg θ η $\vec{t}'_1$ $\vec{t}'_2$ x_o y_o

sf=(1) P1g1 90 2 2t1+ 0t2 ; 0t1+ 1t2 0. -0.67 0. (5) 0.
sf=(1) P1g1 90 2 2t1+ 0t2 ; 0t1+ 1t2 1.00 -0.33 0. (5) 0.

sf=(1) P111 63 4 0t1+-1t2 ; 2t1+-1t2 0.25 0.25
sf=(1) P111 90 4-2t1+ 0t2 ; 0t1+-1t2 0.25 0.25

elem $\Gamma_k : G_o$ = P1g1 e c2z c4z- c4z+ mx my da db
star 1 ,characters 1 0 0 0 -1 0 0 0 for k = 1/2,0

sg θ η $\vec{t}'_1$ $\vec{t}'_2$ x_o y_o

sf=(1) P1g1 90 2 2t1+ 0t2 ; 0t1+ 1t2 0.50 -0.67 1.00(5) 0.

sf=(1) P111 63 4 0t1+-1t2 ; 2t1+-1t2 0.25 0.25
sf=(1) P111 90 4-2t1+ 0t2 ; 0t1+-1t2 0.25 0.25

elem $\Gamma_k : G_o$ = P1g1 e c2z c4z- c4z+ mx my da db
star 2 ,characters 1 0 0 0 1 0 0 0 : for k = 0,1/2

sg θ η $\vec{t}'_1$ $\vec{t}'_2$ x_o y_o

sf=(1) P111 90 4-1t1+ 0t2 ; 0t1+-2t2 0.25 0.25
sf=(1) P111 90 4 0t1+ 2t2 ;-1t1+ 0t2 0.25 0.25

elem $\Gamma_k : G_o$ = P1g1 e c2z c4z- c4z+ mx my da db
star 2 ,characters 1 0 0 0 -1 0 0 0 : for k = 0,1/2

sg θ η $\vec{t}'_1$ $\vec{t}'_2$ x_o y_o

sf=(1) P111 90 4-1t1+ 0t2 ; 0t1+-2t2 0.25 0.25
sf=(1) P111 90 4 0t1+ 2t2 ;-1t1+ 0t2 0.25 0.25

elem $\Gamma_k : G_o$ = P1g1 e c2z c4z- c4z+ mx my da db
star 3 ,characters 1 0 0 0 1 0 0 0 : for k = 1/2,1/2

sg θ η $\vec{t}'_1$ $\vec{t}'_2$ x_o y_o

sf=(1) P1g1 90 4 2t1+-2t2 ; 1t1+ 1t2 0.25 -0.67 1.00(5) 0.
sf=(1) P1g1 90 4-2t1+-2t2 ; 1t1+-1t2 0.75 -0.33 2.00(5)-1.00

sf=(1) P111 45 4 1t1+-1t2 ; 2t1+ 0t2 0.25 0.25
sf=(1) P111 90 4-1t1+ 1t2 ;-1t1+-1t2 0.25 0.25

elem $\Gamma_k : G_o$ = P1g1 e c2z c4z- c4z+ mx my da db
star 3 ,characters 1 0 0 0 -1 0 0 0 : for k = 1/2,1/2

sg θ η $\vec{t}'_1$ $\vec{t}'_2$ x_o y_o

sf=(1) P1g1 90 4-2t1+-2t2 ; 1t1+-1t2 0.25 -0.67 0. (5) 0.
sf=(1) P1g1 90 4 2t1+-2t2 ; 1t1+ 1t2 0.75 -0.33 2.00(5) 0.

sf=(1) P111 45 4 1t1+-1t2 ; 2t1+ 0t2 0.25 0.25
sf=(1) P111 90 4-1t1+ 1t2 ;-1t1+-1t2 0.25 0.25

The 4^{th} line can now be read as follows :

P1g1 is an allowed subgroup with subduction frequency sf = 1 .

The new translations of the unit cell of T' *are* $2t_1, t_2$;

the generator of the subgroup is $\{m_x \mid 0,0 + \vec{r}\}$ and the

non-primitive translation $\vec{r}'' = \vec{r} + \vec{t}_o = \frac{1}{2}, \frac{1}{2}$

The entire printout was then inspected to see whether various settings were consistent with those of the ITC , to remove remaining redundancy and to complete the application of the Chain Subduction Criteria .

(1) *Redundancy* : The 4^{th} and 5^{th} lines of our printout displays identical information for the allowed subgroup $\bar{G} = P1g1$. Though the $\vec{s}$ are different , the generators are the same . Similarly for the 6^{th} and 7^{th} lines even though the θ are different as $\bar{G} = P1$ is oblique .

(2) *Chain Subduction Criteria* : Partial application of these selection rules was done on the computer at the K - step . If we look at the 4^{th} line we see that only the smallest index $\eta = 2$ is retained . Higher values of η all have the same sf = 1 and are discardedd as their translation subgroups $\bar{\bar{T}}$, $\bar{\bar{\bar{T}}}$, . . have $\bar{T}$ with new cell $2\vec{t}_1, \vec{t}_2$ as their maximal supergroup .

(3) *Spurious Entries* : If we look at the listing for the 3^{rd} star or $\mathbf{k} = \frac{1}{2}, \frac{1}{2}$ we find in its 4^{th} or 5^{th} line that P1g1 should be an allowed transition with sf = 1 .

However the new translations are :-

$$\vec{t}_1 = 2\vec{t}_1 - 2\vec{t}_2$$
$$\vec{t}_2 = \vec{t}_1 + \vec{t}_2$$

Even though the angle $\theta = 90°$ indicating a rectangular cell this entry is false as the generator m_x of the P1g1 group must be perpendicular to the X-axis or to one of the $\vec{t}_i$ ' . This is not the case here and we discard this entry . The cure would be additioanal tests to eliminate this misalignment between symmetry elements and basic cell vectors . However we persisted with this approach as we wished to do some direct comparison of our output data with the Internatioanl tables . At this stage we leaned towards some excess rather than have tests that might be too restrictive.

CHAPTER 4

TABLES

4.1 Allowed subgroups for the Diperiodic Groups

We present in the following tables the subgroups G' that allowed in a second - order phase transition for each G_o of the 80 Diperiodic groups. The parent group G_o , allowed subgroup G' , subduction frequency *n or sf* $= 1, 2, 3, \ldots, \Gamma_k$ for each Zone boundary $^*k$ and new translation lattices are given at the head of each table for each space group . The subgroup label G_* refers to the space group type whose family members differ in origin and orientation from one another . This additional information has been compiled only for the 17 - plane space groups and is listed in Section 4.2 .

In the the Centered Rectangular (C) lattice-type space groups the new translations are defined with respect to the primitive translations of the parent cell . This is different from the conventional listing of the basic vectors of the C-cell[3] . This alternative approach makes checking for translational invariance easier as the k vectors are defined with respect to these primitive lattice vectors.

Let us consider table DG 40 , page ; $G_o = Cmmm$.
The primitive translations of its primitive unit cell are

$$\vec{t}_1 = \frac{-1}{2},\frac{1}{2} \quad ; \quad \vec{t}_2 = \frac{1}{2},\frac{1}{2}$$

The **k** - vector S on the Brillouin Zone boundary has two arms ;
$^*k = \frac{1}{2},0 \quad ; \quad 0,\frac{1}{2}$. The *irreps* of Γ_k the multiplier rep of G_k

can be found in APPENDIX II . We have only one *irrep* R_1 for this star-k in table DG 40 . The allowed subgroups for this *irrep* in *Hermann-Mauguin* notation [3], subduction frequency n and new translation sublattice T' are indicated as integer multiples of the above primitive basic vectors $\vec{t}_1$ and $\vec{t}_2$.

For $^*k = \frac{1}{2}, \frac{1}{2}$, there is only one arm .

The *irreps* are all 1- D , R_1 , R_2 , ,.. R_8 .

The subduction frequencies for each irrep is obviously $n = 1$ and there is only one allowed subgroup for each irrep after application of the *Chain Subduction Criteria* .

TABLE 1

1 Go = P1

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P1	2t1,t2
* k = 0 , 1/2			
R1	1	P1	t1,2t2
* k = 1/2 , 1/2			
R1	1	P1	t1-t2,t1+t2

TABLE 2

2 Go = P$\bar{1}$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P$\bar{1}$	2t1,t2
R2	1	P$\bar{1}$	2t1,t2
* k = 0 , 1/2			
R1	1	P$\bar{1}$	t1,2t2
R2	1	P$\bar{1}$	t1,2t2
* k = 1/2 , 1/2			
R1	1	P$\bar{1}$	t1-t2,t1+t2
R2	1	P$\bar{1}$	2t1,t1+t2

TABLE 3

#3 Go = P211

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P211	2t1,t2
R2	1	P211	2t1,t2
* k = 0 , 1/2			
R1	1	P211	t1,2t2
R2	1	P211	t1,2t2
* k = 1/2 , 1/2			
R1	1	P211	t1-t2,t1+t2
R2	1	P211	2t1,t1+t2

TABLE 4

#4 Go = Pm11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	Pm11	2t1,t2
R2	1	Pa11	2t1,t2
* k = 0 , 1/2			
R1	1	Pm11	t1,2t2
R2	1	Pb11	t1,2t2
* k = 1/2 , 1/2			
R1	1	Pm11	t1-t2,t1+t2
R2	1	Pa11	2t1,t1+t2

TABLE 5

#5 Go = Pb11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	Pb11	2t1,t2
R2	1	Pb11	2t1,2t1+t2
* k = 0 , 1/2			
R1	1	P1	t1,2t2
R2	1	P1	t1,2t2
* k = 1/2 , 1/2			
R1	1	P1	t1-t2,t1+t2
R2	1	P1	t1-t2,t1+t2

TABLE 6

#6 Go = P2/m11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P2/m11	2t1,t2
R2	1	P2/a11	2t1,t2
R3	1	P2/a11	2t1,t2
R4	1	P2/m11	2t1,t2
* k = 0 , 1/2			
R1	1	P2/m11	t1,2t2
R2	1	P2/b11	t1,2t2
R3	1	P2/b11	t1,2t2
R4	1	P2/m11	t1,2t2

* k = 1/2 , 1/2

R1	1	P2/m11	t1-t2,t1+t2
R2	1	P2/a11	t1-t2,t1+t2
R3	1	P2/a11	t1-t2,t1+t2
R4	1	P2/m11	t1-t2,t1+t2

TABLE 7

#7 Go = P2/b11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P2/b11	2t1,t2
R2	1	P2/b11	2t1+t2,t2
R3	1	P2/b11	2t1+t2,t2
R4	1	P2/b11	2t1,t2
* k = 0 , 1/2			
R1	1	P211	t1,2t2
	1	P$\bar{1}$	t1,2t2
	2	P1	t1,2t2
* k = 1/2 , 1/2			
R1	1	P211	t1-t2,t1+t2
	1	P$\bar{1}$	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 8

8 Go = P112

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112	2t1,t2
R2	1	P112	2t1,t2

* k = 0 , 1/2			
R1	1	P112	t1,2t2
R2	1	P112$_1$	t1,2t2
* k = 1/2 , 1/2			
R1	1	C112	t1-t2,t1+t2
R2	1	C112	t1-t2,t1+t2

TABLE 9

9 Go = P112$_1$

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112$_1$	2t1,t2
R2	1	P112$_1$	2t1,t2
* k = 0 , 1/2			
R1	1	P1	t1,2t2
R2	1	P1	t1,2t2
* k = 1/2 , 1/2			
R1	1	P1	t1-t2,t1+t2
R2	1	P1	t1-t2,t1+t2

TABLE 10

10 Go = C112

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			

R1	1	C112	2t1,2t2
	1	P1	t1,2t2
R2	1	P1	t1,2t2
	2	P1	2t1,2t2

* k = 1/2 , 1/2

R1	1	P112	t1-t2,t1+t2
R2	1	$P112_1$	t1-t2,t1+t2

TABLE 11

11 Go = P11m

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P11m	2t1,t2
R2	1	P11m	2t1,t2
* k = 0 , 1/2			
R1	1	P11m	t1,2t2
R2	1	P11a	t1,2t2
* k = 1/2 , 1/2			
R1	1	C11m	t1-t2,t1+t2
R2	1	C11m	t1-t2,t1+t2

TABLE 12

12 Go = P11a

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P11a	2t1,t2

R2	1	P11a	2t1,t2

* k = 0 , 1/2

R1	1	P1	t1,2t2
R2	1	P1	t1,2t2

* k = 1/2 , 1/2

R1	1	P1	t1-t2,t1+t2
R2	1	P1	t1-t2,t1+t2

TABLE 13

\# 13 Go = C11m

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	C11m	2t1,2t2
	1	P1	t1,2t2
R2	1	P1	1t1,2t2
	2	P1	2t1,2t2
* k = 1/2 , 1/2			
R1	1	P11m	t1-t2,t1+t2
R2	1	P11a	t1-t2,t1+t2

TABLE 14

\# 14 Go = P112/m

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112/m	2t1,t2

R2	1	P112/a	2t1,t2
R3	1	P112/a	2t1,t2
R4	1	P112/m	2t1,t2

* k = 0 , 1/2

R1	1	P112/m	t1,2t2
R2	1	P112/m	t1,2t2
R3	1	P112/a	t1,2t2
R4	1	P112/a	t1,2t2

* k = 1/2 , 1/2

R1	1	C112/m	t1-t2,t1+t2
R2	1	C112/m	t1-t2,t1+t2
R3	1	C112/m	t1-t2,t1+t2
R4	1	C112/m	t1-t2,t1+t2

TABLE 15

\# 15 Go = $P112_1/m$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	$P112_1/m$	2t1,t2
R2	1	$P112_1/a$	2t1,t2
R3	1	$P112_1/a$	2t1,t2
R4	1	$P112_1/m$	2t1,t2
* k = 0 , 1/2			
R1	1	P11m	t1,2t2
	1	$P\bar{1}$	t1,2t2
	2	P1	t1,2t2

* k = 1/2 , 1/2

R1	1	C11m	t1-t2,t1+t2
	1	$P\bar{1}$	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 16

16 Go = C112/m

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	C112/m	2t1,2t2
	1	P1	2t1,t2
	2	$P\bar{1}$	2t1,2t2
R2	1	C112/m	2t1,2t2
	1	P1	2t1,t2
	2	$P\bar{1}$	2t1,2t2
* k = 1/2 , 1/2			
R1	1	P112/m	t1-t2,t1+t2
R2	1	$P112_1/m$	t1-t2,t1+t2
R3	1	$P112_1/a$	t1-t2,t1+t2
R4	1	P112/a	t1-t2,t1+t2

TABLE 17

17 Go = P112/a

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112	2t1,t2
	1	$P\bar{1}$	2t1,t2
	2	P1	2t1,t2
* k = 0 , 1/2			

R1	1	P112/a	t1,2t2
R2	1	P112/a	t1,2t2
R3	1	$P112_1/a$	t1,2t2
R4	1	$P112_1/a$	t1,2t2
* k = 1/2 , 1/2			
R1	1	C112	t1-t2,t1+t2
	1	$P\bar{1}$	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 18

18 Go = $P112_1/a$

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0			
R1	1	$P112_1$	2t1,t2
	1	$P\bar{1}$	2t1,t2
	2	P1	2t1,t2
* k = 0 , 1/2			
R1	1	P11a	t1,2t2
	1	$P\bar{1}$	t1,2t2
	2	P1	t1,2t2
* k = 1/2 , 1/2			
R1	2	$P\bar{1}$	t1-t2,t1+t2
R1	2	$P\bar{1}$	t1-t2,t1+t2

TABLE 19

19 Go = P222

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0			
R1	1	P222	2t1,t2

R2	1	$P222_1$	2t1,t2
R3	1	P222	2t1,t2
R4	1	$P222_1$	2t1,t2
* k = 0 , 1/2			
R1	1	P222	t1,2t2
R2	1	$P222_1$	t1,2t2
R3	1	$P222_1$	t1,2t2
R4	1	P222	t1,2t2
* k = 1/2 , 1/2			
R1	1	C222	t1-t2,t1+t2
R2	1	C222	t1-t2,t1+t2
R3	1	C222	t1-t2,t1+t2
R4	1	C222	t1-t2,t1+t2

TABLE 20

20 Go = $P222_1$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	$P222_1$	2t1,t2
R2	1	$P22_12_1$	2t1,t2
R3	1	$P222_1$	2t1,t2
R4	1	$P22_12_1$	2t1,t2
* k = 0 , 1/2			
R1	1	P121	t1,2t2
	1	P2	t1,2t2
	2	P1	t1,2t2

* k = 1/2 , 1/2

R1	1	C121	t1-t2,t1+t2
	1	P2	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 21

21 Go = $P22_12_1$

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0			
R1	1	$P112_1$	2t1,t2
	1	P2	2t1,t2
	2	P1	2t1,t2
* k = 0 , 1/2			
R1	1	$P112_1$	t1,2t2
	1	P2	t1,2t2
	2	P1	t1,2t2
* k = 1/2 , 1/2			
R1	2	P2	t1-t2,t1+t2
R2	2	P2	t1-t2,t1+t2

TABLE 22

22 Go = C222

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	C222	2t1,2t2
	1	P1	2t1,1t2
	2	P2	2t1,2t2
R2	1	C222	2t1,2t2
	1	P1	2t1,1t2
	2	P2	2t1,2t2

* k = 1/2 , $\bar{1}/2$

R1	1	P222	t1-t2,t1+t2
R2	1	$P22_12_1$	t1-t2,t1+t2
R3	1	$P222_1$	t1-t2,t1+t2
R4	1	$P222_1$	t1-t2,t1+t2

TABLE 23

#23 Go = P2mm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P2mm	2t1,t2
R2	1	P2ma	2t1,t2
R3	1	P2ma	2t1,t2
R4	1	P2mm	2t1,t2
* k = 0 , 1/2			
R1	1	P2mm	t1,2t2
R2	1	P2ma	t1,2t2
R3	1	P2mm	t1,2t2
R4	1	P2ma	t1,2t2
* k = 1/2 , 1/2			
R1	1	C2mm	t1-t2,t1+t2
R2	1	C2mm	t1-t2,t1+t2
R3	1	C2mm	t1-t2,t1+t2
R4	1	C2mm	t1-t2,t1+t2

TABLE 24

24 Go = Pmm2

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	Pmm2	2t1,t2
R2	1	Pam2	2t1,t2
R3	1	Pmm2	2t1,t2
R4	1	Pam2	2t1,t2
* k = 0 , 1/2			
R1	1	Pmm2	t1,2t2
R2	1	Pbb2	t1,2t2
R3	1	$Pab2_1$	2t1,2t2
R4	1	$Pbm2_1$	t1,2t2
* k = 1/2 , 1/2			
R1	1	Cmm2	t1-t2,t1+t2
R2	1	Pam2	2t1,2t2
R3	1	Cmm2	t1-t2,t1+t2
R4	1	Pam2	2t1,2t2

TABLE 25

25 Go = $Pm2_1a$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	Pm11	2t1,t2
R2	1	Pa11	2t1,t2
R3	1	Pm11	2t1,t2

R4	1	Pa11	2t1,t2

* k = 0 , 1/2

R1	1	$Pm2_1a$	t1,2t2
R2	1	$Pb2_1a$	t1,2t2
R3	1	$Pm2_1a$	t1,2t2
R4	1	$Pb2_1a$	t1,2t2

* k = 1/2 , 1/2

R1	1	Pm11	t1-t2,t1+t2
R2	1	Pa11	t1-t2,t1+t2
R3	1	Pm11	t1-t2,t1+t2
R4	1	Pa11	t1-t2,t1+t2

TABLE 26

\# 26 Go = $Pbm2_1$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	$Pbm2_1$	2t1,t2
R2	1	$Pnm2_1$	2t1,t2
R3	1	$Pbm2_1$	2t1,t2
R4	1	$Pnm2_1$	2t1,t2
* k = 0 , 1/2			
R1	1	P1m1	t1,2t2
R2	1	P1b1	t1,2t2
R3	1	P1b1	t1,2t2
R4	1	P1m1	t1,2t2

* k = 1/2 , 1/2

R1	1	C1m1	t1-t2,t1+t2
R2	1	C1m1	t1-t2,t1+t2
R3	1	C1m1	t1-t2,t1+t2
R4	1	C1m1	t1-t2,t1+t2

TABLE 27

27 Go = Pbb2

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	Pbb2	2t1,t2
R2	1	Pnb2	2t1,t2
R3	1	Pbb2	2t1,t2
R4	1	Pnb2	2t1,t2
* k = 0 , 1/2			
R1	1	P112	t1,2t2
R2	1	P112	t1,2t2
R3	1	$P112_1$	t1,2t2
R4	1	$P112_1$	t1,2t2
* k = 1/2 , 1/2			
R1	1	C112	t1-t2,t1+t2
R2	1	C112	t1-t2,t1+t2
R3	1	C112	t1-t2,t1+t2
R4	1	C112	t1-t2,t1+t2

TABLE 28

28 Go = P2ma

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P1m1	2t1,t2
	1	P2	2t1,t2
	2	P1	2t1,t2
* k = 0 , 1/2			
R1	1	P2ma	t1,2t2
R2	1	P2ba	t1,2t2
R3	1	P2ma	t1,2t2
R4	1	P2ba	t1,2t2
* k = 1/2 , 1/2			
R1	1	C1m1	t1-t2,t1+t2
	1	P2	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 29

29 Go = Pam2

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112	2t1,t2
	1	P1m1	2t1,t2
	2	P2	2t1,t2
* k = 0 , 1/2			
R1	1	Pam2	t1,2t2
R2	1	Pnb2	t1,2t2
R3	1	$Pab2_1$	t1,2t2
R4	1	$Pnm2_1$	t1,2t2

* k = 1/2 , 1/2

R1	1	C112	t1-t2,t1+t2
	1	P1m1	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 30

30 Go = $Pab2_1$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	$P112_1$	2t1,t2
	1	$P1b1^1$	2t1,t2
	2	P1	2t1,t2
* k = 0 , 1/2			
R1	1	Pa11	t1,2t2
R2	1	Pa11	t1-t2,t1+t2
R3	1	Pa11	t1,2t2
R4	1	Pa11	t1-t2,t1+t2
* k = 1/2 , 1/2			
R1	1	$P112_1$	2t1,2t2
	1	$P1b1^1$	2t1,2t2
	2	P1	t1-t2,t1+t2

TABLE 31

31 Go = Pnb2

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112	2t1,t2
	1	P1b1	2t1,t2
	2	P1	2t1,t2

* k = 0 , 1/2

R1	1	P112	t1,2t2
R2	1	P112	t1,2t2
R3	1	$P112_1$	t1,2t2
R4	1	$P112_1$	t1,2t2

* k = 1/2 , 1/2

R1	1	C112	t1-t2,t1+t2
	1	Pa11	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 32

32 Go = $Pnm2_1$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	$P112_1$	2t1,t2
	1	P1m1	2t1,t2
	2	P1	2t1,t2
* k = 0 , 1/2			
R1	1	P1m1	t1,2t2
R2	1	P1b1	t1,2t2
R3	1	P1b1	t1,2t2
R4	1	P1m1	t1,2t2
* k = 1/2 , 1/2			
R1	1	C1m1	t1-t2,t1+t2
	1	Pa11	t1-t2,t1+t2
	2	P2	t1-t2,t1+t2

TABLE 33

33 Go = P2ba

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice

* k = 1/2 , 0				
	R1	1	P1b1	2t1,t2
		1	P2	2t1,t2
		2	P1	2t1,t2
* k = 0 , 1/2				
	R1	1	P11a	t1,2t2
		1	P2	t1,2t2
		2	P1	t1,2t2
* k = 1/2 , 1/2				
	R1	2	P2	t1-t2,t1+t2
	R2	2	P2	t1-t2,t1+t2

TABLE 34

34 Go = C2mm

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

	irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2				
	R1	1	C2mm	2t1,2t2
		1	P2	2t1,t2
		2	P2	2t1,2t2
	R2	1	C2mm	2t1,2t2
		1	P2	2t1,t2
		2	P2	2t1,2t2
* k = 1/2 , 1/2				
	R1	1	P2mm	t1-t2,t1+t2
	R2	1	P2ba	t1-t2,t1+t2
	R3	1	P2ma	t1-t2,t1+t2
	R4	1	P2ma	t1-t2,t1+t2

TABLE 35

35 Go = Cmm2

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	Cmm2	2t1,2t2
	1	P1	t1,2t2
	2	Pm11	2t1,2t2
R2	1	Cam2	2t1,2t2
	1	P1	t1,2t2
	2	Pa11	2t1,2t2
* k = 1/2 , 1/2			
R1	1	Pmm2	t1-t2,t1+t2
R2	1	Cam2	2t1,2t2
R3	1	Pmm2	t1-t2,t1+t2
R4	1	Cam2	2t1,2t2

TABLE 36

36 Go = Cam2

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	C112	2t1,2t2
	1	C1m1	2t1,2t2
	1	P1	t1,2t2
	2	P2	2t1,2t2
R2	1	C112	2t1,2t2
	1	P1	t1,2t2
	1	C1m1	2t1,2t2
	2	P1	2t1,2t2

* k = 1/2 , 1/2

R1	1	Pam2	t1-t2,t1+t2
R2	1	Pam2	t1-t2,t1+t2
R3	1	$Pbm2_1$	t1-t2,t1+t2
R4	1	$Pab2_1$	t1-t2,t1+t2

TABLE 37

37 Go = Pmmm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	Pmmm	2t1,t2
R2	1	Pmma	2t1,t2
R3	1	Pama	2t1,t2
R4	1	Pamm	2t1,t2
R5	1	Pama	2t1,t2
R6	1	Pamm	2t1,t2
R7	1	Pmmm	2t1,t2
R8	1	Pmma	2t1,t2
* k = 0 , 1/2			
R1	1	Pmmm	t1,2t2
R2	1	Pmma	t1,2t2
R3	1	Pama	t1,2t2
R4	1	Pamm	t1,2t2
R5	1	Pamm	t1,2t2
R6	1	Pama	t1,2t2
R7	1	Pmma	t1,2t2
R8	1	Pmmm	t1,2t2

R1	1	Cmmm	t1-t2,t1+t2
R2	1	Cmmm	t1-t2,t1+t2
R3	1	Camm	t1-t2,t1+t2
R4	1	Camm	t1-t2,t1+t2
R5	1	Camm	t1-t2,t1+t2
R6	1	Camm	t1-t2,t1+t2
R7	1	Cmmm	t1-t2,t1+t2
R8	1	Cmmm	t1-t2,t1+t2

TABLE 38

38 Go = Pama

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112/m	2t1,t2
	1	P222	2t1,t2
	2	P121	2t1,t2
R2	1	$P112_1/m$	2t1,t2
	1	$P222_1$	2t1,t2
	2	$P12_11$	2t1,t2
* k = 0 , 1/2			
R1	1	Pama	t1,2t2
R2	1	Paba	t1,2t2
R3	1	Pnma	t1,2t2
R4	1	Pnba	t1,2t2
R5	1	Pnba	t1,2t2
R6	1	Pnma	t1,2t2
R7	1	Paba	t1,2t2
R8	1	Pama	t1,2t2

* k = 1/2 , 1/2

R1	1	C12/m1	t1-t2,t1+t2
	1	C222	t1-t2,t1+t2
	2	C121	t1-t2,t1+t2
R2	1	C12/m1	t1-t2,t1+t2
	1	C222	t1-t2,t1+t2
	2	C121	t1-t2,t1+t2

TABLE 39

39 Go = Pnba

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0			
R1	1	P222	2t1,t2
	1	$P\bar{1}$	2t1,t2
	2	P121	2t1,t2
R2	1	$P222_1$	2t1,t2
	1	$P\bar{1}$	2t1,t2
	2	$P12_11$	2t1,t2
* k = 0 , 1/2			
R1	1	P222	t1,2t2
	1	$P\bar{1}$	t1,2t2
	2	P112	t1,2t2
R2	1	$P222_1$	t1,2t2
	1	$P\bar{1}$	t1,2t2
	2	$P112_1$	t1,2t2
* k = 1/2 , 1/2			
R1	1	C222	t1-t2,t1+t2
	1	P2/a11	t1-t2,t1+t2
	2	P2	t1-t2,t1+t2
R2	1	C222	t1-t2,t1+t2
	1	P2/a11	t1-t2,t1+t2
	2	P2	t1-t2,t1+t2

TABLE 40

40 Go = Pmma

irrep	Subduction	Subgroup G'	Translation

	Frequency		Sublattice
* k = 1/2 , 0			
R1	1	Pmm2	2t1,t2
	1	P2/m11	2t1,t2
	2	Pm11	2t1,t2
R2	1	Pam2	2t1,t2
	1	P2/a11	2t1,t2
	2	Pa11	2t1,t2
* k = 0 , 1/2			
R1	1	Pmma	t1,2t2
R2	1	Pmba	t1,2t2
R3	1	Paba	t1,2t2
R4	1	Pabm	t1,2t2
R5	1	Pabm	t1,2t2
R6	1	Paba	t1,2t2
R7	1	Pmba	t1,2t2
R8	1	Pmma	t1,2t2
* k = 1/2 , 1/2			
R1	1	Pnm21	t1-t2,t1+t2
	1	P2/m11	t1-t2,t1+t2
	2	Pm11	t1-t2,t1+t2
R2	1	Pam2	t1-t2,t1+t2
	1	P2/a11	t1-t2,t1+t2
	2	Pa11	t1-t2,t1+t2

TABLE 41

#41 Go = Pamm

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0			
R1	1	P2mm	2t1,t2
	1	P112/m	2t1,t2

	2	P11m	2t1,t2
R2	1	P2ma	2t1,t2
	1	P112/a	2t1,t2
	2	P11a	2t1,t2
* k = 0 , 1/2			
R1	1	Pamm	t1,2t2
R2	1	Pabm	t1,2t2
R3	1	Pnmm	t1,2t2
R4	1	Pnbm	t1,2t2
R5	1	Pnbm	t1,2t2
R6	1	Pnmm	t1,2t2
R7	1	Pabm	t1,2t2
R8	1	Pamm	t1,2t2
* k = 1/2 , 1/2			
R1	1	C2mm	t1-t2,t1+t2
	1	C112/m	t1-t2,t1+t2
	2	C11m	t1-t2,t1+t2
R2	1	C2mm	t1-t2,t1+t2
	1	C112/m	t1-t2,t1+t2
	2	C11m	t1-t2,t1+t2

TABLE 42

#42 Go = Pnma

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P222$_1$1	2t1,t2
	1	P12$_1$/m	2t1,t2
	2	P112	2t1,t2
R2	1	P22121	2t1,t2
	1	P121/m	2t1,t2
	2	P112$_1$1	2t1,t2

* k = 0 , 1/2			
R1	1	P2ma	t1,2t2
	1	P112/m	t1,2t2
	2	P1m1	t1,2t2
R2	1	P2ba	t1,2t2
	1	P112/a	t1,2t2
	2	P1b1	t1,2t2
* k = 1/2 , 1/2			
R1	1	C12/m1	t1-t2,t1+t2
	1	P2/a11	t1-t2,t1+t2
	2	P$\bar{1}$	t1-t2,t1+t2
R2	1	C12/m1	t1-t2,t1+t2
	1	P2/a11	t1-t2,t1+t2
	2	P$\bar{1}$	t1-t2,t1+t2

TABLE 43

43 Go = Paba

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P12/a1	2t1,t2
	1	P112$_1$	2t1,t2
	2	P121	2t1,t2
R2	1	P22$_1$2$_1$	2t1,t2
	1	P121/a	2t1,t2
	2	P12$_1$1	2t1,t2
* k = 0 , 1/2			
R1	1	Pbb2	t1,2t2
	1	P2/a11	t1,2t2
	2	Pa11	t1,2t2
R2	1	Pnb2	t1,2t2
	1	P2/a11	t1,2t2
	2	Pa11	t1,2t2
* k = 1/2 , 1/2			
R1	1	C121	t1-t2,t1+t2
	1	P2	t1-t2,t1+t2

	1	P$\bar{1}$	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2
R2	1	C121	t1-t2,t1+t2
	1	P2	t1-t2,t1+t2
	1	P$\bar{1}$	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 44

44 Go = Pmba

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P2/m11	2t1,t2
	1	P1b1	2t1,t2
	1	P112$_1$1	2t1,t2
	2	Pm11	2t1,t2
R2	1	P2/a11	2t1,t2
	1	P1b1	2t1,t2
	1	P112$_1$1	2t1,t2
	2	Pa11	2t1,t2
* k = 0 , 1/2			
R1	1	Pm2$_1$1a	t1,2t2
	1	P2/m11	t1,2t2
	2	Pm11	t1,2t2
R2	1	Pab2$_1$1	t1,2t2
	1	P2/a11	t1,2t2
	2	Pa11	t1,2t2
* k = 1/2 , 1/2			
R1	2	P2/a11	2t1,t1+t2
R2	2	P2/m11	t1-t2,2t1
R3	2	P2/a11	2t1,-t1+t2
R4	2	P2/m11	t1-t2,t1+t2

TABLE 45

45 Go = Pabm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P2ma	2t1,t2
	1	P112$_1$/m	2t1,t2
	2	P11m	2t1,t2

R2	1	P2ba	2t1,t2
	1	P112$_1$/a	2t1,t2
	2	P11a	2t1,t2
* k = 0 , 1/2			
R1	1	Pa2$_1$m	t1,2t2
	1	P2/a11	t1,2t2
	2	Pa11	t1,2t2
R2	1	Pn2$_1$m	t1,2t2
	1	P2/a11	t1,t1-2t2
	2	Pa11	t1,t1+2t2
* k = 1/2 , 1/2			
R1	1	C11m	t1-t2,t1+t2
	1	P2	t1-t2,t1+t2
	1	P$\bar{1}$	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2
R2	1	C11m	t1-t2,t1+t2
	1	P2	t1-t2,t1+t2
	1	P$\bar{1}$	t1-t2,t1+t2
	2	P1	t1-t2,t1+t2

TABLE 46

46 Go = Pnmm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0			
R1	1	P112$_1$/m	2t1,t2
	1	P2mm	2t1,t2
	2	P11m	2t1,t2
R2	1	P112$_1$/a	2t1,t2
	1	P2ma	2t1,t2
	2	P11a	2t1,t2
* k = 0 , 1/2			
R1	1	P12$_1$/m1	t1,2t2
	1	P2mm	t1,2t2
	2	P1m1	t1,2t2
R2	1	P12$_1$/a1	t1,2t2
	1	P2ma	t1,2t2

	2	P1b1	t1,2t2

* k = 1/2 , 1/2

R1	1	C2mm	t1-t2,t1+t2
	1	P2/a11	t1-t2,t1+t2
	2	P2	t1-t2,t1+t2
R2	1	C2mm	t1-t2,t1+t2
	1	P2/a11	t1-t2,t1+t2
	2	P2	t1-t2,t1+t2

TABLE 47

\# 47 Go = Cmmm

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	Cmmm	2t1,2t2
	1	P1	t1,2t2
	2	P2/m11	2t1,2t2
R2	1	Camm	2t1,2t2
	1	P1	t1,2t2
	2	P2/a11	2t1,2t2
R3	1	Camm	2t1,2t2
	1	P1	t1,2t2
	2	P2/a11	2t1,2t2
R4	1	Cmmm	2t1,2t2
	1	P1	t1,2t2
	2	P2/m11	2t1,2t2
* k = 1/2 , 1/2			
R1	1	Pmmm	t1-t2,t1+t2
R2	1	Pmba	t1-t2,t1+t2
R3	1	Pnma	t1-t2,t1+t2
R4	1	Pnbm	t1-t2,t1+t2
R5	1	Pnba	t1-t2,t1+t2
R6	1	Pnmm	t1-t2,t1+t2

R7	1	Pmma	t1-t2,t1+t2
R8	1	Pmma	t1-t2,t1+t2

TABLE 48

48 Go = Camm

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	C112/m	2t1,2t2
	1	C12/m1	2t1,2t2
	1	C2mm	2t1,2t2
	1	P1	t1,2t2
	2	C112	2t1,2t2
	2	C121	2t1,2t2
	2	C11m	2t1,2t2
	2	C1m1	2t1,2t2
	2	P$\bar{1}$	2t1,2t2
	4	P1	2t1,2t2
* k = 1/2 , 1/2			
R1	1	Pama	t1-t2,t1+t2
R2	1	Pabm	t1-t2,t1+t2
R3	1	Pama	t1-t2,t1+t2
R4	1	Pabm	t1-t2,t1+t2
R5	1	Paba	t1-t2,t1+t2
R6	1	Pamm	t1-t2,t1+t2
R7	1	Pamm	t1-t2,t1+t2
R8	1	Paba	t1-t2,t1+t2

TABLE 49

#49 Go = P411

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P411	2t1 , 2t2
	1	P211	2t1 , t2
	2	P211	2t1 , 2t2
R2	1	P411	2t1 , 2t2
	1	P211	2t1 , t2
	2	P211	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P411	t1 - t2,t1 + t2
R2	1	P411	t1 - t2,t1 + t2
R3	2	P211	t1 - t2,t1 + t2

TABLE 50

#50 Go = P$\bar{4}$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P$\bar{4}$	2t1 , 2t2
	1	P2	2t1 , t2
	2	P2	2t1 , 2t2
R2	1	P$\bar{4}$	2t1 , 2t2
	1	P2	2t1 , t2
	2	P2	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P$\bar{4}$	t1 - t2,t1 + t2
R2	1	P4	t1 - t2,t1 + t2
R3	2	P2	t1 - t2,t1 + t2

TABLE 51

#51 Go = P4/m11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
#51 Go = P4/m11			
R1	1	P4/m11	2t1 , 2t2
	1	P1	2t1 , t2
	2	P2/m11	2t1 , 2t2
R2	1	P4/n11	2t1 , 2t2
	1	P1	2t1 , t2
	2	P2/b11	2t1 , 2t1 + 2t2
R3	1	P4/n11	2t1 , 2t2
	1	P1	2t1 , t2
	2	P2/b11	2t1 , 2t1 + 2t2
R4	1	P4/m11	2t1 , 2t2
	1	P1	2t1 , t2
	2	P2/m11	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P4/m11	t1 - t2,t1 + t2
R2	1	P4/n11	t1 - t2,t1 + t2
R3	1	P4/m11	t1 - t2,t1 + t2
R4	1	P4/n11	t1 - t2,t1 + t2
R5	2	P2/m11	t1 - t2,t1 + t2
R6	2	P2/b11	t1 - t2,t1 + t2

TABLE 52

52 Go = P4/n11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P$\bar{4}$	2t1 , 2t2
	1	P4	2t1 , 2t2
	1	P$\bar{1}$	2t1 , t2
	2	P$\bar{1}$	2t1 , 2t2
	2	P2	2t1 , 2t2
	4	P1	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P$\bar{4}$	t1 - t2,t1 + t2
	1	P2/b11	t1 - t2,t1 + t2
	2	P2	t1 - t2,t1 + t2
R2	1	P4	t1 - t2,t1 + t2
	1	P2/b11	t1 - t2,t1 + t2
	2	P2	t1 - t2,t1 + t2

TABLE 53

#53 Go = P422

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P422	2t1 , 2t2
	1	P1	2t1 , t2
	2	P222	2t1 , 2t2
R2	1	$P42_12$	2t1 , 2t2
	1	P1	2t1 , t2
	2	$P22_12_1$	2t1 , 2t2
R3	1	P422	2t1 , 2t2
	1	P1	2t1 , t2
	2	P222	2t1 , 2t2
R4	1	$P42_12$	2t1 , 2t2
	1	P1	2t1 , t2
	2	$P22_12_1$	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P422	t1 - t2,t1 + t2
R2	1	$P42_12$	t1 - t2,t1 + t2
R3	1	$P42_12$	t1 - t2,t1 + t2
R4	1	P422	t1 - t2,t1 + t2
R5	1	$P222_1$	t1 - t2,t1 + t2
	1	$P222_1$	2t1 , 2t2
	2	P2	t1 - t2,t1 + t2

TABLE 54

54 Go = $P42_12$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P4	2t1 , 2t2
	1	C222	2t1 , 2t2
	1	C112	2t1 , 2t2
	1	P1	2t1 , t2
	2	P2	2t1 , 2t2
	4	P1	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P4	t1 - t2,t1 + t2
	2	P222	t1 - t2,t1 + t2
R2	1	P4	t1 - t2,t1 + t2
	2	$P22_12_1$	t1 - t2,t1 + t2
R3	1	P4	t1 - t2,t1 + t2
	1	$P222_1$	t1 - t2 ,t1 + t2
	2	P2	t1 - t2,t1 + t2

TABLE 55

#55 Go = P4mm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P4mm	2t1 , 2t2
	1	P2mm	2t1 , t2
	2	P2mm	2t1 , 2t2
R2	1	P4bm	2t1 , 2t2
	1	P2ma	2t1 , t2
	2	P2ba	2t1 , 2t2
R3	1	P4bm	2t1 , 2t2
	1	P2ma	2t1 , t2
	2	P2ba	2t1 , 2t2
R4	1	P4mm	2t1 , 2t2
	1	P2mm	2t1 , t2
	2	P2mm	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P4mm	t1 - t2,t1 + t2
R2	1	P4bm	t1 - t2,t1 + t2
R3	1	P4bm	t1 - t2,t1 + t2
R4	1	P4mm	t1 - t2,t1 + t2
R5	1	C2mm	t1 - t2,t1 + t2
	1	P2ma	t1 - t2,t1 + t2
	2	P2	t1 - t2,t1 + t2

TABLE 56

56 Go = P4bm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P411	2t1 , 2t2
	1	C2mm	2t1 , 2t2
	2	C1m1	2t1 , 2t2
	2	C11m	2t1 , 2t2
	1	P1b1	2t1 , t2
	1	P11a	t1 , 2t2
	1	P2	2t1 , t2
	2	P2	2t1 , 2t2
	2	P1	t1 , 2t2
	4	P1	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P4	t1 -t2 , t1 + t2
	1	P2ma	t1 - t2,t1 + t2
	2	P2	t1 -t2 , t1 + t2
R2	1	P2mm	t1 - t2,t1 + t2
R3	1	P2ba	t1 - t2,t1 + t2

TABLE 57

57 Go = $P\bar{4}2m$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	$P\bar{4}2m$	2t1 , 2t2
	1	P1	2t1 , t2
	2	P222	2t1 , 2t2
R2	1	$P\bar{4}2_1m$	2t1 , 2t2
	1	P1	2t1 , t2
	2	$P22_12_1$	2t1 , 2t2
R3	1	$P\bar{4}2m$	2t1 , 2t2
	1	P1	2t1 , t2
	2	P222	2t1 , 2t2
R4	1	$P\bar{4}2_1m$	2t1 , 2t2
	1	P1	2t1 , t2
	2	$P22_12_1$	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	$P\bar{4}m2$	t1 - t2,t1 + t2
R2	1	$P\bar{4}2_1m$	t1 - t2,t1 + t2
R3	1	$P\bar{4}m2$	t1 - t2,t1 + t2
R4	1	$P\bar{4}2_1m$	t1 - t2,t1 + t2
R5	1	P2ma	t1 - t2,t1 + t2
	1	$P222_1$	t1 - t2,t1 + t2
	2	P2	t1 - t2,t1 + t2

TABLE 58

#58 Go = $P\bar{4}2_1m$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P4	2t1 , 2t2
	1	C2mm	2t1 , 2t2
	2	C1m1	2t1 , 2t2
	2	C11m	2t1 , 2t2
	1	$P112_1$	2t1 , t2
	2	P2	2t1 , 2t2
	4	P1	2t1 , 2t2
* k = 1/2 , 1/2			
R1	2	P2ba	t1 -t2 , t1 + t2
R2	2	P2mn	t1 - t2,t1 + t2
R3	1	$P\bar{4}$	t1 - t2,t1 + t2
	1	P2ma	t1 - t2,t1 + t2
	2	P2	t1 - t2,t1 + t2

TABLE 59

59 Go = P$\bar{4}$m2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P$\bar{4}$m2	2t1 , 2t2
	1	P2mm	2t1 , t2
	2	P2mm	2t1 , 2t2
R2	1	P$\bar{4}$	2t1 , 2t2
	1	P2ma	t1 , 2t2
	1	P222	2t1 , 2t2
	2	P11a	2t1 , 2t2
	2	P1b1	2t1 , 2t2
	2	P2	2t1 , 2t2
R3	1	P$\bar{4}$	2t1 , 2t2
	1	P2ma	t1 , 2t2
	1	P222	2t1 , 2t2
	2	P11a	2t1 , 2t2
	2	P1b1	2t1 , 2t2
	2	P2	2t1 , 2t2
R4	1	P$\bar{4}$m2	2t1 , 2t2
	1	P2mm	2t1 , t2
	2	P2mm	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P$\bar{4}$2m	t1 - t2,t1 + t2
R2	1	P$\bar{4}$2m	t1 - t2,t1 + t2
R3	1	P$\bar{4}$b2	t1 - t2,t1 + t2
R4	1	P$\bar{4}$b2	t1 - t2,t1 + t2
R5	1	P2mm	t1 - t2,t1 + t2
	1	P112	t1 - t2,t1 + t2
	1	P121	t1 - t2,t1 + t2
	2	P2	t1 - t2,t1 + t2

TABLE 60

60 Go = $P\bar{4}b2$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	$P\bar{4}$	2t1 , 2t2
	1	C222	2t1 , 2t2
	1	P1b1	t1 , 2t2
	2	P112	2t1 , 2t2
	2	P2	2t1 , 2t2
	4	P1	2t1 , 2t2
* k = 1/2 , 1/2			
R1	2	P222	t1 -t2 , t1 + t2
	2	$P22_12_1$	t1 - t2,t1 + t2
R2	1	$P22_12_1$	t1 - t2,t1 + t2
R3	1	$P\bar{4}$	t1 - t2,t1 + t2
	1	$P222_1$	t1 - t2,t1 + t2
	2	P2	t1 - t2,t1 + t2

TABLE 61

#61 Go = P4/mmm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P4/mmm	2t1,2t2
	1	P1	t1 , 2t2
	2	P2/mmm	2t1,2t2
R2	1	P4/mbm	2t1,2t2
	1	P1	t1 , 2t2
	2	P2/mba	2t1 , 2t2
R3	1	P4/nbm	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/nba	2t1 , 2t2
R4	1	P4/nmm	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/nmm	2t1 , 2t2
R5	1	P4/nbm	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/nba	2t1 , 2t2
R6	1	P4/nmm	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/nmm	2t1 , 2t2
R7	1	P4/mmm	2t1 , 2t2
	1	.P1	t1 , 2t2
	2	P2/mmm	2t1 , 2t2
R8	1	P4/mbm	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/mba	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P4/mmm	t1-t2,t1+t2
R2	1	P4/mbm	t1-t2,t1+t2
R3	1	P4/mbm	t1-t2,t1+t2
R4	1	P4/mmm	t1-t2,t1+t2
R5	1	P2ma	t1-t2,t1+t2
	1	Cam2	t1-t2,t1+t2

	1	C222	t1-t2,t1+t2
	1	Pam2	2t1 , 2t2
	2	P2/b11	2t1 , 2t2
R6	1	P4/nmm	t1-t2,t1+t2
R7	1	P4/nmm	t1-t2,t1+t2
R8	1	P4/nmm	t1-t2,t1+t2
R9	1	P4/nmm	t1-t2,t1+t2
R10	1	C2/mmm	t1 - t2,t1 + t2
	2	P2/m11	2t1 , 2t2

TABLE 62

#62 Go = P4/nbm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2			
R1	1	P4	2t1 , 2t2
	1	P112/a	t1 , 2t2
	2	P222	2t1 , 2t2
	3	P112	2t1 , 2t2
	4	P1	2t1 , 2t2
R2	1	P4	2t1 , 2t2
	1	$P112_1/a$	t1 , 2t2
	2	$P22_12_1$	2t1 , 2t2
	3	$P112_1$	2t1 , 2t2
	4	P1	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P4	t1 -t2 , t1 + t2
	1	C222	t1 - t2,t1 + t2
	1	P2/b11	t1 - t2,t1 + t2
	1	P2ma	t1 - t2,t1 + t2
	2	C222	2t1 , 2t2

TABLE 63

63 Go = P4/mbm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2			
R1	1	P4/m11	2t1 , 2t2
	1	$Pmb2_1$	2t1 , 2t2
	1	$Pm2_1a$	t1 , 2t2
	2	P2/m11	2t1-2t2 ,2t1
	4	Pm11	
R2	1	P4/n11	2t1 , 2t2
	1	$Pab2_1$	2t1 , 2t2
	1	$Pb2_1a$	t1 , 2t2
	2	P2/b11	2t1-2t2 ,2t1
	4	Pb11	
* k = 1/2 , 1/2			
R1	2	P2/b11	2t1 , t1 + t2
R2	2	P2/b11	2t1 , t1 + t2
R3	2	P2/m11	t1 - t2 , 2t1
R4	2	P2/m11	t1 - t2 , 2t1
R5	1	P4/m11	t1 - t2 , t1 + t2
	2	P2/m11	t1 - t2 , t1 + t2
R6	1	P4/n11	t1 - t2 , t1 + t2
	2	P2/b11	t1 - t2 , t1 + t2

TABLE 64

64 Go = P4/nmm

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P$\bar{4}$m2	2t1 , 2t2
	1	P4	2t1 , 2t2
	1	P2mm	t1 , 2t2
	1	P112$_1$	2t1 , t2
	2	P$\bar{1}$	2t1 , 2t2
	2	P2mm	2t1 , 2t2
	3	P1m1	2t1 , 2t2
	3	P11m	2t1 , 2t2
	4	P1	2t1 , 2t2
R2	1	P$\bar{4}$m2	2t1 , 2t2
	1	P4	2t1 , 2t2
	1	P2mm	2t1 , t2
	1	P112$_1$	2t1 , t2
	2	P$\bar{1}$	2t1 , 2t2
	2	P2mm	2t1 , 2t2
	3	P1m1	2t1 , 2t2
	3	P11m	2t1 , 2t2
	4	P1	2t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P$\bar{4}$m2	t1 -t2 , t1 + t2
	1	P2/b11	t1 -t2 , t1 + t2
R2	1	P2/b11	t1 -t2 , t1 + t2
R3	1	P4bm	t1 -t2 , t1 + t2
	1	P2/b11	t1 -t2 , t1 + t2
R4	1	P4/mm	t1 -t2 , t1 + t2
	1	P2/b11	t1 -t2 , t1 + t2

TABLE 65

65 Go = P3

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P3	2t1 , 2t2
	1	P1	t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3			
R1	1	P3	t1 -t2 ,t1 + 2t2
R2	1	P3	t1 -t2 ,t1 + 2t2
	2	P1	t1 -t2 ,t1 + 2t2

TABLE 66

66 Go = P$\bar{3}$

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P$\bar{3}$	2t1 , 2t2
	1	P1	t1 , 2t2
	3	P1	2t1 , 2t2
R2	1	P3	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P$\bar{1}$	t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P$\bar{3}$	2t1 +t2 ,-t1 + t2
	2	P3	2t1 +t2 ,-t1 + t2
R2	2	P3	2t1 +t2 ,-t1 + t2
	2	P$\bar{1}$	2t1 +t2 ,-t1 + t2
	4	P1	2t1 +t2 ,-t1 + t2

TABLE 67

67 Go = P312

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P312	2t1 , 2t2
	1	P1	t1 , 2t2
	2	C112	2t1 , 2t2
	3	P1	2t1 , 2t2
R2	1	P3	2t1 , 2t2
	1	P1	t1 , 2t2
	2	C112	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P321	2t1 +t2 ,-t1 + t2
	1	C112	2t1 +t2 ,-t1 + t2
	2	P3	2t1 +t2 ,-t1 + t2
R2	1	P321	2t1 +t2 ,-t1 + t2
	2	P3	2t1 +t2 ,-t1 + t2
	2	C112	2t1 +t2 ,-t1 + t2
	4	P1	2t1 +t2 ,-t1 + t2

TABLE 68

68 Go = P321

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P321	2t1 , 2t2
	1	P1	t1 , 2t2
	1	P112	t1 -t2 ,t1 + t2
	2	C112	2t1 , 2t2
	3	P1	2t1 , 2t2
R2	1	P3	2t1 , 2t2
	1	P1	t1 , 2t2
	1	$P112_1$	t1 -t2 ,t1 + t2
	2	C112	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3			
R1	1	P312	2t1 +t2 ,-t1 + t2
R2	1	P3	2t1 +t2 ,-t1 + t2
R3	1	P3	2t1 +t2 ,-t1 + t2
	1	P112	3t1 , t1 + 2t2
	2	P1	2t1 +t2 ,-t1 + t2

TABLE 69

#69 Go = P3m1

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P3m1	2t1 , 2t2
	1	Pm11	t1 - t2 , t1 + t2
	1	P1	
	2	Cm	
	3	P1	
R2	1	P3	
	1	Pg	t1 - t2 , t1 + t2
	1	Cm	
	1	P1	
	3	Pi	
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P31m	t1 -t2 ,t1 + 2t2
	2	P3	t1 -t2 ,t1 + 2t2
R2	1	P31m	t1 -t2 ,t1 + 2t2
	2	P3	t1 -t2 ,t1 + 2t2
	2	Cm	2t1 + t2 , -t1 + t2
	4	P1	2t1 + t2 , -t1 + t2

TABLE 70

#70 Go = P31m

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P31m	2t1 , 2t2
	1	Pm11	t1 - t2 , t1 + t2
	1	P1	
	2	Cm	
	3	P1	
R2	1	P3	
	1	P1	
	1	Pg	t1 - t2 , t1 + t2
	1	Cm	
	3	P1	
* k = 1/3 , -2/3			
R1	1	P3m1	t1 -t2 ,t1 + 2t2
R2	1	P3	t1 -t2 ,t1 + 2t2
R3	1	P3	t1 -t2 ,t1 + 2t2
	1	Cm	2t1 + t2 , -t1 + t2
	2	P1	2t1 + t2 , -t1 + t2

TABLE 71

\# 71 Go = P$\bar{3}$12/m

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P$\bar{3}$12/m	2t1 , 2t2
	1	P1	t1 , 2t2
	2	C112/m	2t1 , 2t2
	2	C12/m1	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R2	1	P$\bar{3}$	2t1 , 2t2
	1	P1	t1 , 2t2
	2	C112/m	2t1 , 2t2
	2	C12/m1	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R3	1	P312	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P112/m	t1 , 2t2
	2	C112	2t1 , 2t2
	2	P$\bar{1}$	2t1 , 2t2
	3	P1	2t1 , 2t2
R4	1	P31m	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P112/m	t1 , 2t2
	2	C11m	2t1 , 2t2
	2	C112	2t1 , 2t2
	2	P$\bar{1}$	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P$\bar{3}$2/m1	2t1 +t2 ,-t1 + t2
	2	P31m	2t1 +t2 ,-t1 + t2
R2	1	P31m	2t1 +t2 ,-t1 + t2
	1	P321	2t1 +t2 ,-t1 + t2
	1	P$\bar{3}$	2t1 +t2 ,-t1 + t2
	2	P3	2t1 +t2 ,-t1 + t2
R3	1	P31m	2t1 +t2 ,-t1 + t2
	1	P321	2t1 +t2 ,-t1 + t2
	2	P3	2t1 + t2 , -t1 + t2
	2	C11m	2t1 + t2 , -t1 + t2
	2	C112	2t1 + t2 , -t1 + t2
	2	P$\bar{1}$	2t1 + t2 , -t1 + t2
	4	P1	2t1 + t2 , -t1 + t2

TABLE 72

#72 Go = P$\bar{3}$2/m1

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P$\bar{3}$2/m1	2t1 , 2t2
	1	P1	t1 , 2t2
	2	C12/m1	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R2	1	P$\bar{3}$	2t1 , 2t2
	1	P1	t1 , 2t2
	1	P112/m	t1 , t1 + 2t2
	2	C12/m1	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R3	1	P321	2t1 , 2t2
	1	P1	t1 , 2t2
	1	P12/m1	2(t1-t2),2(t1+ t2)
	2	C11m	2t1 , 2t2
	2	P$\bar{1}$	2t1 , 2t2
	3	P1	2t1 , 2t2
R4	1	P3m1	2t1 , 2t2
	1	P1	t1 , 2t2
	1	P112/m	t1 , t1 + 2t2
	2	C11m	2t1 , 2t2
	2	C112	2t1 , 2t2
	2	P$\bar{1}$	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P31m	2t1 +t2 ,-t1 + t2
	1	P312	2t1 +t2 ,-t1 + t2
	1	P$\bar{3}$	2t1 +t2 ,-t1 + t2
	2	P3	2t1 +t2 ,-t1 + t2
R2	1	P31m	2t1 +t2 ,-t1 + t2
	1	P312	2t1 +t2 ,-t1 + t2
	1	P$\bar{3}$	2t1 +t2 ,-t1 + t2
	2	P3	2t1 +t2 ,-t1 + t2
R3	1	P31m	2t1 +t2 ,-t1 + t2
	1	P312	2t1 +t2 ,-t1 + t2
	1	C112/m	2t1 +t2 ,-t1 + t2
	2	P3	2t1 + t2 , -t1 + t2
	2	C11m	2t1 + t2 , -t1 + t2
	2	C112	2t1 + t2 , -t1 + t2
	2	P$\bar{1}$	2t1 + t2 , -t1 + t2
	4	P1	2t1 + t2 , -t1 + t2

TABLE 73

#73 Go = P6̄11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P6	2t1 , 2t2
	1	P2	t1 , 2t2
	3	P2	2t1 , 2t2
R2	1	P3	2t1 , 2t2
	1	P2	t1 , 2t2
	2	P2	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P6	t1 -t2 ,t1 + 2t2
	2	P3	t1 - t2 ,t1 + 2t2
R2	2	P3	t1 - t2 ,t1 + 2t2
	2	P2	t1 - t2 ,t1 + 2t2
	4	P1	t1 - t2 ,t1 + 2t2

TABLE 74

#74 Go = P$\bar{6}$11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P$\bar{6}$	2t1 , 2t2
	1	P1	t1 , 2t2
	3	P1	2t1 , 2t2
R2	1	P3	2t1 , 2t2
	1	P1	t1 , 2t2
	2	Pm11	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3			
R1	1	P$\bar{6}$	t1 -t2 ,t1 + 2t2
R2	1	P3	t1 -t2 ,t1 + 2t2
R3	1	P$\bar{6}$	t1 - t2 ,t1 + 2t2
	2	P1	t1 - t2 ,t1 + 2t2
R4	1	P3	t1 - t2 ,t1 + 2t2
	1	Pm11	t1 - t2 ,t1 + 2t2
	2	P1	t1 - t2 ,t1 + 2t2

TABLE 75

#75 Go = P6/m11

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P6/m11	2t1 , 2t2
	1	P1	t1 , 2t2
	3	P2/m11	2t1 , 2t2
R2	1	P$\bar{3}$	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/b11	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R3	1	P6	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/b11	2t1 , 2t2
	3	P2	2t1 , 2t2
R4	1	P$\bar{6}$	2t1 , 2t2
	1	P1	t1 , 2t2
	2	P2/m11	2t1 , 2t2
	3	Pm11	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P6/m11	t1 -t2 ,t1 + 2t2
	2	P$\bar{6}$	t1 -t2 ,t1 + 2t2
R2	1	P6	t1 -t2 ,t1 + 2t2
	2	P3	t1 -t2 ,t1 + 2t2
R3	1	P3	t1 - t2 ,t1 + 2t2
	1	Pm11	t1 - t2 ,t1 + 2t2
	2	P2	t1 - t2 ,t1 + 2t2
	2	P$\bar{1}$	t1 - t2 ,t1 + 2t2
	4	P1	t1 - t2 ,t1 + 2t2
R4	1	P$\bar{6}$	t1 - t2 ,t1 + 2t2
	2	P3	t1 - t2 ,t1 + 2t2
	2	P2	t1 - t2 ,t1 + 2t2
	2	P$\bar{1}$	t1 - t2 ,t1 + 2t2
	3	Pm11	t1 - t2 ,t1 + 2t2
	4	P1	t1 - t2 ,t1 + 2t2

TABLE 76

#76 Go = P622

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P622	2t1 , 2t2
	1	P1	t1 , 2t2
	2	C222	2t1 , 2t2
	3	P2	2t1 , 2t2
R2	1	P321	2t1 , 2t2
	1	P222	t1 , t1 + 2t2
	2	C112	2t1 , 2t2
	2	P2	2t1 , 2t2
	3	P1	2t1 , 2t2
R3	1	P6	2t1 , 2t2
	1	P222	t1 , t1 + 2t2
	2	C222	2t1 , 2t2
	3	P2	2t1 , 2t2
R4	1	P312	2t1 , 2t2
	1	P222	t1 , t1 + 2t2
	2	C112	2t1 , 2t2
	2	P2	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P622	2t1 + t2 ,-t1 + t2
	2	P312	2t1 + t2 ,-t1 + t2
	2	C112	2t1 + t2 ,-t1 + t2
	2	C121	2t1 + t2 ,-t1 + t2
R2	1	P6	2t1 + t2 ,-t1 + t2
	1	$P222_1$	3(t1+t2),2(-t1+t2)
	2	P3	2t1 + t2 ,-t1 + t2
R3	1	P321	2t1 + t2 ,-t1 + t2
	1	C222	2t1 + t2 ,-t1 + t2
	2	C112	2t1 + t2 ,-t1 + t2
	2	P3	2t1 + t2 ,-t1 + t2
	2	P2	2t1 + t2 ,-t1 + t2
	4	P1	2t1 + t2 ,-t1 + t2

TABLE 77

77 Go = P6mm

irrep	Subduction Frequency	Subgroup G′	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P6mm	2t1 , 2t2
	1	P2mm	t1 -t2 ,t1 + t2
	1	C2mm	2t1 , 2t2
	3	P2	2t1 , 2t2
R2	1	P6	2t1 , 2t2
	1	P2ba	t1 -t2 ,t1 + t2
	1	C2mm	2t1 , 2t2
	3	P2	2t1 , 2t2
R3	1	P31m	2t1 , 2t2
	1	P2ma	t1 -t2 ,t1 + t2
	1	C2mm	2t1 , 2t2
	2	Cm	2t1 , 2t2
	2	P2	2t1 , 2t2
	3	P1	2t1 , 2t2
R4	1	P3m1	2t1 , 2t2
	1	P2ma	t1 -t2 ,t1 + t2
	1	C2mm	2t1 , 2t2
	2	Cm	2t1 , 2t2
	2	P2	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P6mm	t1 -t2 ,t1 + 2t2
	2	P3m1	t1 - t2 ,t1 + 2t2
R2	1	P6	t1 - t2 ,t1 + 2t2
	1	P31m	t1 - t2 ,t1 + 2t2
	3	P3	t1 - t2 ,t1 + 2t2
R3	1	P31m	t1 - t2 ,t1 + 2t2
	1	C2mm	3t1 , 3t2
	2	P3	t1 - t2 ,t1 + 2t2
	2	Cm	3t1 , 3t2
	2	P2	t1 - t2 ,t1 + 2t2
	4	P1	t1 - t2 ,t1 + 2t2

TABLE 78

78 Go = P$\bar{6}$m2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P$\bar{6}$m2	2t1 , 2t2
	1	P1	2t1 , t2
	2	Cmm2	2t1 , 2t2
	3	Pm11	2t1 , 2t2
R2	1	P$\bar{6}$	2t1 , 2t2
	1	P1	2t1 , t2
	1	Cam2	2t1 , 2t2
	2	Cmm2	2t1 , 2t2
	3	Pm11	2t1 , 2t2
R3	1	P3m1	2t1 , 2t2
	1	P1	2t1 , t2
	1	Cam2	2t1 , 2t2
	2	Cm	2t1 , 2t2
	2	C112	2t1 , 2t2
	3	P1	2t1 , 2t2
R4	1	P312	2t1 , 2t2
	1	P1	2t1 , t2
	1	Cam2	2t1 , 2t2
	2	Cm	2t1 , 2t2
	2	C112	2t1 , 2t2
	3	P1	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P$\bar{6}$2m	t1 - t2 ,t1 + 2t2
	2	P$\bar{6}$	t1 - t2 ,t1 + 2t2
R2	1	P321	t1 - t2 ,t1 + 2t2
	1	P31m	t1 - t2 ,t1 + 2t2
	2	P3	t1 - t2 ,t1 + 2t2
R3	1	P$\bar{6}$2m	t1 - t2 ,t1 + 2t2
	2	P$\bar{6}$	t1 - t2 ,t1 + 2t2
R4	1	P321	t1 - t2 ,t1 + 2t2
	1	P31m	t1 - t2 ,t1 + 2t2
	2	P3	t1 - t2 ,t1 + 2t2
R5	1	P$\bar{6}$2m	t1 - t2 ,t1 + 2t2
	2	P$\bar{6}$	t1 - t2 ,t1 + 2t2
R6	1	P321	t1 - t2 ,t1 + 2t2
	1	P31m	t1 - t2 ,t1 + 2t2
	2	P3	t1 - t2 ,t1 + 2t2

TABLE 79

79 Go = P$\bar{6}$2m

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2			
R1	1	P$\bar{6}$2m	2t1 , 2t2
	1	P1	2t1 , t2
	2	Cm2m	2t1 , 2t2
	3	Pm11	2t1 , 2t2
R2	1	P321	2t1 , 2t2
	1	Cb2m	2t1 , 2t2
	1	P1	2t1 , t2
	2	C1m1	2t1 , 2t2
	2	C121	2t1 , 2t2
	3	P1	2t1 , 2t2
R3	1	P31m	2t1 , 2t2
	1	P1	2t1 , t2
	1	Cb2m	2t1 , 2t2
	2	C1m1	2t1 , 2t2
	2	C121	2t1 , 2t2
	3	P1	2t1 , 2t2
R4	1	P$\bar{6}$	2t1 , 2t2
	1	P1	2t1 , t2
	1	Cm2m	2t1 , 2t2
	3	Pm11	2t1 , 2t2
* k = 1/3 , -2/3 ; -1/3 , -1/3			
R1	1	P$\bar{6}$m2	t1 -t2 ,t1 + 2t2
R2	1	P312	t1 - t2 ,t1 + 2t2
R3	1	P$\bar{6}$	t1 - t2 ,t1 + 2t2
R4	1	P3m1	t1 - t2 ,t1 + 2t2
R5	1	P3	t1 - t2 ,t1 + 2t2
	1	C112	t1 - t2 ,t1 + 2t2
	1	C11m	t1 - t2 ,t1 + 2t2
	2	P1	t1 - t2 ,t1 + 2t2
R6	1	P$\bar{6}$	t1 - t2 ,t1 + 2t2
	1	Cmm2	t1 - t2 ,t1 + 2t2
	2	Pm11	t1 - t2 ,t1 + 2t2

TABLE 80

\# 80 Go = P6/mmm

* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Translation Sublattice
R1	1	P6/mmm	2t1 , 2t2
	1	P1	2t1 , t2
	2	C2/mmm	2t1 , 2t2
	3	P2/m11	2t1 , 2t2
R2	1	P6/m	2t1 , 2t2
	1	P1	2t1 , t2
	2	C2/mmm	2t1 , 2t2
	3	P2/m11	2t1 , 2t2
R3	1	P$\bar{3}$2/m1	2t1 , 2t2
	1	P2/amm	2(t1-t2),2(t1+t2)
	1	P1	2t1 , t2
	2	C112/m	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R4	1	P$\bar{3}$12/m	2t1 , 2t2
	1	P2/amm	2(t1-t2),2(t1+t2)
	1	P1	2t1 , t2
	2	C112/m	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R5	1	P622	2t1 , 2t2
	1	P2/amm	2(t1-t2),2(t1+t2)
	2	C222	2t1 , 2t2
	1	P1	2t1 , t2
	2	C11m	2t1 , 2t2
	2	P2/b11	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R6	1	P6mm	2t1 , 2t2
	1	P2/amm	2(t1-t2),2(t1+t2)
	1	P1	2t1 , t2
	2	C222	2t1 , 2t2
	2	C11m	2t1 , 2t2
	2	P2/b11	2t1 , 2t2
	3	P$\bar{1}$	2t1 , 2t2
R7	1	P$\bar{6}$2m	2t1 , 2t2
	1	P2/mba	2(t1-t2),2(t1+t2)
	1	Pm2m	t1 , t1 + 2t2
	2	C112	2t1 , 2t2
	2	C2mm	2t1 , 2t2
	2	P2/m11	2t1 , 2t2
	3	Pm	2t1 , 2t2

R8	1	P$\bar{6}$m2	2t1 , 2t2
	1	P2/mba	2(t1-t2),2(t1+t2)
	1	P2/nma	2(t1-t2),2(t1+t2)
	2	Cmm2	t1 , t1 + 2t2
	2	C2mm	2t1 , 2t2
	2	P2/m11	2t1 , 2t2
	3	Pm	2t1 , 2t2

* k = 1/3 , -2/3 ; -1/3 , -1/3

R1	1	P6/mmm	t1 -t2 ,t1 + 2t2
	2	P$\bar{6}$m2	t1 -t2 ,t1 + 2t2
	2	Cmm2	2t1 + t2 , -t1 + t2
R2	1	P622	t1 - t2 ,t1 + 2t2
	1	P$\bar{3}$2/m1	t1 - t2 ,t1 + 2t2
	2	P312	t1 - t2 ,t1 + 2t2
R3	1	P6mm	2t1 + t2 ,-t1 + t2
	1	P$\bar{3}$12/m	t1 - t2 ,t1 + 2t2
	2	P3m1	t1 - t2 ,t1 + 2t2
R4	1	P$\bar{6}$m2	2t1 + t2 ,-t1 + t2
	1	P6	t1 - t2 ,t1 + 2t2
	2	P$\bar{6}$	t1 - t2 ,t1 + 2t2
R5	1	P$\bar{6}$m2	2t1 + t2 ,-t1 + t2
	1	Cmmm	t1 - t2 ,t1 + 2t2
	2	Cmm2	t1 - t2 ,t1 + 2t2
	2	C2mm	t1 - t2 ,t1 + 2t2
	2	P$\bar{6}$	t1 - t2 ,t1 + 2t2
	2	C222	t1 - t2 ,t1 + 2t2
	2	P2/m11	t1 - t2 ,t1 + 2t2
	4	Pm11	t1 - t2 ,t1 + 2t2
R5	1	P31m	2t1 + t2 ,-t1 + t2
	1	P321	t1 - t2 ,t1 + 2t2
	1	C222	t1 - t2 ,t1 + 2t2
	1	C112/m	t1 - t2 ,t1 + 2t2
	2	P3	t1 - t2 ,t1 + 2t2
	2	P$\bar{1}$	t1 - t2 ,t1 + 2t2
	2	P2	t1 - t2 ,t1 + 2t2
	4	P1	t1 - t2 ,t1 + 2t2

4.2 Allowed subgroups for the 17 plane space groups

The tables in this section show the additional information on the generators of each subgroup G' allowed in a continuous phase transition Subgroups may have the same space group label yet differ in origin and orientation from each other [3,4]. Apart from the explicit information on how to generate general subgroups for the 17 plane space groups given by *Billiet et al*. [4], such data are excluded from the ITC on the grounds of being too voluminous for the 230 3-D space groups.

Let us consider Table PL7 on page . We have G_o = P2mg :- a rectangular non-symmorphic plane space group with non-primitive translation $r = \{\frac{1}{2},0\}$. The primitive translations of T_o are

$$\vec{t}_1 = (1,0,0) \equiv (1,0) \; ; \; \vec{t}_2 = (0,1,0) \equiv (0,1)$$

The *irreps* Γ_k for Zone boundary points k are listed in APPENDIX II under DG 28 P2ma , its new name in the larger family of Diperiodic groups . There we find the single arm stars

$^*k = \frac{1}{2},0 \; ; \; ^*k = \frac{1}{2},\frac{1}{2}$ each with a single *irrep* R_1

while $^*k = 0,\frac{1}{2}$ has *irreps* R_1 , R_2 , R_3 , R_4 .

For $k = \frac{1}{2},0$ we have 3 subgroups $p1m1$, $p211$, and $p1$ with subduction frequencies 1 , 1 , 2 respectively . However the generators of **p1m1** are given as :-

$$2t_1, \; \{m_x \mid r + 1,0\} \, , t_2 \, , \{m_x \mid r + 0,0\}$$

This implies that there are **2** subgroups G' with the same label **p1m1** viz.

G'	*Subduction Frequency*	*Generators*
$p1m1$	1	$2t_1, t_2, \{m_x \mid r + 1,0\}$
$p1m1$	1	$2t_1, t_2, \{m_x \mid r + 0,0\}$

as the non-primitive translations given in the form $\vec{t_o} + \vec{r}$ of Eq. (3.1.11) are different in each case. It is convenient to give $\vec{t_o} + \vec{r}$ rather than the various origins O' in the parent unit cell of P2mg because of the multiplicity in shift vectors $\vec{s}$ that yield the same information. To obtain an $\vec{s}$ we substitute (Eq. 3.1.11) R = m_x ,$\vec{t_o}$ = 1(*say*),
$\vec{r} = (\frac{1}{2},0)$, $\vec{r}'' = (\frac{1'}{2},0') \equiv \frac{1}{2}(2t_1,0) = t_1$ and *solve* for $\vec{s}$.

TABLE PL 1

1 Go = P1

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0			
R1	1	P1	2t1 , t2
* k = 0 , 1/2			
R1	1	P1	t1 , 2t2
* k = 1/2 , 1/2			
R1	1	P1	t1 - t2,t1 + t2

TABLE PJ, 2

#2 Go = P211

irrep	Subduction Frequency	SubgroupG′	Generators
* k = 1 / 2 , 0			
R1	1	P211	2t1,t2 , {C2z|0,0}
R2	1	P211	2t1,t2 , {C2z|1,0}
* k = 0 , 1 / 2			
R1	1	P211	t1,2t2 , {C2z|0,0}
R2	1	P211	t1,2t2 , {C2z|0,1}
* k = 1 / 2 , 1 / 2			
R1	1	P211	t1-t2,t1+t2 , {C2z|0,0}
R2	1	P211	t1-t2,t1+t2 , {C2z|0,1}

TABLE PL 3

#3 Go = P1m1

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0			
R1	1	P1m1	2t1,t2 , {mx|0,0}
R2	1	P1m1	2t1,t2 , {mx|1,0}
* k = 0 , 1/2			
R1	1	P1m1	t1,2t2 , {mx|0,0}
R2	1	P1g1	t1,2t2 , {mx|0,1}
* k = 1/2 , 1/2			
R1	1	C1m1	t1-t2,t1+t2 , {mx|0,0}
R2	1	C1m1	t1-t2,t1+t2 , {mx|1,0}

TABLE PL 4

5 Go = C1m1

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	C1m1	2 t1, 2t2 , {mx|0,0}
	1	C1m1	2 t1, 2t2 , {mx|1,0}
	1	P1	t1, 2t2 , {E|0,0}
	1	P1	2 t1, t2 , {E|0,0}
	2	P1	2 t1, 2t2 , {E|0,0}
* k = 1/2 , 1/2			
R1	1	P1m1	t1-t2,t1+t2 , {mx|0,0}
R2	1	P1g1	t1-t2,t1+t2 , {mx|1/2,1/2}

TABLE PL 5

4 Go = P1g1 ; r = (0 , 1/2)

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0			
R1	1	P1g1	2t1,t2;{mx|r+0,0}
R2	1	P1g1	2t1,t2,{mx|r+0,0}
* k = 0 , 1/2			
R1	1	P1	t1,2t2;{E|0,0}
R2	1	P1	t1,2t2;{E|0,0}
* k = 1/2 , 1/2			
R1	1	P1	t1-t2;t1+t2{E|0,0}
R2	1	P1	t1-t2;t1+t2{E|0,0}

TABLE PL 6

#6 Go = P2mm

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0			
R1	1	P2mm	2t1,t2 , {mx|0,0},{my|0,0}
R2	1	P2mg	2t1,t2 , {mx|1,0},{my|1,0}
R3	1	P2mg	2t1,t2 , {mx|0,0},{my|1,0}
R4	1	P2mm	2t1,t2 , {mx|1,0},{my|0,0}
* k = 0 , 1/2			
R1	1	P2mm	t1,2t2 , {mx|0,0},{my|0,0}
R2	1	P2mg	t1,2t2 , {mx|0,1},{my|0,1}
R3	1	P2mm	t1,2t2 , {mx|0,0},{my|0,1}
R4	1	P2mg	t1,2t2 , {mx|0,1},{my|0,0}
* k = 1/2 , 1/2			
R1	1	C2mm	t1-t2,t1+t2 , {mx|0,0},{my|0,0}
R2	1	C2mm	t1-t2,t1+t2 , {mx|1,0},{my|1,0}
R3	1	C2mm	t1-t2,t1+t2 , {mx|0,0},{my|1,0}
R4	1	C2mm	t1-t2,t1+t2 , {mx|1,0},{my|0,0}

TABLE PL 7

#7 Go = P2mg ; r = (1/2 ,0)

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0			
R1	1	P1m1	2t1,{mx|r+1,0} t2,{mx|r+0,0}
	1	P211	2t1,{C2z|1,0} t2,{C2z|0,0}
	2	P1	2t1,t2,{E|0,0}
* k = 0 , 1/2			
R1	1	P2mg	2t2,{C2z|0,0} t1,{mx|0,0+r}
R2	1	P2gg	2t2,{C2z|0,0} t1,{mx|0,1+r}
R3	1	P2mg	t1,2t2,{C2z|0,1} {mx|0,0+r}
R4	1	P2gg	t1,2t2,{C2z|0,1} {mx|0,0+r}
* k = 1/2 , 1/2			
R1	1	C1m1	t1-t2,{mx|0,0+r} t1+t2,{mx|1,0+r}
	1	P211	t1-t2,{C2z|0,0} t1+t2,{C2z|1,0}
	2	P1	t1-t2,t1+t2,{E|0,0}

TABLE PL 8

8 Go = P2gg

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0			
R1	1	P1g1	2t1,t2{mx|0,0+r} {mx|1,0+r}
	1	P211	2t1,t2{C2z|0,0} {C2z|1,0}
	2	P1	2t1,t2{E|0,0}
* k = 0 , 1/2			
R1	1	P11g	t1,2t2{my|0,0+r} {my|0,1+r}
	1	P211	t1,2t2{C2z|0,0} {C2z|0,1}
	2	P1	t1,2t2{E|0,0}
* k = 1/2 , 1/2			
R1	2	P211	t1-t2,t1+t2 {C2z|1,0}
R2	2	P211	t1-t2,t1+t2 {C2z|0,0}

TABLE PL 9

9 Go = C2mm

t1 = -1/2 , 1/2
t2 = 1/2 , 1/2

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	C2mm	2t1,2t2 {mx|1,1},{my|1,1} {mx|0,0},{my|0,0}
	1	P211	2t1,t2,{C2z|0,0} t1,2t2,{C2z|0,0}
	2	P211	2t1,2t2,{C2z|0,0}
R2	1	C2mm	2t1,2t2 {mx|1,1},{my|0,0} {mx|0,0},{my|1,1}
	1	P211	2t1,t2,{C2z|1,0} t1,2t2,{C2z|0,1}
	2	P211	2t1,2t2,{C2z|1,1}
* k = 1/2 , 1/2			
R1	1	P2mm	t1-t2,{my|00} t1+t2,{mx|00}
R2	1	P2gg	t1-t2,{my|10} t1+t2,{mx|10},
R3	1	P2mg	t1-t2,{my|10} t1+t2,{mx|00}
R4	1	P2mg	t1-t2,{mx|10} t1+t2,{my|00}

TABLE PL 10

10 Go = P411

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P411	2t1,2t2,{C4Z+I0,0} {C4Z+I1,1}
	1	P211	2t1,t2,{C2ZI0,0}
			t1,2t2,{C2ZI0,0}
	2	P211	2t1,2t2,{C2ZI0,0}
R2	1	P411	2t1,2t2,{C4Z+I1,0} {C4Z+I0,1}
	1	P211	2t1,t2,{C2ZI1,0}
			t1,2t2,{C2ZI0,1}
	2	P211	2t1,2t2,{C2ZI1,1}
* k = 1/2 , 1/2			
R1	1	P411	t1-t2,t1+t2 {C4z+I00}
R2	1	P411	t1-t2,t1+t2 {C4z+I10}
R3	2	P211	t1-t2,t1+t2 {C2zI10}

TABLE PL 11

11 Go = P4mm

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P4mm	2t1,{C2z|0,0} 2t2,{my|0,0} {mdb|0,0}
	1	P4mm	2t1,{C2z|0,0} 2t2,{my|0,0} {mdb|1,1}
	1	P2mm	2t1,{my|0,0} t2,{mx|0,0}
	1	P2mm	t1,{mx|0,0} 2t2,{my|0,0}
	2	P2mm	2t1,{mx|0,0} 2t2,{my|0,0}
R2	1	P4gm	2t1,{C2z|0,0} 2t2,{my|1,1} {mdb|0,0}
	1	P4gm	2t1,{C2z|0,0} 2t2,{my|1,1} {mdb|1,1}
	1	P2mg	2t1,{mx|1,0} t2,{my|1,0}
	1	P2mg	t1,2t2{mx|0,1} 2t2,{my|0,1}
	2	P2gg	2t1,2t2{mx|1,1} 2t2,{my|1,1}
R3	1	P4gm	2t1,{C2z|1,1} 2t2,{my|1,0} {mdb|1,1}
	1	P4gm	2t1,{C2z|1,1} 2t2,{my|1,0} {mdb|0,0}
	1	P2mg	2t1,{my|1,0} t2,{mx|0,0}
	1	P2mg	t1{my|0,0} 2t2,{mx|0,1}
	2	P2gg	2t1,{mx|0,1} 2t2,{my|1,0}

R4	1	P4mm	2t1,{C2z|1,1} 2t2,{my|0,1} {mdb|0,0}
	1	P4mm	2t1,{C2z|1,1} 2t2,{my|0,1} {mdb|1,1}
	1	P2mm	2t1,{mx|1,0} t2,{my|0,0}
	1	P2mm	2t2,{mx|0,0} 1t1,{my|0,1}
	2	P2mm	2t1,{mx|1,0} 2t2,{my|0,1}

* k = 1/2 , 1/2

R1	1	P4mm	t1-t2,t1+t2 {C2z|0,0},{my|0,0} {mdb|0,0}
R2	1	P4gm	t1-t2,t1+t2 {C2z|0,0},{my|1,0} {mdb|1,0}
R3	1	P4gm	t1-t2,t1+t2 {C2z|0,0},{my|0,0} {mdb|1,0}
R4	1	P4mm	t1-t2,t1+t2 {C2z|0,0},{my|1,0} {mdb|0,0}
R5	1	C2mm	t1-t2,t1+t2 {mx|1,0},{my|0,0}
	1	C2mm	t1-t2,t1+t2 {mx|0,0},{my|1,0}
	1	P2mg	t1-t2,t1+t2 {da|0,0},{db|1,0}
	1	P2mg	t1-t2,t1+t2 {da|1,0},{db|0,0}
	1	P211	t1-t2,t1+t2 {C2z|1,0}

TABLE PL 12

\# 12 Go = P4gm ; r = (1/2 ,1/2)

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0 ; 0 , 1/2			
R1	1	P411	2t1,2t2 {C4zl0,0)
	1	P411	2t1,2t2 {C4zl1,0)
	1	P411	2t1,2t2 {C4zl0,1)
	1	P411	2t1,2t2 {C4zl1,1)
	1	C2mm	2t1,2t2 {dalr + 0,0) {dblr + 0,1)
	1	C2mm	2t1,2t2 {dalr + 1,1) {dblr + 0,1)
	1	C2mm	2t1,2t2 {dalr + 0,0) {dblr + 1,0)
	1	C2mm	2t1,2t2 {dalr + 1,1) {dblr + 1,0)
	2	C1m1	2t1,2t2 {dalr + 0,0)
	2	C1m1	2t1,2t2 {dalr + 1,1)
	2	C11m	2t1,2t2 {dblr + 1,0)
	1	C11m	2t1,2t2 {dblr + 0,1)
	1	P1g1	2t1, t2 {mxlr + 0,0)
	1	P1g1	2t1, t2 {mxlr + 1,0)
	1	P11g	t1,2t2 {mylr + 0,0)
	1	P11g	t1,2t2 {mylr + 0,1)
	1	P211	t1,2t2 {C2zl0,0)
	1	P211	t1,2t2 {C2zl0,1)
	1	P211	2t1, t2 {C2zl0,0)
	1	P211	2t1, t2 {C2zl1,0)

<table>
<tr><td></td><td>2</td><td>P211</td><td>2t1,2t2
{C2z|0,0)</td></tr>
<tr><td></td><td>2</td><td>P211</td><td>2t1,2t2
{C2z|1,0)</td></tr>
<tr><td></td><td>2</td><td>P211</td><td>2t1,2t2
{C2z|0,1)</td></tr>
<tr><td></td><td>2</td><td>P211</td><td>2t1,2t2
{C2z|1,1)</td></tr>
<tr><td></td><td>2</td><td>P1</td><td>2t1, t2</td></tr>
<tr><td></td><td>2</td><td>P1</td><td>t1,2t2</td></tr>
<tr><td></td><td>4</td><td>P1</td><td>2t1,2t2</td></tr>
</table>

* k = 1/2 , 1/2

<table>
<tr><td>R1</td><td>1</td><td>P411</td><td>t1-t2,t1+t2
{C4z|0,0}</td></tr>
<tr><td></td><td>1</td><td>P411</td><td>t1-t2,t1+t2
{C4z|1,0}</td></tr>
<tr><td></td><td>1</td><td>P2mg</td><td>t1-t2,t1+t2
{da|r+ 0,0}
{db|r+ 0,0}</td></tr>
<tr><td></td><td>1</td><td>P2mg</td><td>t1-t2,t1+t2
{da|r+ 1,0}
{db|r+ 1,0}</td></tr>
<tr><td></td><td>2</td><td>P211</td><td>t1-t2,t1+t2
{C2z|0,0}</td></tr>
<tr><td>R2</td><td>1</td><td>P2mm</td><td>t1-t2,t1+t2
{da|r + 0,0}
{db|r + 1,0}</td></tr>
<tr><td>R3</td><td>1</td><td>P2gg</td><td>t1-t2,t1+t2
{da|r + 1,0}
{db|r + 0,0}</td></tr>
</table>

TABLE PE 13

13 Go = P311

irrep	Subduction Frequency	Subgroup G′	Generators
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 ,1/2			
R1	1	P311	2t1,2t2 {C3+I0,0)
	1	P311	2t1,2t2 {C3+I1,0)
	1	P311	2t1,2t2 {C3+I0,1)
	1	P311	2t1,2t2 {C3+I1,1)
	2	P1	2t1, t2
	2	P1	t1,2t2
	3	P1	2t1,2t2
* k = -1/3 , 2/3			
R1	1	P311	t1-t2,t1+2t2 {C3+I0,0}
R2	1	P311	t1-t2,t1+2t2 {C3+I1,0}
	1	P311	t1-t2,t1+2t2 {C3+I1,1}
	2	P1	t1-t2,t1+2t2

TABLE PL 14

14 Go = P3m1

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 ,1/2			
R1	1	P3m1	2t1,2t2 {C3+|0,0) {v2 |0,0)
	1	P3m1	2t1,2t2 {C3+|1,0) {v2 |0,0)
	1	P3m1	2t1,2t2 {C3+|0,1) {v2 |0,1)
	1	P3m1	2t1,2t2 {C3+|1,1) {v2 |0,1)
	1	Pm	t1-t2,t1+t2 {v3|0,0)
	1	Pm	2t1+t2,t2 {v2|0,0)
	1	Pm	t1,t1+2t2 {v1|0,0)
	2	Cm	2t1,2t2 {v3|0,0)
	2	Cm	2t1,2t2 {v3|1,1)
	3	P1	2t1,2t2
R2	1	P311	2t1,2t2 {C3+|0,0)
	1	P311	2t1,2t2 {C3+|1,0)
	1	P311	2t1,2t2 {C3+|0,1)
	1	P311	2t1,2t2 {C3+|1,1)
	1	Pg	t1-t2,t1+t2 {v3|1,0)
	1	Pg	2t1+t2,t2 {v2|1,0)
	1	Pg	t1,t1+2t2 {v1|0,1)
	1	Cm	2t1,2t2 {v3|0,0)
	1	Cm	2t1,2t2 {v3|1,1)
	3	P1	2t1,2t2

* k = -1/3 , 2/3 ; -1/3 , 1/3

<table>
<tr><td>R1</td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|0,0}
{v1 |0,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|0,0}
{v1 |1,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|0,0}
{v1 |1,1}</td></tr>
<tr><td></td><td>2</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|0,0}</td></tr>
<tr><td>R2</td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,0}
{v1 |0,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,0}
{v1 |1,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,0}
{v1 |1,1}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,1}
{v1 |0,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,1}
{v1 |1,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,1}
{v1 |1,1}</td></tr>
<tr><td></td><td>2</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|1,0}</td></tr>
<tr><td></td><td>2</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|1,1}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>2t1+t2,-t1+t2
{v1 |0,0}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>2t1+t2,-t1+t2
{v1 |1,0}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>2t1+t2,-t1+t2
{v1 |1,1}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>2t1+t2,-t1+t2
{v2 |0,0}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>2t1+t2,-t1+t2
{v2 |1,0}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>2t1+t2,-t1+t2
{v2 |1,1}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>3t1,3t2
{v3 |0,0}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>3t1,3t2
{v3 |1,1}</td></tr>
<tr><td></td><td>2</td><td>Cm</td><td>3t1,3t2
{v3 |2,2}</td></tr>
<tr><td></td><td>4</td><td>P1</td><td>2t1 + t2
-t1 + t2</td></tr>
</table>

TABLE PL 15

15 Go = P31m

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 ,1/2			
R1	1	P31m	2t1,2t2 {C3+|0,0) {d2 |0,0)
	1	P31m	2t1,2t2 {C3+|1,0) {d2 |0,0)
	1	P31m	2t1,2t2 {C3+|0,1) {d2 |0,1)
	1	P31m	2t1,2t2 {C3+|1,1) {d2 |0,1)
	1	Pm	t1-t2,t1+t2 {d3|0,0)
	1	Pm	2t1+t2,t2 {d2|0,0)
	1	Pm	t1,t1+2t2 {d1|0,0)
	2	Cm	2t1,2t2 {d3|0,0)
	2	Cm	2t1,2t2 {d3|1,1)
	3	P1	2t1,2t2
R2	1	P311	2t1,2t2 {C3+|0,0)
	1	P311	2t1,2t2 {C3+|1,0)
	1	P311	2t1,2t2 {C3+|0,1)
	1	P311	2t1,2t2 {C3+|1,1)
	1	Pg	t1-t2,t1+t2 {d3|0,1)
	1	Pg	2t1+t2,t2 {d2|1,0)
	1	Pg	t1,t1+2t2 {d1|0,1)
	1	Cm	2t1,2t2 {d3|0,0)
	1	Cm	2t1,2t2 {d3|1,1)
	3	P1	2t1,2t2

* k = -1/3 , 2/3

<table>
<tr><td>R1</td><td>1</td><td>P3m1</td><td>t1-t2,t1+2t2
{C3+|0,0}
{d2+|0,0}</td></tr>
<tr><td>R2</td><td>1</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|0,0}</td></tr>
<tr><td>R3</td><td>1</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|1,0}</td></tr>
<tr><td></td><td>1</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|1,1}</td></tr>
<tr><td></td><td>1</td><td>Cm</td><td>2t1+t2,-t1+t2
{d1+|0,0}</td></tr>
<tr><td></td><td>1</td><td>Cm</td><td>t1+2t2,-t1+t2
{d2+|0,0}</td></tr>
<tr><td></td><td>1</td><td>Cm</td><td>3t1,3t2
{d3+|0,0}</td></tr>
<tr><td></td><td>2</td><td>P1</td><td>2t1+t2,-t1+t2</td></tr>
</table>

TABLE PL 16

16 Go = P611

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 ,1/2			
R1	1	P611	2t1,2t2 {C6+I0,0)
	1	P611	2t1,2t2 {C6+I1,0)
	1	P611	2t1,2t2 {C6+I0,1)
	1	P611	2t1,2t2 {C6+I1,1)
	1	P2	t1,2t1 {C2zI0,0)
	1	P2	2t1,t2 {C2zI0,0)
	3	P2	2t1,2t2 {C2zI0,0)
R2	1	P311	2t1,2t2 {C3+I0,0)
	1	P311	2t1,2t2 {C3+I1,0)
	1	P311	2t1,2t2 {C3+I0,1)
	1	P311	2t1,2t2 {C3+I1,1)
	1	P2	t1,2t1 {C2zI0,1)
	1	P2	2t1,t2 {C2zI1,0)
	2	P2	2t1,2t2 {C2zI0,1)
	2	P2	2t1,2t2 {C2zI1,0)
	2	P2	2t1,2t2 {C2zI1,1)
	3	P1	2t1,2t2
* k = -1/3 , 2/3 ; -1/3 , 1/3			
R1	1	P611	t1-t2,t1+2t2 {C6+I0,0}
	1	P31m	t1-t2,t1+2t2 {C3+I0,0} {v1 I1,0}
	2	P311	t1-t2,t1+2t2 {C3+I0,0}

	2	P311	t1-t2,t1+2t2 {C3+I0,0}
R2	2	P311	t1-t2,t1+2t2 {C3+I1,0}
	2	P311	t1-t2,t1+2t2 {C3+I1,1}
	2	P2	2t1+t2,-t1+t2 {C2zI0,0}
	2	P2	2t1+t2,-t1+t2 {C2zI1,0}
	2	P2	2t1+t2,-t1+t2 {C2zI1,1}
	4	P1	2t1+t2,-t1+t2

TABLE PL 17

17   Go = P6mm

irrep	Subduction Frequency	Subgroup G'	Generators
* k = 1/2 , 0 ; 0 , -1/2 ; -1/2 ,1/2			
R1	1	P6mm	2t1,2t2 {C6+|0,0) {d2 |0,0)
	1	P6mm	2t1,2t2 {C6+|1,0) {d2 |1,0)
	1	P6mm	2t1,2t2 {C6+|0,1) {d2 |0,1)
	1	P6mm	2t1,2t2 {C6+|1,1) {d2 |0,0)
	1	P2mm	t1-t2,t1+t2 {d3|0,0) {v3|0,0)
	1	P2mm	2t1+t2,t2 {d2|0,0) {v2|0,0)
	1	P2mm	t1,t1+2t2 {d1|0,0) {v1|0,0)
	2	C2mm	2t1,2t2 {d3|0,0) {v3|0,0)
	2	C2mm	2t1,2t2 {d3|1,1) {v3|1,1)
	3	P2	2t1,2t2 {C2z|0,0}
R2	1	P611	2t1,2t2 {C6+|0,0)
	1	P6mm	2t1,2t2 {C6+|1,0)
	1	P6mm	2t1,2t2 {C6+|0,1)
	1	P6mm	2t1,2t2 {C6+|1,1)
	1	P2gg	t1-t2,t1+t2 {d3|1,0) {C2z|0,0)
	1	P2gg	2t1+t2,t2 {d2|1,0) {C2z|0,0)

	1	P2gg	t1,t1+2t2 {d1|0,1) {C2z|0,0)
	2	C2mm	2t1,2t2 {d3|0,0) {C2z|0,0)
	2	C2mm	2t1,2t2 {d3|1,1) {C2z|1,1)
	3	P2	2t1,2t2 {C2z|0,0}
R3	1	P31m	2t1,2t2 {C3+|0,0) {d2|0,0)
	1	P31m	2t1,2t2 {C3+|1,0) {d2|0,0)
	1	P31m	2t1,2t2 {C3+|0,1) {d2|0,1)
	1	P31m	2t1,2t2 {C3+|1,1) {d2|0,1)
	1	P2mg	t1-t2,t1+t2 {d3|1,0) {C2z|1,0)
	1	P2mg	2t1+t2,t2 {d2|1,0) {C2z|1,0)
	1	P2mg	t1,t1+2t2 {d1|0,1) {C2z|0,1)
	1	C2mm	2t1,2t2 {d3|0,0) {C2z|1,1)
	1	C2mm	2t1,2t2 {d3|1,1) {C2z|1,1)
	2	Cm	2t1,2t2 {d3|0,0}
	2	Cm	2t1,2t2 {d3|1,1}
	2	P2	2t1,2t2 {C2z|0,1}
	2	P2	2t1,2t2 {C2z|1,0}
	2	P2	2t1,2t2 {C2z|1,1}
	3	P1	2t1,2t2
R4	1	P3m1	2t1,2t2 {C3+|0,0) {v2|0,0)

	1	P3m1	2t1,2t2 {C3+|1,0} {v2 |0,0}
	1	P3m1	2t1,2t2 {C3+|0,1} {v2 |0,1}
	1	P3m1	2t1,2t2 {C3+|1,1} {v2 |0,1}
	1	P2mg	t1-t2,t1+t2 {v3|1,0} {C2z|1,0}
	1	P2mg	2t1+t2,t2 {v2|1,0} {C2z|1,0}
	1	P2mg	t1,t1+2t2 {v1|0,1} {C2z|0,1}
	1	C2mm	2t1,2t2 {v3|0,0} {C2z|1,1}
	1	C2mm	2t1,2t2 {v3|1,1} {C2z|1,1}
	2	Cm	2t1,2t2 {v3|0,0}
	2	Cm	2t1,2t2 {v3|1,1}
	2	P2	2t1,2t2 {C2z|0,1}
	2	P2	2t1,2t2 {C2z|1,0}
	2	P2	2t1,2t2 {C2z|1,1}
	3	P1	2t1,2t2

* k = -1/3 , 2/3 ; -1/3 , 1/3

R1	1	P6mm	t1-t2,t1+2t2 {C6+|0,0} {d2 |0,0}
	1	P6mm	t1-t2,t1+2t2 {C6+|1,1} {d2 |0,0}
	1	P6mm	t1-t2,t1+2t2 {C6+|1,0} {d2 |0,0}
	1	P3m1	t1-t2,t1+2t2 {C3+|0,0} {d2 |0,0}
R2	1	P31m	t1-t2,t1+2t2 {C3+|0,0} {v2 |0,0}

<table>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|0,0}
{v2 |1,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|0,0}
{v2 |1,1}</td></tr>
<tr><td></td><td>1</td><td>P611</td><td>t1-t2,t1+2t2
{C6+|1,0}</td></tr>
<tr><td></td><td>1</td><td>P611</td><td>t1-t2,t1+2t2
{C6+|1,1}</td></tr>
<tr><td></td><td>2</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|0,0}</td></tr>
<tr><td>R3</td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,0}
{v2 |0,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,0}
{v2 |0,1}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,0}
{v2 |1,1}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,1}
{v2 |0,0}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,1}
{v2 |0,1}</td></tr>
<tr><td></td><td>1</td><td>P31m</td><td>t1-t2,t1+2t2
{C3+|1,1}
{v2 |1,1}</td></tr>
<tr><td></td><td>2</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|1,0}</td></tr>
<tr><td></td><td>2</td><td>P311</td><td>t1-t2,t1+2t2
{C3+|1,1}</td></tr>
<tr><td></td><td>2</td><td>C2mm</td><td>2t1+t2,-t1+t2
{d1 |0,0}
{v1 |0,0}</td></tr>
<tr><td></td><td>2</td><td>C2mm</td><td>2t1+t2,-t1+t2
{d1 |0,0}
{v1 |1,0}</td></tr>
<tr><td></td><td>2</td><td>C2mm</td><td>2t1+t2,-t1+t2
{d1 |0,0}
{v1 |1,1}</td></tr>
<tr><td></td><td>2</td><td>C2mm</td><td>t1-t2,t1+2t2
{d1 |0,0}
{v1 |0,0}</td></tr>
<tr><td></td><td>2</td><td>C2mm</td><td>t1-t2,t1+2t2
{d1 |0,0}
{v1 |1,0}</td></tr>
<tr><td></td><td>2</td><td>C2mm</td><td>t1-t2,t1+2t2
{d1 |0,0}
{v1 |1,1}</td></tr>
<tr><td></td><td>2</td><td>C2mm</td><td>3t1,3t2</td></tr>
</table>

		{d3 |0,0}
		{v3 |0,0}
2	C2mm	3t1,3t2
		{d3 |2,1}
		{v3 |1,1}
2	C2mm	3t1,3t2
		{d3 |1,2}
		{v3 |2,2}
2	Cm	2t1+t2,-t1+t2
		{d2 |0,0}
2	Cm	2t1+t2,-t1+t2
		{v2 |0,0}
2	Cm	2t1+t2,-t1+t2
		{v2 |1,0}
2	Cm	2t1+t2,-t1+t2
		{v2 |1,1}
2	Cm	2t1+t2,-t1+t2
		{d1 |0,0}
2	Cm	2t1+t2,-t1+t2
		{v1 |0,0}
2	Cm	2t1+t2,-t1+t2
		{v1 |1,0}
2	Cm	2t1+t2,-t1+t2
		{v1 |1,1}
2	Cm	3t1,3t2
		{d3 |0,0}
2	Cm	3t1,3t2
		{d3 |1,1}
2	Cm	3t1,3t2
		{d3 |2,2}
2	Cm	3t1,3t2
		{v3 |0,0}
2	Cm	3t1,3t2
		{v3 |1,1}
2	Cm	3t1,3t2
		{v3 |2,2}
2	P2	t1-t2,t1+2t2
		{C2z|0,0}
2	P2	t1-t2,t1+2t2
		{C2z|1,0}
2	P2	t1-t2,t1+2t2
		{C2z|1,1}
4	P1	2t1+t2,-t1+t2

CONCLUSION

The past few years have witnessed a marked resurgence of interest in surface phenomena [48,49,50] . Studies range from fields (catalysis , oxidation and corrosiom) *outside* traditional solid state physics to present day micro-electronics and the physics of thin films or of monolayers adsorbed on thin films .

Much of our understanding however, had been empirical because of the difficulty in obtaining atomically pure surfaces . With improvements in vacuum technology and in surface probes via LEED [9,51] , photo-electron spectroscopy [52] and synchrotron radiation - observations can be made on surface features different from that of an atomic plane in a bulk crystal , we can study the various types of long-range order which are possible in 2D and test some of the recent theoretical work in statistical mechanics , with the discovery of 2D critical phenomena in chemisorbed systems [53] .

An important step in a program leading to an understanding of surface physics comparable to that of bulk matter is the knowledge and application of the relevant space groups . Just as the 230 space groups were essential in elucidating bulk properties , the planar groups are appropriate for surface analysis . Because of the asymmetry in force fields that an atom on a *smooth* interface experiences , one could argue that the ordinary 17 2-D space groups should suffice . However *Zallen et el.* [14] have shown that the 80 diperiodic groups in 3-D *Wood* [5] are essential in the interpretation of the observed spectra in layer crystals having the orpiment structure (As_2S_3, As_2Se_3) .

Their experiments demonstarted the dominance of layer symmetry over bulk symmetry . Since an experimental probe samples a layer of finite thickness (*the selvedge* [5]), the existence of an aperiodic 3^{rd} dimension allows us to include glide planes an 2-fold screw axes parallel to and in the diperiodic layer . Low dimensional (1-D and 2-D) systems have proven to be rich as in physical phenomena as the familiar world of 3-D . The electron diffractogram has shown conclusively the existence of Fermi-driven distortions in 2-D (charge-density waves) [54] . In the the 1970's it was shown how 1-D diffuse x-ray scattering must accompany a Peierls distortion , thus establishing a mechanism for the metal-insulator transition which had been surmised earlier for the 1-D crystal system T.T.F.-T.C.N.Q [55]. Additional interest in 2-D systems comes from the field of high energy physics . It appears that by understanding the mechanism and conditions under which phase transition occur in 2-D , we can gain insight into the problem of quark - confinement by drawing analogies between the theories of phase transitions in 2-D and Quantum Field theory in 4 - D space-time [13] .

Applications

Several experiments have shown that surface reconstruction is reversible with temperature [56,57] . The experimental evidence of a 2^{nd} order phase transition on a Tungsten (100) surface was reported by *Debe & King* [38] and analysed by us [1] . Atoms adsorbed on a crystal surface can also adopt different arrangements [58] . However it is only recently that transitions between the polymorphic states have been studied in any experimental detail or a theoretical classification made :- adsorption of Xenon on $NiCl_2$ [59];

adsorption of Helium on exfoliated graphite (Graphoil) [60] .

Graphite Intercalation Compounds {*GIC's* } form a natural testing ground for 2-D phenomenaa because of the large variety of available interlayer couplings [10] . With dimensionality playing a key role in the critical properties of structural and magnetic phase transitions , one may question the extent to which a real material approximates a 2-D system . The stage index of a GIC is the number of carbon layers that separate some intercalant species . The relatively weak interlayer coupling in high stage (> 2) compounds such as $C_x FeCl_3$, CsC_8 imply that the Diperiodic groups would be the relevant groups to consider in studying intralayer phase transitions .

While there are widescale reports of phase transitions in *GIC's* :- Commensurate - Incommensurate transitions in $SbCl_5$ -intercalated graphite (stage 2 - stage 6) [61] , Order - Disorder phase transitions in Graphite - Potassium Compounds [62] ,there are no reports so far of commensurate - commensurate phase transitions which would fall within the purvey of our Group Thoery Criteria . Since research interest in *GIC's* are at an all-time high and with work ranging from basic physics and chemistry to engineering applications [63,64] it is appropriate that powerful Group Theoretical Methods based partly on the diperiodic groups be applied to clarify the wealth of experimental data being accumulated .

Phase transitions in magnetic sysyems and in adsorbed surface layers have been studied in terms of both phenomenological theories (e.g. Landau theory of phase transitions) and the statistical mechanics of simple models

(Ising -like)[6] . Apart from the asymmetry of a surface layer , the microscopic interactions close to the surface may have values which are quite different from those in the interior of a crystal . As a consequence a surface may undergo a phase transition before the the bulk or may display an ordering different from the bulk e.g. an antiferromagnetic ordering on a ferromagnetic sample . Very recently experiments on *literally* 2-D magnetic lipid layers created by the Langmuir - Blodgett technique have been performed [11] . Evidence of order in these 2-D systems would be a challenge to our understanding of phase transitions [65,66] . Magnetic 2-D groups may be related to the 80 Diperiodic groups if the *Color-changing* operator (black - white) is substituted for the inversion operator . Problems arise however as the former are antiunitary while the latter is unitary ; this will influence our use of co-representations or ordinary representations in the Landau theory . This connection will be explored in future work .

Liquid crystals are another form of 2-D matter under study [67] . Liquid crystals (Smectic-A phase) have a layered structure in which the molecules are fluid-like within the layer and orient with their long axes normal to the layer . Free-standing films of liquid crystals a few molecules thick are being studied with the aim of studying the nature of the ordering in these films . However liquid crystals composed of disc-like molecules display a rich polymorphism - in the HAT series temperature induced phase transitions have been detected [68] . The parent phase is Hexagonal (G_o = P6/mmm) for this layered family [69] . Based on our tables (DG 1- DG 80) , if we are given that a phase transition is 2^{nd} order we can predict the symmetry of the low-temperature phase(s) or assign possible irreps (order parameters) if an identification of G' has been reported .

Recently a sequence of phase transitions in the layer compound $RbVF_4$ has been reported [70] . We studied before [71] the symmetry aspect of a transition step in this sequence using the Selection Rules (A - C6) via hand - computation . Our computer results are consistent with the conclusion there on the nature of the stage I ($D_{4h}^{1} - P4/\ mmm$) to stage II ($D_{4h}^{6} - P4/\ mbm$) transition as being probably 2^{nd} order . In our notation the *irreps* R_2 , and , R_3 are associated with this transitionand provide labels for the hypothesized [70] soft - phonon mechanism that may drive the transition .

APPENDIX I

Computer Program for G_o = Plgl

```
##      PROGRAM FOR CALCULATING THE SUBDUCTION FREQUENCIES FOR
                        SUBGROUPS OF  Go = P1g1

# rectangular / oblique systems
integer subfs1(12,10),ns111(12,10),ns112(12,10),ns121(12,10),ns122(12,10)
integer subfs2(12,10),ns211(12,10),ns212(12,10),ns221(12,10),ns222(12,10)
integer subfs3(12,10),ns311(12,10),ns312(12,10),ns321(12,10),ns322(12,10)
integer subfs4(12,10),ns411(12,10),ns412(12,10),ns421(12,10),ns422(12,10)
integer ang1(12,10),ang2(12,10),ang3(12,10),ang4(12,10)
integer ldet1(12,10),ldet2(12,10),ldet3(12,10),ldet4(12,10)
real xrs1(12,10),yrs1(12,10)
real xrs2(12,10),yrs2(12,10)
real xrs3(12,10),yrs3(12,10)
real xrs4(12,10),yrs4(12,10)
real xrr(12,10,8),yrr(12,10,8)
integer p,q
integer elem(12),char1(12),char2(12),char3(12)
real xro,yro,vectx(8),vecty(8)
integer ord,ordd,detm,detm1,detm12,detm13,detm14
integer chec,chec1a,chec1b,chec2a,chec2b,chec3,chec4
real xar(10,8),yar(10,8),alx(8),aly(8),alpx(8),alpy(8),xall(7),yall(14)
real xr11(10),xr22(10),xr33(10),xr44(10)
real yr11(10),yr22(10),yr33(10),yr44(10)
integer input(4),output(4),nusg(30),list(8)
integer subf1(10),subf2(10),subf3(10),subf4(10)
integer nc111(10),nc112(10),nc121(10),nc122(10)
integer nc211(10),nc212(10),nc221(10),nc222(10)
integer nc311(10),nc312(10),nc321(10),nc322(10)
integer nc411(10),nc412(10),nc421(10),nc422(10)
dimension inv(8)
complex t1,t2,t1p,t2p,t1pc
complex add,sadd
real dot
integer angle
complex hp0(8),hp1(8),hp2(8),hp3(8)
complex cfn11,cfn12,cfn21,cfn22
complex phas11,phas12,phas21,phas22,phas31,phas32
complex k0,k1,k2,k3,zero,xo,yo,f,sum
complex el(8)
data xall(1),xall(2),xall(3),xall(4),xall(5),xall(6),xall(7)/0.0000,0.2500,
                         0.3333,0.5000,0.6667,0.7500,1.0000/
data yall(1),yall(2),yall(3),yall(4),yall(5),yall(6),yall(7)/0.0000,0.2500,
                         0.3333,0.5000,0.6667,0.7500,1.0000/
data inv(1),inv(2),inv(3),inv(4),inv(5),inv(6),inv(7),inv(8)/1,2,4,3,5,
```

```
                                        6,7,8/
do jm = 8,14
yall(jm) = -yall(jm - 7)

pi = 3.14159
t2 = cmplx(0.00,1.00)
t1 = cmplx(1.000,0.000)
#international tables
zero = cmplx(0.00,0.00).
do itot = 1,3   # number of stars
$(
call data0(ordd,input,itot,inew,ma,n1,n2,n3)
#inew = 1
do ire = 1,inew    # number of irreps in each star
 $(
do k = 1,8
$(
elem(k) = 0
char1(k) = 0
char2(k) = 0
char3(k) = 0
$)
call data1(itot,ire,elem,alx,aly)
# delta h'k,k test here
if (itot==1| itot==2 | itot==3)
$(
for(n=1;n <=1;n=n+3)
     $(
for(m=1;m <=8;m=m+1)
    $(
    l = inv(n)
call sqtab(l,m,n,k)
if(n==n1)
  char1(m) = elem(k)
    $)
      $)

       $)
call hwri12(input,itot,char1,char2,char3,im,jm)
for(iall = ma;iall >=1 ;iall = iall-1)
$(   # for various subgroups
write(15,900)

js1 = 0
js2 = 0
js3 = 0
js4 = 0
do k1 = 1,10
$(
```

```
do km = 1,12
$(
 subfs1(km,kl) = 0
 ns111(km,kl) = 0
 ns112(km,kl) = 0
 ns121(km,kl) = 0
 ns122(km,kl) = 0
 subfs2(km,kl) = 0
 ns211(km,kl) = 0
 ns212(km,kl) = 0
 ns221(km,kl) = 0
 ns222(km,kl) = 0
 subfs3(km,kl) = 0
 ns311(km,kl) = 0
 ns312(km,kl) = 0
 ns321(km,kl) = 0
 ns322(km,kl) = 0
 subfs4(km,kl) = 0
 ns411(km,kl) = 0
 ns412(km,kl) = 0
 ns421(km,kl) = 0
 ns422(km,kl) = 0
 ang1(km,kl)  = 0
 ldet1(km,kl) = 0
 ang2(km,kl)  = 0
 ldet2(km,kl) = 0
 ang3(km,kl)  = 0
 ldet3(km,kl) = 0
 ang4(km,kl)  = 0
 ldet4(km,kl) = 0
$)
$)
do kl = 1,12
$(
do km = 1,10
$(
do kn = 1,8
$(
 xrr(kl,km,kn) = 0.0000
 yrr(kl,km,kn) = 0.0000
$)
$)
$)
do kl = 1,12
$(
do km = 1,10
$(
 xrs1(kl,km) = 0.0000
 yrs1(kl,km) = 0.0000
```

```
 xrs2(k1,km) = 0.0000
 yrs2(k1,km) = 0.0000
 xrs3(k1,km) = 0.0000
 yrs3(k1,km) = 0.0000
 xrs4(k1,km) = 0.0000
 yrs4(k1,km) = 0.0000
$)
$)
if(iall == 1)
$(
limx = 2
limy = 2
$)
else
$(
limx = 7
limy = 14
$)

    do im = 1,limx
              $(
      do jm = 1,limy
        $(
# to be changed


do l = 1,10
$(
xr11(l) = 0.000
xr22(l) = 0.000
xr33(l) = 0.000
xr44(l) = 0.000
yr11(l) = 0.000
yr22(l) = 0.000
yr33(l) = 0.000
yr44(l) = 0.000
nc111(l) = 0
nc112(l) = 0
nc121(l) = 0
nc122(l) = 0
nc211(l) = 0
nc212(l) = 0
nc221(l) = 0
nc222(l) = 0
nc311(l) = 0
nc312(l) = 0
nc321(l) = 0
nc322(l) = 0
nc411(l) = 0
```

```
nc412(1) = 0
nc421(1) = 0
nc422(1) = 0
subf1(1) = 0
subf2(1) = 0
subf3(1) = 0
subf4(1) = 0
$)
isf1a =0
isf2a =0
isf1b =0
isf2b =0
isf3 =0
isf4 =0


chec = 0
chec1a = 0
chec1b = 0
chec2a = 0
chec2b = 0
chec3 = 0
chec4 = 0
jc1 = 0
jc2 = 0
jc3 = 0
jc4 = 0
detm1 = 16
detm12 = 16
detm13 = 16
detm14 = 16
n11pa =0
n12pa =0
n21pa =0
n22pa =0
n11p2a =0
n12p2a =0
n21p2a =0
n22p2a =0
n11pb =0
n12pb =0
n21pb =0
n22pb =0
n11p2b =0
n12p2b =0
n21p2b =0
n22p2b =0
n11p3 =0
n12p3 =0
```

```
n21p3 =0
n22p3 =0
n11p4 =0
n12p4 =0
n21p4 =0
n22p4 =0
xo = cmplx(0.00,xall(im))
yo = cmplx(0.00,yall(jm))
for(nxx= 2;iabs(nxx) <=2;nxx= nxx-1)
  $(
for(nxy= 2;iabs(nxy) <=2;nxy= nxy-1)
         $(
for(nyx= 2;iabs(nyx) <=2;nyx= nyx-1)
           $(
for(nyy= 2;iabs(nyy) <=2;nyy= nyy-1)
         $(
 #is detm = > *** ?

call m1(nxx,nxy,nyx,nyy,n11,n12,n21,n22,detm)
if ( detm <= 0 )
     next
 #select suitable arms
fn11 = float(n11)
fn12 = float(n12)
fn21 = float(n21)
fn22 = float(n22)
cfn11 = cmplx(0.00,fn11)
cfn12 = cmplx(0.00,fn12)
cfn21 = cmplx(0.00,fn21)
cfn22 = cmplx(0.00,fn22)


# to be changed
if(itot==1)
$(
call arm1(cfn11,cfn12,cfn21,cfn22,phas11,phas12,k1)
if (cabs(k1) ==0.00 )
next
$)
else if(itot==2)
$(
call arm2(cfn11,cfn12,cfn21,cfn22,phas21,phas22,k2)
if (cabs(k2) ==0.00)
next
$)
else if(itot==3)
$(
call arm3(cfn11,cfn12,cfn21,cfn22,phas31,phas32,k3)
if (cabs(k3) ==0.00)
```

```
next
$)


# to be changed
#calculation of subduction frequencies
xr = aimag(xo)
yr = aimag(yo)
xro = 12.0*xr
yro = 12.0*yr
call sg12(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
 #to get alpha'—. alpx,alpy
call tran(vectx,vecty,xro,yro)
je = 0
for(jk1 = 1;jk1 <= max ;jk1 = jk1+1)
#for(jk1 = 1;list(jk1) !=0 ;jk1 = jk1+1)
$(
jd = list(jk1)
xa = abs(alpx(jd)*n11+alpy(jd)*n21 - alx(jd) + vectx(jd)/12.0)
if(xa <= 0.01) xa = 0.00
else if((xa <= 1.01)&(xa >= 0.99)) xa = 1.00
else if((xa <= 2.01)&(xa >= 1.99)) xa = 2.00
else if((xa <= 3.01)&(xa >= 2.99)) xa = 3.00
else if((xa <= 4.01)&(xa >= 3.99)) xa = 4.00
else if((xa <= 5.01)&(xa >= 4.99)) xa = 5.00
else   xa = 2.500
ya = abs(alpx(jd)*n12+alpy(jd)*n22 - aly(jd) + vecty(jd)/12.0)
if(ya <= 0.01) ya = 0.00
else if((ya <= 1.01)&(ya >= 0.99)) ya = 1.00
else if((ya <= 2.01)&(ya >= 1.99)) ya = 2.00
else if((ya <= 3.01)&(ya >= 2.99)) ya = 3.00
else if((ya <= 4.01)&(ya >= 3.99)) ya = 4.00
else if((ya <= 5.01)&(ya >= 4.99)) ya = 5.00
else ya = 2.500
if((xa!=0.00)&(xa!=1.00)&(xa!=2.00)&(xa!=3.00)&(xa!=4.00)&(xa!=5.00))
break
if((ya!=0.00)&(ya!=1.00)&(ya!=2.00)&(ya!=3.00)&(ya!=4.00)&(ya!=5.00))
break
je = je + 1
$)
if(je < max )
next

if (itot==1)
$(
k0 = k1
xk = 0.50
yk = 0.00
call sg12(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
```

```
call phs0(k0,xk,yk,hp0,xo,yo)
do j1 = 1,8
hp1(j1) = hp0(j1)*e1(j1)
$)

else if(itot==2)
$(
k0 = k2
xk = 0.00
yk = 0.50
call sg12(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
call phs0(k0,xk,yk,hp0,xo,yo)
do j2 = 1,8
hp2(j2) = hp0(j2)*e1(j2)
$)


else if(itot==3)
$(
k0 = k3
xk = 0.50
yk = 0.50
call sg12(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
call phs0(k0,xk,yk,hp0,xo,yo)
do j3 = 1,8
hp3(j3) = hp0(j3)*e1(j3)
$)


t1p = n11*t1 + n12*t2
t2P = n21*t1 + n22*t2
t1pc = conjg(t1p)
dot = real(t1pc*t2p)/(cabs(t1p)*cabs(t2p))
angle = (180/3.14159)*acos(dot)
#if((angle<=88|angle>=92)&(nsg==8|nsg==9|nsg==10|nsg==11|nsg==12))
if((angle<=88|angle>=92)&(nsg>=3&nsg<=21))
next

if(ord==8) inc =2
else inc =1

# to be changed
f = zero
sum = zero
# to be changed
for(k=1;k<=8;k=k+1)
$(
if (itot==1)
sum =(float(1)/float(ord))*(hp1(k)*char1(k))
```

```
else if(itot==2)
sum =(float(1)/float(ord))*(hp2(k)*char1(k))
else if(itot==3)
sum =(float(1)/float(ord))*(hp3(k)*char1(k))
f = f+sum
$)



sf = real(f)
# note truncation error
isf = sf + 0.1250
chec = n11*n11+n12*n12+n21*n21+n22*n22
chec1a = n11pa*n11pa+n12pa*n12pa+n21pa*n21pa+n22pa*n22pa
chec1b = n11pb*n11pb+n12pb*n12pb+n21pb*n21pb+n22pb*n22pb
chec2a = n11p2a*n11p2a+n12p2a*n12p2a+n21p2a*n21p2a+n22p2a*n22p2a
chec2b = n11p2b*n11p2b+n12p2b*n12p2b+n21p2b*n21p2b+n22p2b*n22p2b
chec3 = n11p3*n11p3+n12p3*n12p3+n21p3*n21p3+n22p3*n22p3
chec4 = n11p4*n11p4+n12p4*n12p4+n21p4*n21p4+n22p4*n22p4
if (isf == 1)
  $(
if((detm <detm1)|((detm==detm1)&((chec <chec1a)|(chec <chec1b))))
  $(
 if(n11 > n22)
  $(
n11pa  = n11
n21pa  = n21
n12pa  = n12
n22pa  = n22
detm1 = detm
isf1a  = isf
xr1a  = xr
yr1a  = yr
$)
 else
  $(
n11pb = n11
n21pb = n21
n12pb = n12
n22pb = n22
detm1 = detm
isf1b = isf
xr1b = xr
yr1b = yr
$)
$)
$)
else if(isf ==2)
  $(
```

```
if((detm <detm12)|((detm==detm12)&((chec <chec2a)|(chec <chec2b))))
  $(
 if(n11 >n22)
  $(
n11p2a = n11
n21p2a = n21
n12p2a = n12
n22p2a = n22
detm12 = detm
isf2a = isf
xr2a = xr
yr2a = yr
$)
else
  $(
n11p2b = n11
n21p2b = n21
n12p2b = n12
n22p2b = n22
detm12 = detm
isf2b = isf
xr2b = xr
yr2b = yr
$)
$)
$)
else if(isf ==3)
  $(
if((detm <detm13)|((detm==detm13)&(chec <chec3)))
  $(
n11p3 = n11
n21p3 = n21
n12p3 = n12
n22p3 = n22
detm13 = detm
isf3 = isf
xr3 = xr
yr3 = yr
$)
$)
else if(isf==4)
  $(
if((detm <detm14)|((detm==detm14)&(chec <chec4)))
  $(
n11p4 = n11
n21p4 = n21
n12p4 = n12
n22p4 = n22
detm14 = detm
```

```
isf4 = isf
xr4 = xr
yr4 = yr
$)
$)
next
  $)    # for nxx
     $)       #for nxy
     $)       #for nyx
          $)       #for nyy
if(isf1a !=0 )
$(
jc1 = jc1 + 1
nusg(jc1) = nsg
subf1(jc1) = isf1a
xr11(jc1) = xr1a
yr11(jc1) = yr1a
nc111(jc1) = n11pa
nc112(jc1) = n12pa
nc121(jc1) = n21pa
nc122(jc1) = n22pa
$)
if(isf1b !=0 )
$(
jc1 = jc1 + 1
nusg(jc1) = nsg
subf1(jc1) = isf1b
xr11(jc1) = xr1b
yr11(jc1) = yr1b
nc111(jc1) = n11pb
nc112(jc1) = n12pb
nc121(jc1) = n21pb
nc122(jc1) = n22pb
$)
if(isf2a !=0 )
$(
jc2 = jc2 + 1
nusg(jc2) = nsg
subf2(jc2) = isf2a
xr22(jc2) = xr2a
yr22(jc2) = yr2a
nc211(jc2) = n11p2a
nc212(jc2) = n12p2a
nc221(jc2) = n21p2a
nc222(jc2) = n22p2a
$)
if(isf2b !=0 )
$(
jc2 = jc2 + 1
```

```
nusg(jc2) = nsg
subf2(jc2) = isf2b
xr22(jc2) = xr2b
yr22(jc2) = yr2b
nc211(jc2) = n11p2b
nc212(jc2) = n12p2b
nc221(jc2) = n21p2b
nc222(jc2) = n22p2b
$)
if(isf3 !=0 )
$(
jc3 = jc3 + 1
nusg(jc3) = nsg
subf3(jc3) = isf3
xr33(jc3) = xr3
yr33(jc3) = yr3
nc311(jc3) = n11p3
nc312(jc3) = n12p3
nc321(jc3) = n21p3
nc322(jc3) = n22p3
$)
if(isf4 !=0 )
$(
jc4 = jc4 + 1
nusg(jc4) = nsg
subf4(jc4) = isf4
xr44(jc4) = xr4
yr44(jc4) = yr4
nc411(jc4) = n11p4
nc412(jc4) = n12p4
nc421(jc4) = n21p4
nc422(jc4) = n22p4
$)
116 format(" sf=(",i2,")",4a1,i4,i3,i2,"t1+",i2,"t2 ;",i2,"t1+",i2,"t2",f6.2,f6.2,8(f5.2,"(",i2,")",f5.2))
900 format(/)
do l = 1,10
$(
ldet = nc111(l)*nc122(l) - nc112(l)*nc121(l)
 if(subf1(l) !=0 & ldet !=0)
 $(
msg = nusg(l)
xro = xr11(l)
yro = yr11(l)
t1p = nc111(l)*t1 + nc112(l)*t2
t2p = nc121(l)*t1 + nc122(l)*t2
t1pc = conjg(t1p)
dot = real(t1pc*t2p)/(cabs(t1p)*cabs(t2p))
angle = (180/3.14159)*acos(dot)
call sgn(msg,output)
```

```
call tran(vectx,vecty,xro,yro)
#for(jl = 1;list(jl) != 0 ; jl = jl +1)
for(jl = 1; jl <= max ; jl = jl +1)
$(
jel = list(jl)
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
for(q= 2;iabs(q)<=2;q=q-1)
$(
xar(l,jel) = alpx(jel)*nc111(l)+alpy(jel)*nc121(l) - alx(jel) + vectx(jel)
yar(l,jel) = alpx(jel)*nc112(l)+alpy(jel)*nc122(l) - aly(jel) + vecty(jel)
add = cmplx(p*nc111(l),p*nc112(l)) + cmplx(q*nc121(l),q*nc122(l))
if(cmplx(xar(l,jel),yar(l,jel)) == add)
$(
xar(l,jel) = 0.0000
yar(l,jel) = 0.0000
mud = 98
break
$)
$) #             q loop
$)         #       p loop
$)
#write(15,116) subf1(l),(output(j),j=1,4),angle,ldet,
#nc111(l),nc112(l),nc121(l),nc122(l),xr11(l),yr11(l),
#(xar(l,list(m)),yar(l,list(m)),m = 1,max)
 js1 = js1 +1
 xrs1(js1,l)  =  xr11(l)
 yrs1(js1,l)  =  yr11(l)
 ldet1(js1,l) = ldet*ordd/ord
 ang1(js1,l)    = angle
 subfs1(js1,l) =  subf1(l)
 ns111(js1,l) =  nc111(l)
 ns112(js1,l) =  nc112(l)
 ns121(js1,l) =  nc121(l)
 ns122(js1,l) =  nc122(l)
do m = 1,max
$(
xrr(js1,l,list(m)) = xar(l,list(m))
yrr(js1,l,list(m)) = yar(l,list(m))
$)
$)
$)
do l = 1,10
$(
ldet = nc211(l)*nc222(l) - nc212(l)*nc221(l)
 if(subf2(l) !=0 & ldet !=0)
 $(
```

```
msg = nusg(1)
xro = xr22(1)
yro = yr22(1)
t1p = nc211(1)*t1 + nc212(1)*t2
t2p = nc221(1)*t1 + nc222(1)*t2
t1pc = conjg(t1p)
dot = real(t1pc*t2p)/(cabs(t1p)*cabs(t2p))
angle = (180/3.14159)*acos(dot)
call sgn(msg,output)
call tran(vectx,vecty,xro,yro)
for(jl = 1; jl <= max ; jl = jl +1)
$(
jel = list(jl)
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
for(q= 2;iabs(q)<=2;q=q-1)
$(
xar(1,jel) = alpx(jel)*nc211(1)+alpy(jel)*nc221(1) - alx(jel) + vectx(jel)
yar(1,jel) = alpx(jel)*nc212(1)+alpy(jel)*nc222(1) - aly(jel) + vecty(jel)
add = cmplx(p*nc211(1),p*nc212(1)) + cmplx(q*nc221(1),q*nc222(1))
if(cmplx(xar(1,jel),yar(1,jel)) == add)
$(
xar(1,jel) = 0.0000
yar(1,jel) = 0.0000
mud = 98
break
$)
$) #             q loop
$)        #       p loop
$)
#write(15,116) subf2(1),(output(j),j=1,4),angle,ldet,
#nc211(1),nc212(1),nc221(1),nc222(1),xr22(1),yr22(1),
#(xar(1,list(m)),yar(1,list(m)),m = 1,max)
 js2 = js2 +1
 xrs2(js2,1)  =  xr22(1)
 yrs2(js2,1)  =  yr22(1)
 ldet2(js2,1) = ldet*ordd/ord
 ang2(js2,1)    = angle
 subfs2(js2,1) =  subf2(1)
 ns211(js2,1) =  nc211(1)
 ns212(js2,1) =  nc212(1)
 ns221(js2,1) =  nc221(1)
 ns222(js2,1) =  nc222(1)
do m = 1,max
$(
xrr(js2,1,list(m)) = xar(1,list(m))
yrr(js2,1,list(m)) = yar(1,list(m))
```

```
$)
$)
$)
do l = 1,10
$(
ldet = nc311(l)*nc322(l) - nc312(l)*nc321(l)
 if(subf3(l) !=0 & ldet !=0)
 $(
msg = nusg(l)
xro = xr33(l)
yro = yr33(l)
t1p = nc311(l)*t1 + nc312(l)*t2
t2p = nc321(l)*t1 + nc322(l)*t2
t1pc = conjg(t1p)
dot = real(t1pc*t2p)/(cabs(t1p)*cabs(t2p))
angle = (180/3.14159)*acos(dot)
call sgn(msg,output)
call tran(vectx,vecty,xro,yro)
#for(jl = 1;list(jl) != 0 ; jl = jl +1)
for(jl = 1; jl <= max ; jl = jl +1)
$(
jel = list(jl)
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
for(q=2;iabs(q)<=2;q=q-1)
#do q = -2,2
$(
xar(l,jel) = alpx(jel)*nc311(l)+alpy(jel)*nc321(l) - alx(jel) + vectx(jel)
yar(l,jel) = alpx(jel)*nc312(l)+alpy(jel)*nc322(l) - aly(jel) + vecty(jel)
add = cmplx(p*nc311(l),p*nc312(l)) + cmplx(q*nc321(l),q*nc322(l))
if(cmplx(xar(l,jel),yar(l,jel)) == add)
$(
xar(l,jel) = 0.0000
yar(l,jel) = 0.0000
mud = 98
break
$)
$) #            q loop
$)       #       p loop
$)
#write(15,116) subf3(l),(output(j),j=1,4),angle,ldet,
#nc311(l),nc312(l),nc321(l),nc322(l),xr33(l),yr33(l),
#(xar(l,list(m)),yar(l,list(m)),m = 1,max)
 js3 = js3 +1
 xrs3(js3,l)  =  xr33(l)
 yrs3(js3,l)  =  yr33(l)
 ldet3(js3,l) = ldet*ordd/ord
```

```
 ang3(js3,l)    = angle
 subfs3(js3,l) =  subf3(l)
 ns311(js3,l) =  nc311(l)
 ns312(js3,l) =  nc312(l)
 ns321(js3,l) =  nc321(l)
 ns322(js3,l) =  nc322(l)
do m = 1,max
$(
xrr(js3,l,list(m)) = xar(l,list(m))
yrr(js3,l,list(m)) = yar(l,list(m))
$)
$)
$)
do l = 1,10
$(
ldet = nc411(l)*nc422(l) - nc412(l)*nc421(l)
 if(subf4(l) !=0 & ldet !=0)
 $(
msg = nusg(l)
xro = xr44(l)
yro = yr44(l)
t1p = nc411(l)*t1 + nc412(l)*t2
t2p = nc421(l)*t1 + nc422(l)*t2
t1pc = conjg(t1p)
dot = real(t1pc*t2p)/(cabs(t1p)*cabs(t2p))
angle = (180/3.14159)*acos(dot)
call sgn(msg,output)
call tran(vectx,vecty,xro,yro)
#for(jl = 1;list(jl) != 0 ; jl = jl +1)
for(jl = 1; jl <= max ; jl = jl +1)
$(
jel = list(jl)
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
for(q=2;iabs(q)<=2;q=q-1)
#do q = -2,2
$(
xar(l,jel) = alpx(jel)*nc411(l)+alpy(jel)*nc421(l) - alx(jel) + vectx(jel)
yar(l,jel) = alpx(jel)*nc412(l)+alpy(jel)*nc422(l) - aly(jel) + vecty(jel)
add = cmplx(p*nc411(l),p*nc412(l)) + cmplx(q*nc421(l),q*nc422(l))
if(cmplx(xar(l,jel),yar(l,jel)) == add)
$(
xar(l,jel) = 0.0000
yar(l,jel) = 0.0000
mud = 98
break
$)
```

```
$) #            q loop
$)        #      p loop
$)
#write(15,116) subf4(l),(output(j),j=1,4),angle,ldet,
#nc411(l),nc412(l),nc421(l),nc422(l),xr44(l),yr44(l),
#(xar(l,list(m)),yar(l,list(m)),m = 1,max)
 js4 = js4 +1
 xrs4(js4,l)  =  xr44(l)
 yrs4(js4,l)  =  yr44(l)
 ldet4(js4,l) = ldet*ordd/ord
 ang4(js4,l)    = angle
 subfs4(js4,l) =  subf4(l)
 ns411(js4,l) =  nc411(l)
 ns412(js4,l) =  nc412(l)
 ns421(js4,l) =  nc421(l)
 ns422(js4,l) =  nc422(l)
do m = 1,max
$(
xrr(js4,l,list(m)) = xar(l,list(m))
yrr(js4,l,list(m)) = yar(l,list(m))
$)
$)
$)

  next
            $)   #for limx xo
                      $)   #for limy yo
#write(15,33)
#33 format ("                              xo   yo  <- new origin")

# compare

do kq= 1,12
$(
do kr= 1,10
$(
if(subfs1(kq,kr) != 0)
$(
do ks= kq + 1,12
$(
do kt= 1,10
$(
if( (cmplx(kq,kr) != cmplx(ks,kt))  & (subfs1(ks,kt) != 0) )
$(
if((subfs1(kq,kr)==subfs1(ks,kt))&(ns111(kq,kr)==ns111(ks,kt))&(ns112(kq,kr)==
ns112(ks,kt))&(ns121(kq,kr) == ns121(ks,kt)) & (ns122(kq,kr) == ns122(ks,kt)))
$(  # put gen in new write
for(jel = 1;jel <= max ; jel = jel +1)
$(
```

```
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
#for(q=2;iabs(q)<=2;q=q-1)
do q = -2,2
$(
# before sadd
sadd=cmplx(p*ns111(ks,kt),p*ns112(ks,kt))+cmplx(q*ns121(ks,kt),q*ns122(ks,kt))
if( cmplx(xrr(kq,kr,jel),yrr(kq,kr,jel)) == sadd + cmplx(xrr(ks,kt,jel),yrr(ks,kt,jel)))
$(
# Equating them if  linear comb DID NOT WORK
mud = 99
if(jel == max)
subfs1(kq,kr) = 0
break
$)
$)  #               q loop
$)          #        p loop
$)  # list,  jel
$)
$)
$)
$)
$)
$)
$)
do kq = 1,12
$(
do kr = 1,10
$(
if(subfs1(kq,kr) !=0)
write(15,116) subfs1(kq,kr),(output(j),j=1,4),ang1(kq,kr),ldet1(kq,kr),
ns111(kq,kr),ns112(kq,kr),ns121(kq,kr),ns122(kq,kr),xrs1(kq,kr),yrs1(kq,kr),
(xrr(kq,kr,list(m)),list(m),yrr(kq,kr,list(m)),m = 2,max,inc)
$)
$)


do kq= 1,12
$(
do kr= 1,10
$(
if(subfs2(kq,kr) != 0)
$(
do ks= kq + 1,12
$(
do kt= 1,10
$(
```

```
if( (cmplx(kq,kr) != cmplx(ks,kt)) & (subfs2(ks,kt) != 0) )
$(
if((subfs2(kq,kr)==subfs2(ks,kt))&(ns211(kq,kr)==ns211(ks,kt))&(ns212(kq,kr)==
ns212(ks,kt))&(ns221(kq,kr) == ns221(ks,kt)) & (ns222(kq,kr) == ns222(ks,kt)))
$( #put gen in new write
for(jel = 1;jel <= max ; jel = jel +1)
$(
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
#for(q=2;iabs(q)<=2;q=q-1)
do q = -2,2
$(
# before sadd
sadd=cmplx(p*ns211(ks,kt),p*ns212(ks,kt))+cmplx(q*ns221(ks,kt),q*ns222(ks,kt))
if( cmplx(xrr(kq,kr,jel),yrr(kq,kr,jel)) == sadd + cmplx(xrr(ks,kt,jel),yrr(ks,kt,jel)))
$(
mud = 99
if(jel == max)
subfs2(kq,kr) = 0
break
$)
$) #          q loop
$)      #     p loop
$) # list,  jel
$)
$)
$)
$)
$)
$)
$)
do kq = 1,12
$(
do kr = 1,10
$(
if(subfs2(kq,kr) !=0)
write(15,116) subfs2(kq,kr),(output(j),j=1,4),ang2(kq,kr),ldet2(kq,kr),
ns211(kq,kr),ns212(kq,kr),ns221(kq,kr),ns222(kq,kr),xrs2(kq,kr),yrs2(kq,kr),
(xrr(kq,kr,list(m)),list(m),yrr(kq,kr,list(m)),m = 2,max,inc)
$)
$)


do kq= 1,12
$(
do kr= 1,10
$(
```

```
if(subfs3(kq,kr) != 0)
$(
do ks= kq + 1,12
$(
do kt= 1,10
$(
if( (cmplx(kq,kr) != cmplx(ks,kt))  & (subfs3(ks,kt) != 0) )
$(
if((subfs3(kq,kr)==subfs3(ks,kt))&(ns311(kq,kr)==ns311(ks,kt))&(ns312(kq,kr)
== ns312(ks,kt))&(ns321(kq,kr) == ns321(ks,kt)) & (ns322(kq,kr) ==
ns322(ks,kt)))
$(  # put gen in new write
for(jel = 1;jel <= max ; jel = jel +1)
$(
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
#for(q=2;iabs(q)<=2;q=q-1)
do q = -2,2
$(
# before sadd
sadd=cmplx(p*ns311(ks,kt),p*ns312(ks,kt))+cmplx(q*ns321(ks,kt),q*ns322(ks,kt))
if( cmplx(xrr(kq,kr,jel),yrr(kq,kr,jel)) == sadd + cmplx(xrr(ks,kt,jel),yrr(ks,kt,jel)))
$(
mud = 99
if(jel == max)
subfs3(kq,kr) = 0
break
$)
$) #            q loop
$)        #       p loop
$) # list,  jel
$)
$)
$)
$)
$)
$)
$)
do kq = 1,12
$(
do kr = 1,10
$(
if(subfs3(kq,kr) !=0)
write(15,116) subfs3(kq,kr),(output(j),j=1,4),ang3(kq,kr),ldet3(kq,kr),
ns311(kq,kr),ns312(kq,kr),ns321(kq,kr),ns322(kq,kr),xrs3(kq,kr),yrs3(kq,kr),
(xrr(kq,kr,list(m)),list(m),yrr(kq,kr,list(m)),m = 2,max,inc)
$)
```

```
$)

do kq= 1,12
$(
do kr= 1,10
$(
if(subfs4(kq,kr) != 0)
$(
do ks= kq + 1,12
$(
do kt= 1,10
$(
if( (cmplx(kq,kr) != cmplx(ks,kt))  & (subfs4(ks,kt) != 0) )
$(
if((subfs4(kq,kr)==subfs4(ks,kt))&(ns411(kq,kr)==ns411(ks,kt))&(ns412(kq,kr)==
ns412(ks,kt))&(ns421(kq,kr) == ns421(ks,kt)) & (ns422(kq,kr) == ns422(ks,kt)))
$(  # put gen in new write
for(jel = 1;jel <= max ; jel = jel +1)
$(
mud = 0
for(p=2;iabs(p)<=2;p=p-1)
$(
if(mud==0)
#for(q=2;iabs(q)<=2;q=q-1)
do q = -2,2
$(
# before sadd
sadd=cmplx(p*ns411(ks,kt),p*ns412(ks,kt))+cmplx(q*ns421(ks,kt),q*ns422(ks,kt))
if( cmplx(xrr(kq,kr,jel),yrr(kq,kr,jel)) == sadd + cmplx(xrr(ks,kt,jel),yrr(ks,kt,jel)))
$(
mud = 99
if(jel == max)
subfs4(kq,kr) = 0
break
$)
$)  #              q loop
$)         #       p loop
$)  # list,  jel
$)
$)
$)
$)
$)
$)
$)
do kq = 1,12
$(
do kr = 1,10
```

```
$(
if(subfs4(kq,kr) !=0)
write(15,116) subfs4(kq,kr),(output(j),j=1,4),ang4(kq,kr),ldet4(kq,kr),
ns411(kq,kr),ns412(kq,kr),ns421(kq,kr),ns422(kq,kr),xrs4(kq,kr),yrs4(kq,kr),
(xrr(kq,kr,list(m)),list(m),yrr(kq,kr,list(m)),m = 2,max,inc)
$)
$)
$)   # for the various subgroups
$)   # for  ire reps
                    $)    # for itot     stars
end


subroutine phs0(k0,xk,yk,hp0,xo,yo)
complex k0,hp0(8),xo,yo,zero
zero = cmplx(0.00,0.00)
pi = 3.14159
if (cabs(k0) == 0.000)
   $(
do i=1,8
hp0(i) = zero
   $)
else
     $(
hp0(1) = cexp(2.0*pi*(xk*zero + yk*zero))
hp0(2) = cexp(2.0*pi*(xk*2*xo + yk*2*yo))
hp0(3) = cexp(2.0*pi*(xk*(xo-yo) + yk*(yo+xo)))
hp0(4) = cexp(2.0*pi*(xk*(xo+yo) + yk*(yo-xo)))
hp0(5) = cexp(2.0*pi*(xk*(2.0*xo) + yk*(zero)))
hp0(6) = cexp(2.0*pi*(xk*zero + yk*2*yo))
hp0(7) = cexp(2.0*pi*(xk*(xo+yo) + yk*(yo+xo)))
hp0(8) = cexp(2.0*pi*(xk*(xo-yo) + yk*(yo-xo)))
     $)
return
end
subroutine arm1(cfn11,cfn12,cfn21,cfn22,phas11,phas12,k1)
# k1 = 1/2,0
complex cfn11,cfn12,cfn21,cfn22,phas11,phas12,k1
#k1 = cmplx(0.50,0.00)
pi = 3.14159
zero = cmplx(0.00,0.00)
phas11 = cexp(2.0*pi*(0.50*cfn11 + 0.00*cfn12))
phas12 = cexp(2.0*pi*(0.50*cfn21 + 0.00*cfn22))
if (real(phas11) == +1.000 & real(phas12) == +1.000)
$(
k1 = cmplx(0.50,0.00)
  #write(15,104) k1,phas11,phas12
$)
else
```

```
  $(
  #write(15,105) k1, phas11,phas12
 k1 = zero
  $)
 104 format(" arm k = ",g8.4,g8.4," phase factors = ",g8.4,g8.4, "and ",g8.4,g8.4)
105 format(/,"   arm k ",g8.4,g8.4,"  not allowed  because of phase factors ",g8.4,g8.4," and ",g8.4,g8.4)
 return
 end
 subroutine arm2(cfn11,cfn12,cfn21,cfn22,phas21,phas22,k2)
 # k2 = 0,1/2
 complex cfn11,cfn12,cfn21,cfn22,phas21,phas22,k2
 #k2 = cmplx(0.00,0.50)
 zero = cmplx(0.000,0.000)
 pi = 3.14159
 phas21 = cexp(2.0*pi*(0.00*cfn11 + 0.50*cfn12))
 phas22 = cexp(2.0*pi*(0.00*cfn21 + 0.50*cfn22))
  if (real(phas21)== +1.000 & real(phas22)== +1.000)
 $(
 k2 = cmplx(0.00,0.50)
     #write(15,204) k2,phas21,phas22
 $)
  else
      $(
  #write(15,205) k2, phas21,phas22
 k2 = zero
      $)
 204 format(" arm k = ",g8.4,g8.4," phase factors = ",g8.4,g8.4, "and ",g8.4,g8.4)
205 format(/,"   arm k ",g8.4,g8.4,"  not allowed  because of phase factors ",g8.4,g8.4," and ",g8.4,g8.4)
 return
 end
 subroutine arm3(cfn11,cfn12,cfn21,cfn22,phas31,phas32,k3)
 # k3 = 1/2,1/2
 complex cfn11,cfn12,cfn21,cfn22,phas31,phas32,k3
 #k3 = cmplx(0.50,0.50)
 pi = 3.14159
 zero = cmplx(0.00,0.00)
 phas31 = cexp(2.0*pi*(0.50*cfn11 + 0.50*cfn12))
 phas32 = cexp(2.0*pi*(0.50*cfn21 + 0.50*cfn22))
  if (real(phas31)== +1.000 & real(phas32)== +1.000)
   $(
     #write(15,304) k3,phas31,phas32
    k3 = cmplx(0.50,0.50)
    $)
 else
      $(
  #write(15,305) k3, phas31,phas32
k3 = zero
      $)
 304 format(" arm k = ",g8.4,g8.4," phase factors = ",g8.4,g8.4, "and ",g8.4,g8.4)
```

```
 305 format(/,"   arm k ",g8.4,g8.4,"  not allowed  because of phase factors ",g8.4,g8.4," and ",g8.4)
return
end
subroutine sqtab(l,m,n,k)
integer t(8,8)

t(1,1)=1;t(1,2)=2;t(1,3)=3;t(1,4)=4;t(1,5)=5;t(1,6)=6;t(1,7)=7;t(1,8)=8
t(2,1)=2;t(2,2)=1;t(2,3)=4;t(2,4)=3;t(2,5)=6;t(2,6)=5;t(2,7)=8;t(2,8)=7
t(3,1)=3;t(3,2)=4;t(3,3)=2;t(3,4)=1;t(3,5)=8;t(3,6)=7;t(3,7)=5;t(3,8)=6
t(4,1)=4;t(4,2)=3;t(4,3)=1;t(4,4)=2;t(4,5)=7;t(4,6)=8;t(4,7)=6;t(4,8)=5
t(5,1)=5;t(5,2)=6;t(5,3)=7;t(5,4)=8;t(5,5)=1;t(5,6)=2;t(5,7)=3;t(5,8)=4
t(6,1)=6;t(6,2)=5;t(6,3)=8;t(6,4)=7;t(6,5)=2;t(6,6)=1;t(6,7)=4;t(6,8)=3
t(7,1)=7;t(7,2)=8;t(7,3)=6;t(7,4)=5;t(7,5)=4;t(7,6)=3;t(7,7)=1;t(7,8)=2
t(8,1)=8;t(8,2)=7;t(8,3)=5;t(8,4)=6;t(8,5)=3;t(8,6)=4;t(8,7)=2;t(8,8)=1;
k = t(t(l,m),n)
return
end
subroutine p111(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
#   #1
complex k0,zero,cfn11,cfn12,cfn21,cfn22,el(8)
integer ord,list(8)
real alpx(8),alpy(8)
ord = 1
nsg = 1
max = 1
pi = 3.14159
zero = cmplx(0.00,0.00)
do lk = 1,8
$(
list(lk) = 0
el(lk) = zero
alpx(lk) = 0.0000
alpy(lk) = 0.0000
$)
el(1) = cexp(2.0*pi*(zero + zero))
list(1) = 1
return
end
subroutine p211(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
#   #2
complex  k0,zero,cfn11,cfn12,cfn21,cfn22,el(8)
integer ord,list(8)
real alpx(8),alpy(8)
ord = 2
nsg = 2
max = 2
pi = 3.14159
zero = cmplx(0.00,0.00)
do lk = 1,8
```

```
$(
list(1k) = 0
el(1k) = zero
alpx(1k) = 0.0000
alpy(1k) = 0.0000
$)
el(1) = cexp(2.0*pi*(zero + zero))
el(2) = cexp(2.0*pi*(zero + zero))
list(1) = 1
list(2) = 2
return
end
subroutine p411(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
#   #10
complex  k0,zero,cfn11,cfn12,cfn21,cfn22,el(8)
integer ord,list(8)
real alpx(8),alpy(8)
ord = 4
nsg = 10
max = 4
pi = 3.14159
zero = cmplx(0.00,0.00)
do 1k = 1,8
$(
list(1k) = 0
el(1k) = zero
alpx(1k) = 0.0000
alpy(1k) = 0.0000
$)
el(1) = cexp(2.0*pi*(zero + zero))
el(2) = cexp(2.0*pi*(zero + zero))
el(3) = cexp(2.0*pi*(zero + zero))
el(4) = cexp(2.0*pi*(zero + zero))
list(1) = 1
list(2) = 2
list(3) = 3
list(4) = 4
return
end
subroutine p1m1(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
#sigmax(0,1/2)  for p1g1
#   3
complex  k0,zero,cfn11,cfn12,cfn21,cfn22,el(8)
integer ord,list(8)
real alpx(8),alpy(8)
ord = 2
nsg = 3
max = 2     #for sigx
pi = 3.14159
```

```
zero = cmplx(0.00,0.00)
do lk = 1,8
$(
list(lk) = 0
el(lk) = zero
alpx(lk) = 0.0000
alpy(lk) = 0.0000
$)
el(1) = cexp(2.0*pi*(zero + zero))
el(5) = cexp(2.0*pi*(zero + zero))
list(1) = 1
list(2) = 5
return
end
subroutine c1m1(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
#    5
complex  k0,zero,cfn11,cfn12,cfn21,cfn22,el(8)
integer ord,list(8)
real alpx(8),alpy(8)
ord = 2
nsg = 5
max = 2
pi = 3.14159
zero = cmplx(0.00,0.00)
do lk = 1,8
$(
list(lk) = 0
el(lk) = zero
alpx(lk) = 0.0000
alpy(lk) = 0.0000
$)
el(1) = cexp(2.0*pi*(zero + zero))
el(5) = cexp(2.0*pi*(zero + zero))
list(1) = 1
list(2) = 5
return
end
subroutine p1g1(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
#sigmax(0,1/2)
integer ord,list(8)
complex  k0,k1,k2,k3,zero,cfn11,cfn12,cfn21,cfn22,el(8)
real alpx(8),alpy(8)
ord = 2
nsg = 4
max = 2
pi = 3.14159
zero = cmplx(0.00,0.00)
do lk = 1,8
$(
```

```
list(1k) = 0
el(1k) = zero
alpx(1k) = 0.0000
alpy(1k) = 0.0000
$)
alpx(5) = 0.0000
alpy(5) = 0.5000
k1 = cmplx(0.50,0.00)
k2 = cmplx(0.00,0.50)
k3 = cmplx(0.50,0.50)
if (k0 == k1)
   $(
     xk = 0.50
     yk = 0.00
   $)
else if (k0 == k2)
       $(
         xk = 0.00
         yk = 0.50
       $)
else if (k0 == k3)
     $(
xk = 0.50
yk = 0.50
     $)
el(1) = cexp(2.0*pi*(zero + zero))
#el(5) = cexp(2.0*pi*(xk*(cfn11*0.00+cfn21)*0.50+yk*(cfn12*0.00+cfn22)*0.50))
el(5) = cexp(2.0*pi*(xk*(cfn11*0.00+cfn12)*0.50+yk*(cfn21*0.00+cfn22)*0.50))
list(1) = 1
list(2) = 5
return
end
subroutine tran(vectx,vecty,xro,yro)
real xro,yro,vectx(8),vecty(8)
do l = 1,8
$(
vectx(l) = 0.00000
vecty(l) = 0.00000
$)
vectx(1) = 0.00000
vectx(2) = 2*xro
vectx(3) = xro - yro
vectx(4) = xro+yro
vectx(5) = 2*xro
vectx(6) = 0.0000
vectx(7) = xro+yro
vectx(8) = xro -yro
vecty(1) = 0.00000
vecty(2) = 2*yro
```

```
vecty(3) = yro+xro
vecty(4) = yro-xro
vecty(5) = 0.000
vecty(6) = 2*yro
vecty(7) = yro + xro
vecty(8) = yro -xro
return
end
subroutine info
# remember to change divisor in ......>sum/1,2,3,6,12....
# itot for 1-arm,2-arm,3-arm,...
# --iall, new , 71 f --- ,call origin , call matrices
# char( ) depends on how many elements are in the subgroup
# ---the group to be subduced onto
# elem( ) depends on how many elements are in the gk1( ) ---- the group
# of the wave-vector.



# t1 = (0,1)
# t2 = (1,0)
#   e = 1 = (x,y,z)
# c2z = 2 = (-x,-y,z)
# c4z- = 3 = (y,-x,z)
# c4z+ = 4 = (-y,+x,z)
# sigx = 5 = (-x,y,z)
# sigy = 6 = (x,-y,z)
# sigda = 7 = (-y,-x,z)
# sigdb = 8 = (y,x,z)
#
#
#
# main program is only   -----   500 lines ????
#  p4mm
# l= 1,3  m = 1,2     n= 1,4(c4z+ == -y,x)   # first star  k=1/2,0  0,1/2
# l = 1   m = 1,2,3,4    n = 1   # second star  k = 1/2 , 1/2
# m    --- the elements of gk1
# n    --- the elements sending k2 ===> k1
# l    --- the inverse of n
return
end
subroutine m1(nxx,nxy,nyx,nyy,n11,n12,n21,n22,detm)
integer detm
n11 = nxx
n21 = nxy
n12 = nyx
n22 = nyy
detm = n11*n22 - n21*n12
if (detm < 1)
```

```
detm = 0
return
end
subroutine sg12(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
complex  k0,cfn11,cfn12,cfn21,cfn22,el(8)
integer ord,list(8)
real alpx(8),alpy(8)
if(iall==1)
call p111(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
else if(iall==2)
call p1g1(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
else if(iall==3)
call c1m1(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
else if(iall==4)
call p1g1(k0,iall,ord,nsg,el,alpx,alpy,cfn11,cfn12,cfn21,cfn22,list,max)
return
end
subroutine hwri12(input,itot,char1,char2,char3,im,jm)
integer char1(8),char2(8),char3(8)
integer input(4)

 if(itot==1)
$(
write(15,121) (input(l),l=1,4)
write(15,201) (char1(k), k = 1,8)
write(15,122)
$)
 if(itot==2)
$(
write(15,121) (input(l),l=1,4)
write(15,202) (char1(k), k = 1,8)
write(15,122)
$)
else if(itot==3)
$(
write(15,121) (input(l),l=1,4)
write(15,203) (char1(k), k = 1,8)
write(15,122)
$)
201 format(" star 1 ,character of elements", 8i6," for k = 1/2 , 0")
202 format(" star 2 ,character of elements", 8i6," for k = 0 , 1/2")
203 format(" star 3 ,character of elements", 8i6," for k = 1/2 , 1/2")
121 format(/," elem gk <g = ",4a1,"           e    c2z   c4z-  c4z+",
"  mx    my    da    db")
122 format(/,"       sg    0   x    t1'     t2'    xo    yo",
    "    E        C2Z     C4Z-      C4Z+    SIGX     SIGY",
    "     SIGDA     SIGDB ")
return
end
```

```
subroutine data0(ordd,input,itot,inew,ma,n1,n2,n3)
integer ordd,input(4)
#n1 = 1
#    e     sigx
#arm   1
#change   :: for( ma    ....>>>>> in main program ???
ordd = 2
input(1) = 'p'
input(2) = '1'
input(3) = 'g'
input(4) = '1'
ma = 2
n1 = 1
inew = 2    # number of reps in star 1
return
end
subroutine data1(itot,ire,elem,alx,aly)
real alx(8),aly(8)
integer elem(8)
#alx = alpha for to = a' -a + s -h*s    test
#aly = alpha for to = a' -a + s -h*s    test
do lk = 1,8
$(
alx(lk) = 0.0000
aly(lk) = 0.0000
$)

alx(5) = 0.000
aly(5) = 0.500
 if (ire == 1)
$(
elem(1) = 1
elem(5) = 1
$)
else if (ire == 2 )
$(
elem(1) = 1
elem(5) = -1
$)
return
end
subroutine sgn(nsg,output)
integer output(4)
if(nsg==1)
$(
output(1) = 'p'
output(2) = '1'
output(3) = '1'
output(4) = '1'
```

```
$)
else if(nsg==2)
$(
output(1) = 'p'
output(2) = '2'
output(3) = '1'
output(4) = '1'
$)
else if(nsg==3)
$(
output(1) = 'p'
output(2) = '1'
output(3) = 'm'
output(4) = '1'
$)
else if(nsg==4)
$(
output(1) = 'p'
output(2) = '1'
output(3) = 'g'
output(4) = '1'
$)
else if(nsg==5)
$(
output(1) = 'c'
output(2) = '1'
output(3) = 'm'
output(4) = '1'
$)
else if(nsg==6)
$(
output(1) = 'p'
output(2) = '2'
output(3) = 'm'
output(4) = 'm'
$)
else if(nsg==7)
$(
output(1) = 'p'
output(2) = '2'
output(3) = 'm'
output(4) = 'g'
$)
else if(nsg==8)
$(
output(1) = 'p'
output(2) = '2'
output(3) = 'g'
output(4) = 'g'
```

```
$)
else if(nsg==9)
$(
output(1) = 'c'
output(2) = '2'
output(3) = 'm'
output(4) = 'm'
$)
else if(nsg==10)
$(
output(1) = 'p'
output(2) = '4'
output(3) = '1'
output(4) = '1'
$)
else if(nsg==11)
$(
output(1) = 'p'
output(2) = '4'
output(3) = 'm'
output(4) = 'm'
$)
else if(nsg==12)
$(
output(1) = 'p'
output(2) = '4'
output(3) = 'g'
output(4) = 'm'
$)
else if(nsg==13)
$(
output(1) = 'p'
output(2) = '3'
output(3) = '1'
output(4) = '1'
$)
else if(nsg==14)
$(
output(1) = 'p'
output(2) = '3'
output(3) = 'm'
output(4) = '1'
$)
else if(nsg==15)
$(
output(1) = 'p'
output(2) = '3'
output(3) = '1'
output(4) = 'm'
```

```
$)
else if(nsg==16)
$(
output(1) = 'p'
output(2) = '6'
output(3) = '1'
output(4) = '1'
$)
else if(nsg==17)
$(
output(1) = 'p'
output(2) = '6'
output(3) = 'm'
output(4) = 'm'
$)
return
end
```

APPENDIX II

Character Tables for the Diperiodic Groups

Multiplier reps (R) of G_{k_o} :- the point group of the wave-vector group $G_k \subseteq G_o$ for the 80 diperiodic groups G_o at points of high symmetry .

#1 P1 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

G_{k_o}	E
R1	1

#2 P$\bar{1}$ *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

G_{k_o}	E	I
R1	1	1
R2	1	-i

#3 P211 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

G_{k_o}	E	C2z
R1	1	1
R2	1	-1

#4 Pm11 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2
#5 Pb11

G_{k_o}	E	mz
R1	1	1
R2	1	-1

#6 P2/m11 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

G_{k_o}	E	C2z	I	mz
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

#7 P2/b11 *k = 1/2 ,0 SEE #6 P2/m11

*k = 0,1/2 ; *k = 1/2,1/2

Gko	E	C2z	I	mz
R1	2	0	0	0

#8 P112 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2
#9 P112$_1$

Gko	E	C2y
R1	1	1
R2	1	-1

#10 C112 *k = 1/2,0 ; 0,1/2 : SEE #1

*k = 1/2 , 1/2 : SEE #8

#11 P11m *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2
#12 P11a

Gko	E	my
R1	1	1
R2	1	-1

#13 C11m *k = 1/2,0 ; 0,1/2 : SEE #1

*k = 1/2 ,1/2 : SEE #11

#14 P112/m *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2y	I	my
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

#15 $P112_1/m$ *k = 1/2,0 : SEE #14

*k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2y	I	my
R1	2	0	0	0

#16 C112/m *k = 1/2,0 ; 0,1/2 : SEE #2

*k = 1/2 ,1/2 : SEE #2

#17 P112/a *k = 0,1/2 : SEE #14

*k = 1/2 ,0 ; *k = 1/2 ,1/2

Gko	E	C2y	I	my
R1	2	0	0	0

#18 $P112_1/a$ *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2y	I	my
R1	2	0	0	0

#19 P222 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2z	C2x	C2y
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

#20 $P222_1$ *k = 1/2,0 : SEE #19

*k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2z	C2x	C2y
R1	2	0	0	0

21 $P22_12_1$ *k = 1/2 , 0 ; *k = 0 ,1/2

Gko	E	C2z	C2x	C2y
R1	2	0	0	0

*k = 1/2 ,1/2

Gko	E	C2z	C2x	C2y
R1	2	2	0	0
R2	2	-2	0	0

22 C222 *k = 1/2,0 ; 0,1/2 : SEE # 3

*k = 1/2 ,1/2 : SEE # 19

23 P2mm *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2z	mx	mx
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

24 Pmm2 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2y	mz	mx
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

25 Pm_1a *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2x	mz	my
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

26 Pbm_1 *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2 SEE : # 24
27 Pbb2

#28 P2ma *k = 1/2 , 0 ; *k = 1/2 ,1/2

Gko	E	C2z	mx	my
R1	2	0	0	0

*k = 0 , 1/2 : SEE #23

#29 Pam2 *k = 1/2 , 0 ; *k = 1/2 ,1/2
#30 $Pab2_1$

#31 Pnb2

#32 $Pnm2_1$

Gko	E	C2y	mz	mx
R1	2	0	0	0

*k = 0 , 1/2 : SEE #24

#33 P2ba *k = 1/2 , 0 ; *k = 0 ,1/2

Gko	E	C2z	mx	my
R1	2	0	0	0

*k = 1/2 , 1/2

Gko	E	C2z	mx	my
R1	2	2	0	0
R2	2	-2	0	0

#34 C2mm *k = 1/2 , 0 ; *k = 0 ,1/2 SEE : #3

*k = 1/2 ,1/2 SEE : #23

#35 Cmm2 *k = 1/2 , 0 ; *k = 0 ,1/2 SEE : #4
#36 Cam2

*k = 1/2 ,1/2 SEE : #24

#37 Pmmm *k = 1/2,0 ; *k = 0,1/2 ; *k = 1/2 ,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	1	1	1	1	1	1	1	1
R2	1	1	-1	-1	1	1	-1	-1
R3	1	-1	1	-1	1	-1	1	-1
R4	1	-1	-1	1	1	-1	-1	1
R5	1	1	1	1	-1	-1	-1	-1
R6	1	1	-1	-1	-1	-1	1	1
R7	1	-1	1	-1	-1	1	-1	1
R8	1	-1	-1	1	-1	1	1	-1

38 Pama *k = 0,1/2 SEE : # 37

*k = 1/2,0 ; *k = 1/2 ,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	2	0	0	0	0	0
R2	2	0	-2	0	0	0	0	0

39 Pama *k = 1/2,0

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	2	0	0	0	0	0
R2	2	0	-2	0	0	0	0	0

*k = 0,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	2	0	0	0	0
R2	2	0	0	-2	0	0	0	0

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	2	0	0	0	0	0	0
R2	2	-2	0	0	0	0	0	0

40 Pmma *k = 0,1/2 SEE:# 37

*k = 1/2,0 ; *k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	2	0	0
R2	2	0	0	0	0	-2	0	0

41 Pamm *k = 0,1/2 SEE:# 37

*k = 1/2,0 ; *k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	0	0	2
R2	2	0	0	0	0	0	0	-2

42 Pnma *k = 1/2,0

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	2	0	0	0	0	0
R2	2	0	-2	0	0	0	0	0

*k = 0,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	0	0	2
R2	2	0	0	0	0	0	0	-2

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my

R1	2	0	0	0	2	0	0	0
R2	2	0	0	0	-2	0	0	0

43 Paba

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	2	0	0	0	0	0
R2	2	0	-2	0	0	0	0	0

*k = 0,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	2	0	0
R2	2	0	0	0	0	-2	0	0

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	0	0	2
R2	2	0	0	0	0	0	0	-2

44 Pmba *k = 1/2,0 ; *k = 0,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	2	0	0
R2	2	0	0	0	0	-2	0	0

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	2	0	0	-2	-2	0	0
R2	2	-2	0	0	-2	2	0	0
R3	2	-2	0	0	2	-2	0	0
R4	2	2	0	0	2	2	0	0

45 Pabm *k = 1/2,0

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	0	0	2
R2	2	0	0	0	0	0	0	-2

*k = 0,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	2	0	0
R2	2	0	0	0	0	-2	0	0

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	2	0	0	0	0	0
R2	2	0	-2	0	0	0	0	0

46 Pnmm *k = 1/2,0

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	0	0	2
R2	2	0	0	0	0	0	0	-2

*k = 0,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	0	2	0
R2	2	0	0	0	0	0	-2	0

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my

R1	2	2	0	0	0	0	0	0
R2	2	-2	0	0	0	0	0	0

47Cmmm *k = 1/2,0 ; k = 0,1/2 SEE:# 19

*k = 1/2,1/2 SEE:# 37

48 Camm *k = 1/2,1/2 SEE:# 37

*k = 1/2,0 ; k = 0,1/2

Gko	E	C2z	C2x	C2y	I	mz	mx	my
R1	2	0	0	0	0	0	0	0

49 P4 *k = 1/2,0 ; k = 0,1/2 SEE:# 3

*k = 1/2,1/2

Gko	E	C2z	C4z+	C4z-
R1	1	1	1	1
R2	1	1	-1	-1
R3	2	-2	0	0

50 P$\bar{1}$ *k = 1/2,0 ; k = 0,1/2 SEE:# 3

*k = 1/2,1/2

Gko	E	C2z	S4z+	S4z-
R1	1	1	1	1
R2	1	1	-1	-1
R3	2	-2	0	0

51 P4/m11 *k = 1/2,0 ; k = 0,1/2 SEE:# 6

*k = 1/2,1/2

Gko	E	C2z	C4z	C4z	-I	mz	S4z-	S4z+
R1	1	1	1	1	1	1	1	1

R2	1	1	1	1	-1	-1	-1	-1
R3	1	1	-1	-1	1	1	-1	-1
R4	1	1	-1	-1	-1	-1	1	1
R5	2	-2	0	0	-2	2	0	0
R6	2	-2	0	0	2	-2	0	0

52 P4/n11 *k = 1/2,0 ; k = 0,1/2

Gko	E	C2z	C4z	C4z-	I	mz	S4z-	S4z+
R1	2	0	0	0	0	0	0	0

*k = 1/2,1/2

Gko	E	C2z	C4z	C4z-	I	mz	S4z-	S4z+
R1	2	2	0	0	0	0	0	0
R2	2	-2	0	0	0	0	0	0

53 P422 *k = 1/2,0 ; k = 0,1/2 : SEE# 19

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	C2a	C2b	C4z	C4z-
R1	1	1	1	1	1	1	1	1
R2	1	1	1	1	-1	-1	-1	-1
R3	1	1	-1	-1	1	1	-1	-1
R4	1	1	-1	-1	-1	-1	1	1
R5	2	-2	0	0	0	0	0	0

54 $P42_12$ *k = 1/2,0 ; k = 0,1/2

Gko	E	C2z	C2x	C2y	C2a	C2b	C4z	C4z-
R1	2	0	0	0	0	0	0	0

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	C2a	C2b	C4z	C4z-
R1	2	2	0	0	2	2	0	0
R2	2	2	0	0	-2	-2	0	0
R3	2	-2	0	0	0	0	0	0

55 P4mm *k = 1/2,0 ; k = 0,1/2 : SEE # 23

*k = 1/2,1/2

Gko	E	C2z	C4z	C4z-	mx	my	ma	mb
R1	1	1	1	1	1	1	1	1
R2	1	1	1	1	-1	-1	-1	-1
R3	1	1	-1	-1	1	1	-1	-1
R4	1	1	-1	-1	-1	-1	1	1
R5	2	-2	0	0	0	0	0	0

56 P4bm *k = 1/2,0 ; k = 0,1/2

Gko	E	C2z	C4z	C4z-	mx	my	ma	mb
R1	2	0	0	0	0	0	0	0

*k = 1/2,1/2

Gko	E	C2z	C4z	C4z-	mx	my	ma	mb
R1	22	0	0	0	0	0	0	
R2	2	-2	0	0	0	0	-2	2
R3	2	-2	0	0	0	0	2	2

57 P$\bar{4}$2m *k = 1/2,0 ; k = 0,1/2 : SEE# 19

*k = 1/2,1/2

Gko	E	C2z	C2x	C2y	S4z+	S4z-	ma	mb
R1	1	1	1	1	1	1	1	1
R2	1	1	1	1	-1	-1	-1	-1

R3	1	1	-1	-1	-1	-1	1	1
R4	1	1	-1	-1	1	1	-1	-1
R5	2	-2	0	0	0	0	0	0

58 P4bm *k = 1/2,0 ; k = 0,1/2

Gko	E	C2z	C4z	C4z-	mx	my	ma	mb
R1	2	0	0	0	0	0	0	0

*k = 1/2,1/2

Gko	E	C2z	C4z	C4z-	mx	my	ma	mb
R1	2	-2	0	0	0	0	2	-2
R2	2	-2	0	0	0	0	-2	2
R3	2	2	0	0	0	0	0	0

59 P$\bar{4}$m2 *k = 1/2,0 ; k = 0,1/2:SEE# 23

*k = 1/2,1/2

Gko	E	C2z	mx	my	S4z+	S4z-	C2a	C2b
R1	1	1	1	1	1	1	1	1
R2	1	1	1	1	-1	-1	-1	-1
R3	1	1	-1	-1	-1	-1	1	1
R4	1	1	-1	-1	1	1	-1	-1
R5	2	-2	0	0	0	0	0	0

60 P$\bar{4}$b2 *k = 1/2,0 ; k = 0,1/2

Gko	E	C2z	mx	my	S4z+	S4z-	C2a	C2b
R1	2	0	0	0	0	0	0	0

*k = 1/2,1/2

Gko	E	C2z	mx	my	S4z+	S4z-	C2a	C2b
R1	2	-2	0	0	0	0	2	-2

R2	2	-2	0	0	0	0	-2	2
R3	2	2	0	0	0	0	0	0

61 P4/mmm *k = 1/2,0 ; k = 0,1/2 : SEE # 37

*k = 1/2,1/2 ; P4/mmm = P422 $\bar{1}$

62 P4/nbm *k = 1/2,0 ; k = 0,1/2
{non-zero characters only}

Gko	E	C2x
R1	2	2
R2	2	-2

*k = 1/2,1/2 { non-zero characters only }

Gko	E	C2z	C2a
R1	2	2	2

63 P4/mbm *k = 1/2,0 ; k = 0,1/2
{ non-zero characters only }

Gko	E	mz
R1	2	2
R2	2	-2

*k = 1/2,1/2 { non-zero characters only }

Gko	E	C2z	C2a	C2b	I	mz
R1	2	-2	2	-2	2	-2
R2	2	-2	-2	2	2	-2
R3	2	-2	2	-2	-2	2
R4	2	-2	-2	2	-2	2
R5	2	2	0	0	2	2
R6	2	2	0	0	-2	-2

64 P4/nmm *k = 1/2,0 ; k = 0,1/2
{ non-zero characters only }

Gko	E	mx
R1	2	2
R2	2	-2

*k = 1/2,1/2 { non-zero characters only }

Gko	E	C2z	C2a	C2b	mda	mdb
R1	2	2	2	2	0	0
R2	2	2	0	0	2	-2
R3	2	-2	0	0	-2	2

65 P3 *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2 : SEE # 1

*k = -1/3,2/3 ; -1/3,-1/3

Gko	E	C3+	C3-
R1	1	1	1
R2	2	-1	-1

66 P$\bar{3}$ *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2 : SEE # 2

*k = -1/3,2/3 ; -1/3,-1/3 : SEE # 65

67 P312 *k = -1/3,2/3 ; -1/3,-1/3 : SEE # 65

*k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C22'
R1	1	1
R2	1	-1

68 P321 *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C21"
R1	1	1

R2	1	-1

*k = -1/3,2/3

Gko	E	C3+	C3-	C21"	C22"	C23"
R1	1	1	1	1	1	1
R2	1	1	1	-1	-1	-1
R3	2	-1	-1	0	0	0

69 P3m1 *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	mv2
R1	1	1
R2	1	-1

*k = -1/3,2/3 ; -1/3,-1/3 : SEE # 65

70 P31m *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	md2
R1	1	1
R2	1	-1

*k = -1/3,2/3

Gko	E	C3+	C3-	md1	md2	md3
R1	1	1	1	1	1	1
R2	1	1	1	-1	-1	-1
R3	2	-1	-1	0	0	0

71 P$\bar{3}$12/m *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C22'	I	md2
R1	1	1	1	1
R3	1	-1	1	-1
R2	1	1	-1	-1
R4	1	-1	-1	1

*k = -1/3,2/3 ; -1/3,-1/3

Gko	E	C3+	C3-	md1	md2	md3
R1	1	1	1	1	1	1
R2	1	1	1	-1	-1	-1
R3	2	-1	-1	0	0	0

72 P$\bar{3}$2/m1 *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C22'	'I	mv2
R1	1	1	1	1
R3	1	-1	1	-1
R2	1	1	-1	-1
R4	1	-1	-1	1

*k = -1/3,2/3 ; -1/3,-1/3

Gko	E	C3+	C3-	C21'	C22'	C23'
R1	1	1	1	1	1	1
R2	1	1	1	-1	-1	-1
R3	2	-1	-1	0	0	0

73 P6 *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2 : SEE # 3

*k = -1/3,2/3 ; -1/3,-1/3 : SEE # 65

74 P$\bar{6}$ *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2 : SEE # 4

*k = -1/3,2/3 ; -1/3,-1/3

Gko	E	C3+	C3-	S3-	mz	S3+
R1	1	1	1	1	1	1
R2	1	1	1	-1	-1	-1
R3	2	-1	-1	-1	2	-1
R4	2	-1	-1	1	-2	1

75 P6/m *k = 1/2,0;0,-1/2;1/2,1/2 - see #6

*k = -1/3,2/3 ; -1/3,-1/3 : SEE # 74

76 P622 *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C2z	C22'	C22'
R1	1	1	1	1
R2	1	-1	-1	1
R3	1	1	-1	-1
R4	1	-1	1	-1

*k = -1/3,2/3 ; -1/3,-1/3 : SEE # 68

77 P6mm *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C2z	md2	mv2
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	1	-1
R4	1	-1	-1	1

*k = -1/3,2/3 ; -1/3,-1/3 : SEE # 70

78 P6m2 *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C22'	mz	mv2
R1	1	1	1	1
R2	1	-1	1	-1
R3	1	-1	-1	1
R4	1	1	-1	-1

pi = 3.14159 ; w = exp(-2*pi*1/3)

*k = -1/3,2/3 ; -1/3,-1/3

Gko

R1	1	1	1	1	1	1
R2	1	1	1	-1	-1	-1
R3	1	w	w*	w*	1	w
R4	1	w	w*	-w*	-1	-w

R5	1	w*	w	w	1	w*
R6	1	w*	w	-w	-1	-w*

79 P$\bar{6}$2m *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C22"	mz	md2
R1	1	1	1	1
R2	1	1	-1	-1
R3	1	-1	-1	1
R4	1	-1	1	-1

*k = -1/3,2/3

Gko	E	C3+	C3-	C21"	C22"	C23"	mz	S3-	S3+	md1	md2	md3
R1	1	1	1	1	1	1	1	1	1	1	1	1
R2	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
R3	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
R4	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
R5	2	-1	-1	0	0	0	-2	1	1	1	1	1
R6	2	-1	-1	0	0	0	2	-1	-1	1	1	1

80 P6/mmm *k = 1/2,0 ; 0,-1/2 ; -1/2,1/2

Gko	E	C2z	C22'	C22"	I	mz	md2	mv2
R1	1	1	1	1	1	1	1	1
R2	1	1	-1	-1	1	1	-1	-1
R3	1	-1	1	-1	1	-1	1	-1
R4	1	-1	-1	1	1	-1	-1	1
R5	1	1	1	1	-1	-1	-1	-1
R6	1	1	-1	-1	-1	-1	1	1
R7	1	-1	1	-1	-1	1	-1	1
R8	1	-1	-1	1	-1	1	1	-1

*k = - 1/3,2/3 ; -1/3,-1/3

P6/mmm = P622 x $\bar{1}$

APPENDIX III

Subgroups of the 80 Diperiodic Groups

#	GROUP Go	Z - Subgroup	K - Subgroup
1	P1	P1	P1
2	$P\bar{1}$	P1	$P\bar{1}$
3	P211	P1	P211
4	Pm11	P1	Pm11,Pa11,Pb11
5	Pb11	P1	Pb11
6	P2/m11	Pm11,P211	P2/m11,P2/a11,P2/b11
7	P2/b11	Pb11,P211	P2/b11
8	P112	P1	P112,C112,$P112_1$
9	$P112_1$	P1	$P112_1$
10	C112	P1	C112,P112,$P112_1$
11	P11m	P1	P11m,C11m,P11a
12	P11a	P1	P11a
13	C11m	P1	C11m,P11m,P11a
14	P112/m	P11m,P112 $P\bar{1}$,P1	P112/m,C112/m $P112_1/a$,$P112_1/m$ P112/a
15	$P112_1/m$	P11m,$P112_1$ $P\bar{1}$,P1	$P112_1/m$,$P112_1/a$
16	C112/m	C11m,C112 $P\bar{1}$,P1	C112/m,P112/m $P112_1/a$,$P112_1/m$ P112/a
17	P112/a	P11a,P112 $P\bar{1}$,P1	P112/a,$P112_1/a$
18	$P112_1/a$	P11a, $P\bar{1}$,P1	$P112_1/a$
19	P222	P112,P211,P1	P222,$P222_1$ $P22_12_1$,$P22_12$ C222
20	$P222_1$	$P112_1$,P211,P1	$P222_1$,$P22_12_1$

21	$P22_12_1$	$P112_1$,P211,P1 $P12_11$	$P22_12_1$
22	C222	C112,P211,P1	C222,P222,$P222_1$ $P22_12_1$,$P22_12$
23	P2mm	P11m,P1m1,P211 P1,	P2mm,C2mm,P2ma P2ba
24	Pmm2	P112,P1m1,Pm11 P1	Pmm2,Cmm2,Pnb2 Cam2,Pam2,$Pab2_1$ Pbb2,$Pnm2_1$,$Pbm2_1$ $Pmb2_1$
25	$Pmb2_1$	P1b1,$P112_1$,Pm11 P1	$Pmb2_1$,$Pab2_1$
26	$Pbm2_1$	$P112_1$,Pm11,P1m1 Pb11,P1	$Pbm2_1$,$Pnm2_1$
27	Pbb2	P112,P1b1,Pb11 P1	Pbb2,Pnb2
28	P2ma	P1m1,P11a,P211 P1	P2ma,P2ba
29	Pam2	Pa11,P1m1,P112 P1	Pam2,Pnb2,$Pab2_1$ $Pnm2_1$
30	$Pab2_1$	Pa11,P1b1,$P112_1$ P1	$Pab2_1$
31	Pnb2	Pb11,P1b1,P112 P1	Pnb2
32	$Pnm2_1$	Pb11,P1m1,$P112_1$ P1	$Pnm2_1$
33	P2ba	P1b1,P11a,P211 P1	P2ba
34	C2mm	C11m,C1m1,P211 P1	C2mm,P2mm,P2ma P2ba
35	Cmm2	C1m1,C112,Pm11 P1	Cmm2,Cam2,Pam2 Pnb2,$Pab2_1$,Pbb2 $Pnm2_1$,$Pbm2_1$,$Pbm2_1$ Pmb2,Pmm2
36	Cam2	C1m1,C112,Pb11 P1	Cam2,Pmb2,$Pab2_1$ $Pnm2_1$,Pam2
37	Pmmm	Pmm2,P2mmm,P222 P112/m,P121/m,P1m1	Pmmm,Cmmm,Camm Pnba,Paba,Pabm

		P11m,P112,P121 P2/m11,Pm11,P211 $P\bar{1}$,P1	Pnma,Pama,Pmba Pnmm,Pamm,Pmma
38	Pama	Pbb2,Pam2,P2ma P222,P112/m,$P112_1/a$ Paba,P11a,P1m1, P112,P2/b11,Pb11,$P\bar{1}$ P1	Pama,Pnba,Pnma
39	Pnba	Pnb2,P2ba,P222 P112/a,P1b1,P11a P112,P2/b11,Pb11 P211,$P\bar{1}$,P1	Pnba
40	Pmma	$Pmb2_1$,Pmm2,P2ma $P22_12$,P112/a,$P112_1/m$ Pmba,P2/m11,P1m1 P11a,Pm11,P211,$P\bar{1}$,P1	Pmma,Paba,Pabm

#	GROUP Go	Z - Subgroup	K - Subgroup
41	Pamm	$Pam2, Pbm2_1, P2mm$ $P22_12, P112_1/m$ $P112/m, P11m, P112_1$ $P112, P2/b11, Pb11$ $P211, P\bar{1}, P1$	Pamm,Pnmm,Pabm Pnma
42	Pnma	$Pnb2, Pnm2_1, P2ma$ $P22_12, P112_1/a, P112/m$ $P11a, P1m1, P112_1$ $P112, P2/b11, Pb11$ $P\bar{1}, P1$	Pnma
43	Paba	$Pab2_1, Pbb2, P2ba$ $P22_12, P112_1/a, P112/a$ $P11a, P112_1, P112$ $P1b1, P2/b11, Pb11$ $P211, P\bar{1}, P1$	Paba
44	Pmba	$Pmb2_1, P2ba, P22_12_1$ $P112_1/a, P11a, P1b1$ $P112_1, P2/m11, Pm11$ $P211, P\bar{1}, P1$	Pmba
45	Pabm	$Pab2_1, Pbm2_1, P2ma$ $P22_12_1, P112_1/a, P112_1/m$ $P1b1, P11m, P112_1$ $P2/b11, Pb11, P211$ $P\bar{1}, P1$	Pabm
46	Pnmm	$Pnm2_1, P2mm, P22_12_1$ $P112_1/m, P1m1, P11m$ $P112_1, P2/a11, Pa11$ $P211, P\bar{1}, P1$	Pnmm
47	Cmmm	Cmm2,C2mm,C222 C112/m,C11m,C1m1 C112,P2/m11,Pm11 C121,P211,$P\bar{1}$,P1	Cmmm,Pmmm,Camm Pnba,Paba,Pabm Pnma,Pama,Pmba Pnmm,Pamm,Pmma
48	Camm	Cam2,C2mm,C222 C112/m,C1m1,C11m C112,P2/b11,Pb11 P211,$P\bar{1}$,P1	Camm,Pnba,Paba Pabm,Pnma,Pama Pnmm,Pamm
49	P4	P211,P1	P4
50	$P\bar{4}$	P211,P1	$P\bar{4}$

51	P4/m	$P\bar{4}$,P4,P2/m11 Pm11,P211,$P\bar{1}$,P1	P4/m,P4/n
52	P4/n	$P\bar{4}$,P4,P2/b11 Pb11,P211,$P\bar{1}$,P1	P4/n
53	P422	P4,C222,P222 P112,P121,C121 C112,P211,P1	P422,$P42_12$
54	$P42_12$	P4,C222,$P22_12_1$ $P12_11$,c112,$P2_111$ P1	$P42_12$
55	P4mm	P4,C2mm,P2mm C11m,C1m1,P1m1 P11m,P211,P1	P4mm,P4bm
56	P4bm	P4,C2mm,P2ba C11m,P1b1,P211 P1	P4bm
57	$P\bar{4}2m$	$P\bar{4}$,C2mm,P222 C11m,P121,P211 P1	$P\bar{4}2m$,$P\bar{4}m2$,$P\bar{4}b2$ $P\bar{4}2_1m$
58	$P\bar{4}2_1m$	$P\bar{4}$,C2mm,$P22_12_1$ C11m,$P12_11$,$P2_111$ P1	$P\bar{4}2_1m$
59	$P\bar{4}m2$	$P\bar{4}$,P2mm,C222 P1m1,C112,P211 P1	$P\bar{4}m2$,$P\bar{4}2m$,$P\bar{4}b2$ $P\bar{4}2_1m$
60	$P\bar{4}b2$	$P\bar{4}$,P2ba,C222 P1b1,P112,P211 P1	$P\bar{4}b2$
61	P4/mmm	$P\bar{4}2m$,$P\bar{4}m2$,P4mm P422,P4/m,$P\bar{4}$ P4,Cmmm,Pmmm Cmm2,Cm2m,Pmm2 Pm2m,C2mm,P2mm C222,P222,C112/m C121/m,P112/m,P121/m C11m,C1m1,Pm11 P211,$P\bar{1}$,P1	P4/mmm,P4/nmm,P4/mbm P4/nbm
62	P4/nbm	$P\bar{4}2m$,$P\bar{4}b2$,P4bm P422,P4/n,$P\bar{4}$ P4,Camm,Pnba Cam2,Pnb2,C2mm P2ba,C222,P222 C112/m,P112/a,C11m	P4/nbm

		P1b1,C112,P112 P2/b11,Pb11,P211 $P\bar{1}$,P1	
63	P4/mbm	$P\bar{4}2_1m$,$P\bar{4}b2$,P4bm $P42_12$,P4/m,$P\bar{4}$ P4,Cmmm,Pmba Cmm2,Pam2,C2mm P2ba,C222,$P22_12_1$ $P112_1/a$,C112/m,C11m P11a,C112,$P112_1$ P2/m11,Pm11,$P2_111$ $P\bar{1}$,P1	P4/mbm,P4/nbm,P4/nmm
64	P4/nmm	$P\bar{4}m4$,$P\bar{4}2_1m$,P4mm $P42_12$,P4/n,$P\bar{4}$ P4,Camm,Pnmm Cam2,Cb2m,$Pnm2_1$ $Pn2_1m$,C2mm,P2mm C222,$P22_12_1$,C112/m C121/m,$P112_1/m$,$P12_11/m$ C11m,C1m1,P1m1,P11m C121,C112,$P112_1$,$P12_11$ P2/b11,P2/a11,Pa11 Pb11,P211,$P\bar{1}$,P1	P4/nmm
65	P3	P1	P3
66	$P\bar{3}$	P3,$P\bar{1}$,P1	$P\bar{3}$
67	P312	P3,C112,P1	P312,P321
68	P321	P3,C121,P1	P321,P312
69	P3m1	P3,C1m1,P1	P3m1,P31m
70	P31m	P3,C11m,P1	P31m,P3m1
71	$P\bar{3}1m$	P31m,P312,$P\bar{3}$ P3,C112/m,C11m C112,$P\bar{1}$,P1	$P\bar{3}1m$,$P\bar{3}m1$
72	$P\bar{3}m1$	P3m1,P321,$P\bar{3}$ P3,C12/m1,C1m1 C121,$P\bar{1}$,P1	$P\bar{3}m1$,$P\bar{3}1m$
73	P6	P3,P211,P1	P6
74	$P\bar{6}$	P3,Pm11,P1	$P\bar{6}$
75	P6/m	$P\bar{6}$,P6,$P\bar{3}$ P3,P2/m11 Pm11,P211,$P\bar{1}$ P1	P6/m

76	P622	P6,P321,P312 P3,C222,C121 C112,P211,P1	P622
77	P6mm	P6,P31m,P3m1 P3,C2mm,C1m1 C11m,P211,P1	P6mm
78	P$\bar{6}$m2	P$\bar{6}$,P3m1,P312 P3,Cm2m,C1m1 C112,Pm11,P1	P$\bar{6}$m2,P$\bar{6}$2m
79	P$\bar{6}$2m	P$\bar{6}$,P31m,P321 P3,Cmm2,C11m C121,Pm11,P1	P$\bar{6}$m2,P$\bar{6}$2m
80	P6/mmm	P$\bar{6}$2m,P$\bar{6}$m2,P6mm P622,P6/m,P$\bar{6}$ P6,P$\bar{3}$m1,P$\bar{3}$1m P31m,P3m1,P321 P312,P$\bar{3}$,P3 Cmmm,C2mm,C222 C112/m,C12/m1 C11m,C1m1,C112 C121,P2/m11,Pm11 P211,P$\bar{1}$,P1	P6/mmm

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