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GROUP THEORETICAL CLASSIFICATION OF TWO-DIMENSIONAL LATTICE VIBRATIONS

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Tables of the group theoretical classification of all possible two-dimensional lattice vibrations are presented, using the labeling of the irreducible representations of the two-dimensional space groups. As an example of their use, the group theoretical labeling of the phonon dispersion curves of methane physisorbed on graphite is given.

1. INTRODUCTION

In the study of lattice vibrations in crystals, group theory can predict the degeneracies of the normal modes and can give information on the eigenvalues of the modes[1–4]. For example, the irreducible representations of the three-dimensional space groups provide a labeling scheme for the phonon dispersion curves in three-dimensional crystals and predict the degeneracies of the normal modes. In this paper we use the irreducible representations of the two-dimensional space groups for a labeling scheme of two-dimensional phonon dispersion curves and tabulate the group theoretical labels of all possible two-dimensional lattice vibrations.

A list of the 17 two-dimensional space groups is found in the *International Tables for X-ray Crystallography*, Vol 1 [5]. Tables of the irreducible representations of the two-dimensional space groups have been given by Cracknell[6]. However, not all space groups in the latter tables are given in the same orientation as for those given in ref. 5. Consequently, we have tabulated in Appendix A the irreducible representations of the two-dimensional space groups in the orientation of the *International Tables*. In addition, to rectify ambiguities in the symbols of the irreducible representations[6], we have included in Appendix A explicit character tables of relevant point groups.

2. CLASSIFICATION OF LATTICE VIBRATIONS

The lattice vibrations of a crystal are classified by determining the irreducible representations of the symmetry group of the crystal whose basis functions are linear combinations of the components of a polar vector, the displacements, defined on the atoms of the crystal. These irreducible representations of the symmetry group G of

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the crystal are contained in the direct product of the polar vector representation D_G^{V} and the permutation representation D_G^{PERM} of the atoms of the crystal. The permutation representation characterizes how the atoms of the crystal permute under elements of the symmetry space group of the crystal. To classify all lattice vibrations of all crystals of two-dimensional space group symmetry G, one then must find all irreducible representations of G contained in the direct product $D_G^{\mathrm{PERM}} \times D_G^{\mathrm{V}}$ for every crystal whose symmetry group is one of the 17 two-dimensional space groups.

A crystal of two-dimensional space group symmetry G can be partitioned into "simple crystals"[7]. Each simple crystal consists of all atoms whose atomic positions can be obtained by applying all elements of G to any one atomic position vector $\boldsymbol{r}$ and is said to be generated by G from $\boldsymbol{r}$. A crystal can be considered as consisting of a certain number of simple crystals. No two simple crystals have atoms in common, and the elements of G permute the atoms of each simple crystal among themselves. Consequently, to classify all lattice vibrations of all crystals of two-dimensional space group symmetry G, it is sufficient to determine the irreducible representations of G contained in the direct product $D_G^{\mathrm{PERM}} \times D_G^{\mathrm{V}}$ for each simple crystal whose symmetry group is one of the 17 two-dimensional space groups.

A tabulation of all simple crystals generated by two-dimensional space groups G is given in ref. 5. Each set of equivalent positions found under a two-dimensional space group G corresponds to atomic positions of a single simple crystal generated by G. We choose the first position of each set of equivalent positions as the position vector $\boldsymbol{r}$ from which the simple crystal is generated by G. Each simple crystal will be denoted by the Wyckoff notation of the corresponding set of equivalent positions.

To determine the irreducible representations contained in the direct product $D_G^{\mathrm{PERM}} \times D_G^{\mathrm{V}}$ we used the computational method developed by Litvin[8]. In Table I the irreducible representations contained in this direct product are given for each simple crystal whose symmetry group is one of the 17 two-dimensional space groups. The irreducible representations tabulated in Table I provide a labeling scheme for all possible two-dimensional lattice vibrations.

3. PHYSISORBED METHANE

We consider the two-dimensional phonon dispersion curves of physisorbed methane[9]. We assume that the molecules are rigid tripods with their molecular centers on a two-dimensional triangular lattice with one C—H bond perpendicular to the two-dimensional lattice and the remaining three C—H bonds with projections pointing to nearest-neighbor molecules[10,11]. The molecular centers of these rigid tripod methane molecules can be considered to be a single simple crystal generated by the two-dimensional space group $G = p6m$ from $\boldsymbol{r} = (0,0)$. This is the simple crystal (row a) of the two-dimensional space group $p6m$.

From Table I, subtable 17, row a, the group theoretical labeling of the normal modes is found in terms of the irreducible representations of the two-dimensional space group $p6m$:

$$\Gamma_1, \Gamma_5; 2\Sigma_1, \Sigma_2; 2\mathrm{T}_1, \mathrm{T}_2; \mathrm{K}_1, \mathrm{K}_3; \mathrm{M}_1, \mathrm{M}_2, \mathrm{M}_4; 2\mathrm{T}_1', \mathrm{T}_2' \quad (1)$$

At the point Γ in the Brillouin zone, for example, there are two normal modes: a

TABLE I

PHONON DECOMPOSITION[a]

Subtable 1 p1

	Γ_1	A_1	B_1	Y_1
a (x,y)	3	3	3	3

Subtable 2 p2

	Γ_1	Γ_2	A_1	A_2	B_1	B_2	Y_1	Y_2
a $(0,0)$	1	2	1	2	1	2	1	2
b $(0,\frac{1}{2})$	1	2	1	2	1	2	1	2
c $(\frac{1}{2},0)$	1	2	1	2	1	2	1	2
d $(\frac{1}{2},\frac{1}{2})$	1	2	1	2	1	2	1	2
e (x,y)	3	3	3	3	3	3	3	3

Subtable 3 pm

	Γ_1	Γ_2	Σ_1	Δ_1	Δ_2	X_1	X_2	Y_1	Y_2	S_1	S_2	C_1	D_1	D_2
a $(0,y)$	2	1	3	2	1	2	1	2	1	2	1	3	2	1
b $(\frac{1}{2},y)$	2	1	3	2	1	2	1	2	1	2	1	3	2	1
c (x,y)	3	3	6	3	3	3	3	3	3	3	3	6	3	3

Subtable 4 pg

	Γ_1	Γ_2	Σ_1	Δ_1	Δ_2	X_1	X_2	Y_1	Y_2	S_1	S_2	C_1	D_1	D_2
a (x,y)	3	3	6	3	3	3	3	3	3	3	3	6	3	3

Subtable 5 cm

	Γ_1	Γ_2	Σ_1	Δ_1	Δ_2	Y_1	Y_2	C_1	S_1
a $(0,y)$	2	1	3	2	1	2	1	3	3
b (x,y)	3	3	6	3	3	3	3	6	6

(continued)

TABLE I *(continued)*

Subtable 6 pmm

	Γ_1	Γ_2	Γ_3	Γ_4	Σ_1	Σ_2	Δ_1	Δ_2	X_1	X_2	X_3	X_4	Y_1	Y_2	Y_3	Y_4	S_1	S_2	S_3	S_4	C_1	C_2	D_1	D_2
a (0,0)	1	1	0	1	2	1	2	1	1	1	0	1	1	1	0	1	1	1	0	1	2	1	2	1
b $(0,\frac{1}{2})$	1	1	0	1	2	1	2	1	1	1	0	1	1	1	0	1	1	1	0	1	2	1	2	1
c $(\frac{1}{2},0)$	1	1	0	1	2	1	2	1	1	1	0	1	1	1	0	1	1	1	0	1	2	1	2	1
d $(\frac{1}{2},\frac{1}{2})$	1	1	0	1	2	1	2	1	1	1	0	1	1	1	0	1	1	1	0	1	2	1	2	1
e $(x,0)$	2	1	1	2	4	2	3	3	2	1	1	2	2	1	1	2	2	1	1	2	4	2	4	2
f $(x,\frac{1}{2})$	2	1	1	2	4	2	3	3	2	1	1	2	2	1	1	2	2	1	1	2	4	2	4	2
g $(0,y)$	2	2	1	1	3	3	4	2	2	2	1	1	2	2	1	1	2	2	1	1	3	3	3	3
h $(\frac{1}{2},y)$	2	2	1	1	3	3	4	2	2	2	1	1	2	2	1	1	2	2	1	1	3	3	3	3
i (x,y)	3	3	3	3	6	6	6	6	3	3	3	3	3	3	3	3	3	3	3	3	6	6	6	6

Subtable 7 pmg

	Γ_1	Γ_2	Γ_3	Γ_4	Σ_1	Σ_2	Δ_1	Δ_2	X_1	Y_1	Y_2	Y_3	Y_4	S_1	C_1	C_2	D_1	D_2
a (0,0)	1	2	1	2	3	3	3	3	3	1	2	1	2	3	3	3	3	3
b $(0,\frac{1}{2})$	1	2	1	2	3	3	3	3	3	2	1	2	1	3	3	3	3	3
c $(\frac{1}{4},y)$	2	2	1	1	3	3	4	2	3	2	2	1	1	3	3	3	3	3
d (x,y)	3	3	3	3	6	6	6	6	6	3	3	3	3	6	6	6	6	6

Subtable 8 pgg

	Γ_1	Γ_2	Γ_3	Γ_4	Σ_1	Σ_2	Δ_1	Δ_2	X_1	Y_1	S_1	S_2	S_3	S_4	C_1	C_2	D_1	D_2
a (0,0)	1	2	1	2	3	3	3	3	3	3	1	1	2	2	3	3	3	3
b $(\frac{1}{2},0)$	1	2	1	2	3	3	3	3	3	3	2	2	1	1	3	3	3	3
c (x,y)	3	3	3	3	6	6	6	6	6	6	3	3	3	3	6	6	6	6

(continued)

TABLE I *(continued)*

Subtable 9 cmm

	Γ_1	Γ_2	Γ_3	Γ_4	Σ_1	Σ_2	Δ_1	Δ_2	Y_1	Y_2	Y_3	Y_4	C_1	C_2	S_1	S_2
a (0,0)	1	1	0	1	2	1	2	1	1	1	0	1	2	1	1	2
b $(0,\frac{1}{2})$	1	1	0	1	2	1	2	1	1	1	0	1	2	1	1	2
c $(\frac{1}{4},\frac{1}{4})$	1	2	1	2	3	3	3	3	1	2	1	2	3	3	2	4
d $(x,0)$	2	1	1	2	4	2	3	3	2	1	2	1	4	2	3	3
e $(0,y)$	2	2	1	1	3	3	4	2	2	2	1	1	3	3	3	3
f (x,y)	3	3	3	3	6	6	6	6	3	3	3	3	6	6	6	6

Subtable 10 p4

	Γ_1	Γ_2	Γ_3	Γ_4	Σ_1	Δ_1	M_1	M_2	M_3	M_4	X_1	X_2	Y_1
a (0,0)	1	0	1	1	3	3	1	0	1	1	1	2	3
b $(\frac{1}{2},\frac{1}{2})$	1	0	1	1	3	3	1	0	1	1	1	2	3
c $(\frac{1}{2},0)$	1	1	2	2	6	6	1	1	2	2	2	4	6
d (x,y)	3	3	3	3	12	12	3	3	3	3	6	6	12

Subtable 11 p4m

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Σ_1	Σ_2	Δ_1	Δ_2	M_1	M_2	M_3	M_4	M_5	X_1	X_2	X_3	X_4	Y_1	Y_2
a (0,0)	1	0	0	0	1	2	1	2	1	1	0	0	0	1	1	1	0	1	2	1
b $(\frac{1}{2},\frac{1}{2})$	1	0	0	0	1	2	1	2	1	1	0	0	0	1	1	1	0	1	2	1
c $(\frac{1}{2},0)$	1	0	1	0	2	3	3	4	2	1	0	1	0	2	2	2	0	2	4	2
d $(x,0)$	2	1	2	1	3	6	6	7	5	2	1	2	1	3	4	3	2	3	7	5
e $(x,\frac{1}{2})$	2	1	2	1	3	6	6	7	5	2	1	2	1	3	4	3	2	3	7	5
f (x,x)	2	1	1	2	3	7	5	6	6	2	1	1	2	3	3	3	3	3	6	6
g (x,y)	3	3	3	3	6	12	12	12	12	3	3	3	3	6	6	6	6	6	12	12

(continued)

TABLE I *(continued)*

Subtable 12 p4g

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Σ_1	Σ_2	Δ_1	Δ_2	M_1	M_2	M_3	M_4	M_5	X_1	Y_1	Y_2
a (0,0)	1	1	0	0	2	3	3	3	3	1	1	1	1	1	3	3	3
b ($\frac{1}{2}$,0)	1	0	0	1	2	4	2	3	3	2	1	0	0	1	3	3	3
c ($x,\frac{1}{2}+x$)	2	1	1	2	3	7	5	6	6	3	2	1	1	2	6	6	6
d (x,y)	3	3	3	3	6	12	12	12	12	6	3	3	3	3	12	12	12

Subtable 13 p3

	Γ_1	Γ_2	Γ_3	Σ_1	T_1	K_1	K_2	K_3	M_1	T_1'
a (0,0)	1	1	1	3	3	1	1	1	3	3
b ($\frac{1}{3},\frac{2}{3}$)	1	1	1	3	3	1	1	1	3	3
c ($\frac{2}{3},\frac{1}{3}$)	1	1	1	3	3	1	1	1	3	3
d (x,y)	3	3	3	9	9	3	3	3	9	9

Subtable 14 p3m1

	Γ_1	Γ_2	Γ_3	Σ_1	Σ_2	T	K_1	K_2	K_3	M_1	M_2	T_1'
a (0,0)	1	0	1	2	1	3	1	1	1	2	1	3
b ($\frac{1}{3},\frac{2}{3}$)	1	0	1	2	1	3	1	1	1	2	1	3
c ($\frac{2}{3},\frac{1}{3}$)	1	0	1	2	1	3	1	1	1	2	1	3
d ($x,\bar{x}$)	2	1	3	5	4	9	3	3	3	5	4	9
e (x,y)	3	3	6	9	9	18	6	6	6	9	9	18

Subtable 15 p31m

	Γ_1	Γ_2	Γ_3	Σ_1	T_1	T_2	K_1	K_2	K_3	M_1	M_2	T_1'	T_2'
a (0,0)	1	0	1	3	2	1	1	0	1	2	1	2	1
b ($\frac{1}{3},\frac{2}{3}$)	1	1	2	6	3	3	1	1	2	3	3	3	3
c (x,0)	2	2	4	9	5	4	2	2	4	5	4	5	4
d (x,y)	3	3	6	18	9	9	3	3	6	9	9	9	9

(continued)

TABLE I *(continued)*

Subtable 16 p6

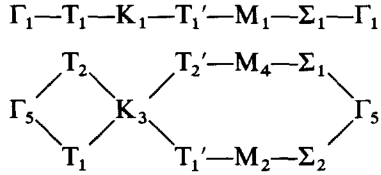
		Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Σ_1	T_1	K_1	K_2	K_3	M_1	M_2	T_1'
a	(0,0)	1	0	0	0	1	1	3	3	1	1	1	1	2	3
b	$(\frac{1}{3},\frac{2}{3})$	1	1	1	1	1	1	6	6	2	2	2	3	3	6
c	$(\frac{1}{2},0)$	1	2	1	1	2	2	9	9	3	3	3	3	6	9
d	(x,y)	3	3	3	3	3	3	18	18	6	6	6	9	9	18

Subtable 17 p6m

		Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Σ_1	Σ_2	T_1	T_2	K_1	K_2	K_3	M_1	M_2	M_3	M_4	T_1'	T_2'
a	(0,0)	1	0	0	0	1	0	2	1	2	1	1	0	1	1	1	0	1	2	1
b	$(\frac{1}{3},\frac{2}{3})$	1	0	0	1	1	1	4	2	3	3	1	1	2	1	1	0	1	3	3
c	$(\frac{1}{2},0)$	1	0	1	1	2	1	5	4	5	4	2	1	3	2	3	1	3	5	4
d	$(x,0)$	2	1	1	2	3	3	9	9	10	8	4	2	6	5	5	4	4	10	8
e	$(x,\bar{x})$	2	1	2	1	3	3	10	8	9	9	3	3	6	5	4	4	5	9	9
f	(x,y)	3	3	3	3	6	6	18	18	18	18	6	6	12	9	9	9	9	18	18

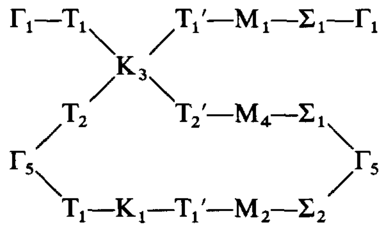
[a] The first column of each subtable corresponding to a two-dimensional space group G gives the Wyckoff notation[5] of the simple crystal generated by G from the atomic position $\boldsymbol{r}$ given in the second column. For each simple crystal the number of lattice vibrational modes labeled by a specific irreducible representation is given at the intersection of the column under the irreducible representation and row alongside the simple crystal.

singly degenerate Γ_1 and a doubly degenerate Γ_5. From this information and the compatibility relations of Table I, subtable 17, a schematic representation of a possible labeling scheme of the phonon dispersion curves is given by



(2)

A second possible labeling scheme is



(3)

The first corresponds to the labeling of the calculated phonon dispersion curves for monolayer CH_4 in the self-consistent harmonic and harmonic approximations and for monolayer CD_4 in the harmonic approximation[9]. The second corresponds to the calculated phonon dispersion curve for monolayer CD_4 in the self-consistent harmonic approximation[9].

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APPENDIX A

Irreducible representations of the two-dimensional space groups

The generating translations of the five two-dimensional Bravais lattices and corresponding reciprocal lattices are given in Table AI. The choice and notation of the points of high symmetry in the Brillouin zone follow those of Zak *et al.*[A1] The two-dimensional Brillouin zones have been taken as the $z = 0$ planes of three-dimensional Brillouin zones found in ref. A1: the $z = 0$ plane of the three-dimensional monoclinic P Brillouin zone for the two-dimensional oblique p Brillouin zone, and those of the orthorhombic P and C, square P and hexagonal P zones for the rectangular p and c, square p and hexagonal p zones respectively. The notations and conventions used in this appendix are those of ref. A1.

In Table AII, for each of the 17 two-dimensional space groups, we list the points of high symmetry of the Brillouin zone, their coordinates and point group elements, and a symbol from which the irreducible representations can be determined. For all

TABLE AI
BRAVAIS LATTICES[a]

	Direct lattice		*Reciprocal lattice*	
	t_1	t_2	K_1	K_2
Oblique	$(d,0)$	(a,b)	$\left(\frac{2\pi}{d}, -\frac{2\pi a}{bd}\right)$	$\left(0,\frac{2\pi}{b}\right)$
Rectangular p	$(a,0)$	$(0,b)$	$\left(\frac{2\pi}{a},0\right)$	$\left(0,\frac{2\pi}{b}\right)$
Rectangular c	$\left(\frac{a}{2},\frac{b}{2}\right)$	$\left(\frac{a}{2},-\frac{b}{2}\right)$	$\left(\frac{2\pi}{a},\frac{2\pi}{b}\right)$	$\left(\frac{2\pi}{a},-\frac{2\pi}{b}\right)$
Square	$(a,0)$	$(0,a)$	$\left(\frac{2\pi}{a},0\right)$	$\left(0,\frac{2\pi}{a}\right)$
Hexagonal	$(a,0)$	$(0,a)$	$\left(\frac{8\pi}{3a},\frac{4\pi}{3a}\right)$	$\left(\frac{4\pi}{3a},\frac{8\pi}{3a}\right)$

[a] The generators of the five two-dimensional Bravais lattices and corresponding reciprocal lattices are given. Cartesian coordinates are used except for the hexagonal p where a hexagonal coordinate system is used.

TABLE AII
SYMMETRY POINTS[a]

Subtable 1	$p1$	*Oblique*	
Γ	$(0,0)$	$(1\|0,0)$	1
A	$\left(\frac{\pi}{d}, -\frac{\pi a}{bd}\right)$	$(1\|0,0)$	1
B	$\left(\frac{\pi}{d},\frac{\pi}{b}-\frac{\pi a}{bd}\right)$	$(1\|0,0)$	1
Y	$\left(0,\frac{\pi}{b}\right)$	$(1\|0,0)$	1
Subtable 2	$p2$	*Oblique*	
Γ	$(0,0)$	$(1\|0,0), (2_z\|0,0)$	2
A	$\left(\frac{\pi}{d}, -\frac{\pi a}{bd}\right)$	$(1\|0,0), (2_z\|0,0)$	2
B	$\left(\frac{\pi}{d},\frac{\pi}{b}-\frac{\pi a}{bd}\right)$	$(1\|0,0), (2_z\|0,0)$	2
Y	$\left(0,\frac{\pi}{b}\right)$	$(1\|0,0), (2_z\|0,0)$	2

(continued)

TABLE AII *(continued)*

Subtable 3	*pm*	*Rectangular p*	
Γ	(0,0)	$(1\|0,0), (\sigma_x\|0,0)$	*m*
Σ	$(k_x,0)$	$(1\|0,0)$	1
Δ	$(0,k_y)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
X	$\left(\frac{\pi}{a},0\right)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
Y	$\left(0,\frac{\pi}{b}\right)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
S	$\left(\frac{\pi}{a},\frac{\pi}{b}\right)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
C	$\left(k_x,\frac{\pi}{b}\right)$	$(1\|0,0)$	1
D	$\left(\frac{\pi}{a},k_y\right)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
Subtable 4	*pg*	*Rectangular p*	
Γ	(0,0)	$(1\|0,0), (\sigma_x\|0,\frac{1}{2})$	*m*
Σ	$(k_x,0)$	$(1\|0,0)$	1
Δ	$(0,k_y)$	$(1\|0,0), (\sigma_x\|0,\frac{1}{2})$	*m*
X	$\left(\frac{\pi}{a},0\right)$	$(1\|0,0), (\sigma_x\|0,\frac{1}{2})$	IR 4.X
Y	$\left(0,\frac{\pi}{b}\right)$	$(1\|0,0), (\sigma_x\|0,\frac{1}{2})$	IR 4.Y
S	$\left(\frac{\pi}{a},\frac{\pi}{b}\right)$	$(1\|0,0), (\sigma_x\|0,\frac{1}{2})$	IR 4.S
C	$\left(k_x,\frac{\pi}{b}\right)$	$(1\|0,0)$	1
D	$\left(\frac{\pi}{a},k_y\right)$	$(1\|0,0), (\sigma_x\|0,\frac{1}{2})$	IR 4.D
Subtable 5	*cm*	*Rectangular c*	
Γ	(0,0)	$(1\|0,0), (\sigma_x\|0,0)$	*m*
Σ	$(k_x,0)$	$(1\|0,0)$	1
Δ	$(0,k_y)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
Y	$\left(0,\frac{2\pi}{b}\right)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
C	$\left(k_x,\frac{2\pi}{b}\right)$	$(1\|0,0)$	1
S	$\left(\frac{\pi}{a},\frac{\pi}{b}\right)$	$(1\|0,0)$	1
Subtable 6	*pmm*	*Rectangular p*	
Γ	(0,0)	$(1\|0,0), (2_z\|0,0), (\sigma_x\|0,0), (\sigma_y\|0,0)$	2*mm*
Σ	$(k_x,0)$	$(1\|0,0), (\sigma_y\|0,0)$	*m*
Δ	$(0,k_y)$	$(1\|0,0), (\sigma_x\|0,0)$	*m*
X	$\left(\frac{\pi}{a},0\right)$	as Γ	2*mm*
Y	$\left(0,\frac{\pi}{b}\right)$	as Γ	2*mm*

(continued)

TABLE AII *(continued)*

S	$\left(\frac{\pi}{a},\frac{\pi}{b}\right)$	as Γ	2*mm*
C	$\left(k_x,\frac{\pi}{b}\right)$	$(1\|0,0),(\sigma_y\|0,0)$	*m*
D	$\left(\frac{\pi}{a},k_y\right)$	$(1\|0,0),(\sigma_x\|0,0)$	*m*
Subtable 7	*pmg*	*Rectangular p*	
Γ	$(0,0)$	$(1\|0,0),(2_z\|0,0),(\sigma_x\|\frac{1}{2},0),(\sigma_y\|\frac{1}{2},0)$	2*mm*
Σ	$(k_x,0)$	$(1\|0,0),(\sigma_y\|\frac{1}{2},0)$	*m*
Δ	$(0,k_y)$	$(1\|0,0),(\sigma_x\|\frac{1}{2},0)$	*m*
X	$\left(\frac{\pi}{a},0\right)$	as Γ	IR 7.X
Y	$\left(0,\frac{\pi}{b}\right)$	as Γ	IR 7.Y
S	$\left(\frac{\pi}{a},\frac{\pi}{b}\right)$	as Γ	IR 7.S
C	$\left(k_x,\frac{\pi}{b}\right)$	$(1\|0,0),(\sigma_y\|\frac{1}{2},0)$	IR 7.C
D	$\left(\frac{\pi}{a},k_y\right)$	$(1\|0,0),(\sigma_x\|\frac{1}{2},0)$	IR 7.D
Subtable 8	*pgg*	*Rectangular p*	
Γ	$(0,0)$	$(1\|0,0),(2_z\|0,0),(\sigma_x\|\frac{1}{2},\frac{1}{2}),(\sigma_y\|\frac{1}{2},\frac{1}{2})$	2*mm*
Σ	$(k_x,0)$	$(1\|0,0),(\sigma_y\|\frac{1}{2},\frac{1}{2})$	*m*
Δ	$(0,k_y)$	$(1\|0,0),(\sigma_x\|\frac{1}{2},\frac{1}{2})$	*m*
X	$\left(\frac{\pi}{a},0\right)$	as Γ	IR 8.X
Y	$\left(0,\frac{\pi}{b}\right)$	as Γ	IR 8.Y
S	$\left(\frac{\pi}{a},\frac{\pi}{b}\right)$	as Γ	IR 8.S
C	$\left(k_x,\frac{\pi}{b}\right)$	$(1\|0,0),(\sigma_y\|\frac{1}{2},\frac{1}{2})$	IR 8.C
D	$\left(\frac{\pi}{a},k_y\right)$	$(1\|0,0),(\sigma_x\|\frac{1}{2},\frac{1}{2})$	IR 8.D
Subtable 9	*cmm*	*Rectangular c*	
Γ	$(0,0)$	$(1\|0,0),(2_z\|0,0),(\sigma_x\|0,0),(\sigma_y\|0,0)$	2*mm*
Σ	$(k_x,0)$	$(1\|0,0),(\sigma_y\|0,0)$	*m*
Δ	$(0,k_y)$	$(1\|0,0),(\sigma_x\|0,0)$	*m*
Y	$\left(0,\frac{2\pi}{b}\right)$	as Γ	2*mm*
C	$\left(k_x,\frac{2\pi}{b}\right)$	$(1\|0,0),(\sigma_y\|0,0)$	*m*
S	$\left(\frac{\pi}{a},\frac{\pi}{b}\right)$	$(1\|0,0),(2_z\|0,0)$	2

(continued)

TABLE AII *(continued)*

Subtable 10 p4		*Square*	
Γ	(0,0)	$(1\|0,0), (4_z\|0,0), (2_z\|0,0), (4_z^{-1}\|0,0)$	4
Σ	(k_x,k_x)	$(1\|0,0)$	1
Δ	$(0,k_y)$	$(1\|0,0)$	1
M	$\left(\frac{\pi}{a},\frac{\pi}{a}\right)$	as Γ	4
X	$\left(0,\frac{\pi}{a}\right)$	$(1\|0,0), (2_z\|0,0)$	2
Y	$\left(k_x,\frac{\pi}{a}\right)$	$(1\|0,0)$	1

Subtable 11 p4m		*Square*	
Γ	(0,0)	$(1\|0,0), (4_z\|0,0), (2_z\|0,0), (4_z^{-1}\|0,0), (\sigma_x\|0,0), (\sigma_y\|0,0), (\sigma_{xy}\|0,0), (\sigma_{\bar{x}y}\|0,0)$	4mm
Σ	(k_x,k_x)	$(1\|0,0), (\sigma_{\bar{x}y}\|0,0)$	m
Δ	$(0,k_y)$	$(1\|0,0), (\sigma_x\|0,0)$	m
M	$\left(\frac{\pi}{a},\frac{\pi}{a}\right)$	as Γ	4mm
X	$\left(0,\frac{\pi}{a}\right)$	$(1\|0,0), (2_z\|0,0), (\sigma_x\|0,0), (\sigma_y\|0,0)$	2mm
Y	$\left(k_x,\frac{\pi}{a}\right)$	$(1\|0,0), (\sigma_y\|0,0)$	m

Subtable 12 p4g		*Square*	
Γ	(0,0)	$(1\|0,0), (4_z\|0,0), (2_z\|0,0), (4_z^{-1}\|0,0), (\sigma_x\|\frac{1}{2},\frac{1}{2}), (\sigma_y\|\frac{1}{2},\frac{1}{2}), (\sigma_{xy}\|\frac{1}{2},\frac{1}{2}), (\sigma_{\bar{x}y}\|\frac{1}{2},\frac{1}{2})$	4mm
Σ	(k_x,k_x)	$(1\|0,0), (\sigma_{\bar{x}y}\|\frac{1}{2},\frac{1}{2})$	m
Δ	$(0,k_y)$	$(1\|0,0), (\sigma_x\|\frac{1}{2},\frac{1}{2})$	m
M	$\left(\frac{\pi}{a},\frac{\pi}{a}\right)$	as Γ	IR 12.M
X	$\left(0,\frac{\pi}{a}\right)$	$(1\|0,0), (2_z\|0,0), (\sigma_x\|\frac{1}{2},\frac{1}{2}), (\sigma_y\|\frac{1}{2},\frac{1}{2})$	IR 12.X
Y	$\left(k_x,\frac{\pi}{a}\right)$	$(1\|0,0), (\sigma_y\|\frac{1}{2},\frac{1}{2})$	IR 12.Y

Subtable 13 p3		*Hexagonal*	
Γ	(0,0)	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0)$	3
Σ	$(k_x,\frac{1}{2}k_x)$	$(1\|0,0)$	1
T	$(k_x,0)$	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0)$	3
K	$\left(\frac{4\pi}{3a},0\right)$	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0)$	3
M	$\left(\frac{4\pi}{3a},\frac{2\pi}{3a}\right)$	$(1\|0,0)$	1
T′	$\left(\frac{4\pi}{3a},k_y\right)$	$(1\|0,0)$	1

(continued)

TABLE AII *(continued)*

Subtable 14 *p3m1*		*Hexagonal*	
Γ	(0,0)	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0), (\sigma_x\|0,0), (\sigma_y\|0,0), (\sigma_{xy}\|0,0)$	3*m*
Σ	$(k_x, \frac{1}{2}k_x)$	$(1\|0,0), (\sigma_y\|0,0)$	*m*
T	$(k_x, 0)$	$(1\|0,0)$	1
K	$\left(\frac{4\pi}{3a}, 0\right)$	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0)$	3
M	$\left(\frac{4\pi}{3a}, \frac{2\pi}{3a}\right)$	$(1\|0,0), (\sigma_y\|0,0)$	*m*
T′	$\left(\frac{4\pi}{3a}, k_y\right)$	$(1\|0,0)$	1
Subtable 15 *p31m*		*Hexagonal*	
Γ	(0,0)	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0), (\sigma_1\|0,0), (\sigma_2\|0,0), (\sigma_3\|0,0)$	3*m*
Σ	$(k_x, \frac{1}{2}k_x)$	$(1\|0,0)$	1
T	$(k_x, 0)$	$(1\|0,0), (\sigma_2\|0,0)$	*m*
K	$\left(\frac{4\pi}{3a}, 0\right)$	as Γ	3*m*
M	$\left(\frac{4\pi}{3a}, \frac{2\pi}{3a}\right)$	$(1\|0,0), (\sigma_1\|0,0)$	*m*
T′	$\left(\frac{4\pi}{3a}, k_y\right)$	$(1\|0,0), (\sigma_1\|0,0)$	*m*
Subtable 16 *p6*		*Hexagonal*	
Γ	(0,0)	$(1\|0,0), (6_z\|0,0), (3_z\|0,0), (2_z\|0,0), (3_z^{-1}\|0,0), (6_z^{-1}\|0,0)$	6
Σ	$(k_x, \frac{1}{2}k_x)$	$(1\|0,0)$	1
T	$(k_x, 0)$	$(1\|0,0)$	1
K	$\left(\frac{4\pi}{3a}, 0\right)$	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0)$	3
M	$\left(\frac{4\pi}{3a}, \frac{2\pi}{3a}\right)$	$(1\|0,0), (2_z\|0,0)$	2
T′	$\left(\frac{4\pi}{3a}, k_y\right)$	$(1\|0,0)$	1
Subtable 17 *p6m*		*Hexagonal*	
Γ	(0,0)	$(1\|0,0), (6_z\|0,0), (3_z\|0,0), (2_z\|0,0), (3_z\|0,0), (6_z^{-1}\|0,0),$ $(\sigma_1\|0,0), (\sigma_2\|0,0), (\sigma_3\|0,0), (\sigma_x\|0,0), (\sigma_y\|0,0), (\sigma_{xy}\|0,0)$	6*mm*
Σ	$(k_x, \frac{1}{2}k_x)$	$(1\|0,0), (\sigma_y\|0,0)$	*m*
T	$(k_x, 0)$	$(1\|0,0), (\sigma_2\|0,0)$	*m*
K	$\left(\frac{4\pi}{3a}, 0\right)$	$(1\|0,0), (3_z\|0,0), (3_z^{-1}\|0,0), (\sigma_1\|0,0), (\sigma_2\|0,0), (\sigma_3\|0,0)$	3*m*
M	$\left(\frac{4\pi}{3a}, \frac{2\pi}{3a}\right)$	$(1\|0,0), (2_z\|0,0), (\sigma_1\|0,0), (\sigma_y\|0,0)$	2*mm*
T′	$\left(\frac{4\pi}{3a}, k_y\right)$	$(1\|0,0), (\sigma_1\|0,0)$	*m*

[a] For each two-dimensional space group we list the symbol and coordinates of each point of high symmetry of the Brillouin zone in the first and second columns. The elements of the corresponding point groups are listed in the third column. In the fourth column is a symbol for the corresponding character table which, for symmorphic space groups and points of high symmetry in the Brillouin zone of non-symmorphic space groups, can be found in ref. A1, and for points of high symmetry on the Brillouin zone of non-symmorphic space groups is found in Table AIII.

TABLE AIII
CHARACTER TABLES[a]

2mm		1	σ_2	σ_x	2_z
		1	σ_1	σ_y	2_z
		1	σ_x	σ_y	2_z
	1	1	1	1	1
	2	1	1	−1	−1
	3	1	−1	−1	1
	4	1	−1	1	−1

IR 4.Y; 4.S	$(1\|0,0)$	$(\sigma_x\|0,\frac{1}{2})$
1	1	i
2	1	−i

IR 4.X	$(1\|0,0)$	$(\sigma_x\|0,\frac{1}{2})$
1	1	1
2	1	−1

IR 4.D	$(1\|0,0)$	$(\sigma_x\|0,\frac{1}{2})$
IR 8.D	$(1\|0,0)$	$(\sigma_x\|\frac{1}{2},\frac{1}{2})$
1	1	q
2	1	$-q$

IR 7.C	$(1\|0,0)$	$(\sigma_y\|\frac{1}{2},0)$
IR 8.C; 12.Y	$(1\|0,0)$	$(\sigma_y\|\frac{1}{2},\frac{1}{2})$
1	1	p
2	1	$-p$

IR 7.X; 7.S	$(1\|0,0)$	$(\sigma_x\|\frac{1}{2},0)$	$(\sigma_y\|\frac{1}{2},0)$	$(2_z\|0,0)$
IR 8.X; 8.Y; 12.Y	$(1\|0,0)$	$(\sigma_x\|\frac{1}{2},\frac{1}{2})$	$(\sigma_y\|\frac{1}{2},\frac{1}{2})$	$(2_z\|0,0)$
1	2	0	0	0

IR 7.Y	$(1\|0,0)$	$(\sigma_x\|\frac{1}{2},0)$	$(\sigma_y\|\frac{1}{2},0)$	$(2_z\|0,0)$
1	1	1	1	1
2	1	1	−1	−1
3	1	−1	−1	1
4	1	−1	1	−1

IR 8.S	$(1\|0,0)$	$(\sigma_x\|\frac{1}{2},\frac{1}{2})$	$(\sigma_y\|\frac{1}{2},\frac{1}{2})$	$(2_z\|0,0)$
1	1	i	i	1
2	1	−i	−i	1
3	1	i	−i	1
4	1	−i	i	−1

IR 12.M	$(1\|0,0)$	$(2_z\|0,0)$	$(4_z\|0,0)$	$(4_z^{-1}\|0,0)$	$(\sigma_y\|\frac{1}{2},\frac{1}{2})$	$(\sigma_x\|\frac{1}{2},\frac{1}{2})$	$(\sigma_{\bar{x}y}\|\frac{1}{2},\frac{1}{2})$	$(\sigma_{xy}\|\frac{1}{2},\frac{1}{2})$
1	2	2	0	0	0	0	0	0
2	1	−1	i	−i	i	−i	−1	1
3	1	−1	i	−i	−i	−i	1	−1
4	1	−1	−i	i	i	i	1	−1
5	1	−1	−i	i	−i	i	−1	1

[a] Character tables are given for the point group 2*mm* and for all points of high symmetry on the Brillouin zone in the case of non-symmorphic space groups. Elements of the point groups are given explicitly. Symbols used are $p = \exp(\frac{1}{2}ik_x a)$ and $q = \exp(\frac{1}{2}ik_y b)$.

symmorphic space groups, and for points of high symmetry inside the Brillouin zone of non-symmorphic space groups, this symbol is that of the corresponding point group whose irreducible representations are tabulated in ref. A1. To avoid ambiguities in indexation, the irreducible representations of the point group *2mm* are given in Table AIII. For points of high symmetry on the Brillouin zone in the case of non-symmorphic space groups, the irreducible representations have been derived and are found in Table AIII under the corresponding symbol.

Reference for Appendix A

A1 J. Zak, A. Casher, M. Gluck and Y. Gur, *The Irreducible Representations of Space Groups*, Benjamin, New York, 1969.