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LETTER TO THE EDITOR

Compatibility relations for two-dimensional space groups

D B Litvin
Department of Physics, The Pennsylvania State University, The Berks Campus, PO Box 2150, Reading, PA 19608, USA

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Abstract. Tables are presented of the compatibility relations between irreducible representations of all two-dimensional space groups.

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 (Maradudin and Vosko 1968). For example, the irreducible representations of the three-dimensional space groups provide a labelling scheme for the lattice vibrations in three-dimensional crystals and predict the degeneracies of the normal modes. Using the irreducible representations of the two-dimensional space groups for a labelling scheme, Litvin (1983) has tabulated the group theoretical labels of all possible two-dimensional lattice vibrations.

In determining the symmetry labelling of phonon dispersion curves, in addition to the labelling of the individual lattice vibrations, the concept of compatibility relations introduced by Bouchaert *et al* (1936) is useful. Compatibility relations provide the information to label correctly branches of phonon dispersion curves which, for example, have split from a single curve. The compatibility relations between irreducible representations of the three-dimensional space groups have been tabulated by Miller and Love (1967). In this Letter we provide the compatibility relations between irreducible representations of the two-dimensional space groups.

Below the number and symbol of each two-dimensional space group we have listed the compatibility relations for that space group. The symbols used to denote the irreducible representations and wavevectors follow the conventions of Zak *et al* (1969). No tables are given for the first two two-dimensional space groups, 1 :p1 and 2 : p2, since all compatibility relations are to wavevectors whose point group symmetry is the identity element. These tables have been used in determining the symmetry labelling of phonon dispersion curves of physisorbed methane (Litvin 1983).

References

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Miller S C and Love W F 1967 *Tables of Irreducible Representations of Space Groups and Co-Representations of Magnetic Space Groups* (Boulder, Colorado: Pruett Press)
Zak J, Casher A, Gluck M and Gur Y 1969 *The Irreducible Representations of Space Groups* (New York: Benjamin)

3: Pm 4: Pg

	Σ	Δ		Δ	C		C	D		Σ	D
Γ_1	Σ_1	Δ_1	Y_1	Δ_1	C_1	S_1	C_1	D_1	X_1	Σ_1	D_1
Γ_2	Σ_1	Δ_2	Y_2	Δ_2	C_1	S_2	C_1	D_2	X_2	Σ_1	D_2

5: Cm

	Σ	Δ		Δ	C
Γ_1	Σ_1	Δ_1	Y_1	Δ_1	C_1
Γ_2	Σ_1	Δ_2	Y_2	Δ_2	C_1

6: Pmm

	Σ	Δ		Δ	C		Σ	D		C	D
Γ_1	Σ_1	Δ_1	Y_1	Δ_1	C_1	X_1	Σ_1	D_1	S_1	C_1	D_1
Γ_2	Σ_2	Δ_1	Y_2	Δ_1	C_2	X_2	Σ_2	D_1	S_2	C_2	D_1
Γ_3	Σ_2	Δ_2	Y_3	Δ_2	C_2	X_3	Σ_2	D_2	S_3	C_2	D_2
Γ_4	Σ_1	Δ_2	Y_4	Δ_2	C_1	X_4	Σ_1	D_2	S_4.	C_1	D_2

7: Pmg

	Σ	Δ		Δ	C		Σ	D		C	D
Γ_1	Σ_1	Δ_1	Y_1	Δ_1	C_1	X_1	Σ_1, Σ_2	D_1, D_2	S_1	C_1, C_2	D_1, D_2
Γ_2	Σ_2	Δ_1	Y_2	Δ_1	C_2						
Γ_3	Σ_2	Δ_2	Y_3	Δ_2	C_2						
Γ_4	Σ_1	Δ_2	Y_4	Δ_2	C_1						

8: Pgg

	Σ	Δ		C	D		Δ	C		Σ	D
Γ_1	Σ_1	Δ_1	S_1	C_1	D_1	Y_1	Δ_1, Δ_2	C_1, C_2	X_1	Σ_1, Σ_2	D_1, D_2
Γ_2	Σ_2	Δ_1	S_2	C_2	D_2						
Γ_3	Σ_2	Δ_2	S_3	C_2	D_1						
Γ_4	Σ_1	Δ_2	S_4	C_1	D_2						

9: Cmm

	Σ	Δ		Δ	C
Γ_1	Σ_1	Δ_1	Y_1	Δ_1	C_1
Γ_2	Σ_2	Δ_1	Y_2	Δ_1	C_2
Γ_3	Σ_2	Δ_2	Y_3	Δ_2	C_2
Γ_4	Σ_1	Δ_2	Y_4	Δ_2	C_1

10: P4

	Σ	Δ		Σ	Y		Y	Δ
Γ_1	Σ_1	Δ_1	M_1	Σ_1	Y_1	X_1	Y_1	Δ_1
Γ_2	Σ_1	Δ_1	M_2	Σ_1	Y_1	X_2	Y_1	Δ_1
Γ_3	Σ_1	Δ_1	M_3	Σ_1	Y_1			
Γ_4	Σ_1	Δ_1	M_4	Σ_1	Y_1			

11: P4m

	Σ	Δ
Γ_1	Σ_1	Δ_1
Γ_2	Σ_2	Δ_2
Γ_3	Σ_2	Δ_1
Γ_4	Σ_1	Δ_2
Γ_5	Σ_1, Σ_2	Δ_1, Δ_2

	Σ	Y
M_1	Σ_1	Y_1
M_2	Σ_2	Y_2
M_3	Σ_2	Y_1
M_4	Σ_1	Y_2
M_5	Σ_1, Σ_2	Y_1, Y_2

	Y	Δ
X_1	Y_1	Δ_1
X_2	Y_2	Δ_1
X_3	Y_2	Δ_2
X_4	Y_1	Δ_2

12: P4g

	Σ	Δ
Γ_1	Σ_1	Δ_1
Γ_2	Σ_2	Δ_2
Γ_3	Σ_2	Δ_1
Γ_4	Σ_1	Δ_2
Γ_5	Σ_1, Σ_2	Δ_1, Δ_2

	Σ	Y
M_1	Σ_1, Σ_2	Y_1, Y_2
M_2	Σ_1	Y_1
M_3	Σ_2	Y_2
M_4	Σ_2	Y_1
M_5	Σ_1	Y_2

	Y	Δ
X_1	Y_1, Y_2	Δ_1, Δ_2

13: P3

	Σ	T
Γ_1	Σ_1	T_1
Γ_2	Σ_1	T_1
Γ_3	Σ_1	T_1

	T	T'
K_1	T_1	T_1'
K_2	T_1	T_1'
K_3	T_1	T_1'

	Σ	T'
M_1	Σ_1	T_1'

14: P3m1

	Σ	T
Γ_1	Σ_1	T_1
Γ_2	Σ_2	T_1
Γ_3	Σ_1, Σ_2	$2T_1$

	Σ	T'
M_1	Σ_1	T_1'
M_2	Σ_1	T_1'

	T	T'
K_1	T_1	T_1'
K_2	T_1	T_1'
K_3	T_1	T_1'

15: P31m

	Σ	T
Γ_1	Σ_1	T_1
Γ_2	Σ_1	T_2
Γ_3	$2\Sigma_1$	T_1, T_2

	Σ	T'
M_1	Σ_1	T_1'
M_2	Σ_1	T_2'

	T	T'
K_1	T_1	T_1'
K_2	T_2	T_2'
K_3	T_1, T_2	T_1', T_2'

16: P6

	Σ	T
Γ_1	Σ_1	T_1
Γ_2	Σ_1	T_1
Γ_3	Σ_1	T_1
Γ_4	Σ_1	T_1
Γ_5	Σ_1	T_1
Γ_6	Σ_1	T_1

	Σ	T'
M_1	Σ_1	T_1'
M_2	Σ_1	T_1'

	T	T'
K_1	T_1	T_1'
K_2	T_1	T_1'
K_3	T_1	T_1'

17: P6m

	Σ	T
Γ_1	Σ_1	T_1
Γ_2	Σ_2	T_2
Γ_3	Σ_1	T_2
Γ_4	Σ_2	T_1
Γ_5	Σ_1, Σ_2	T_1, T_2
Γ_6	Σ_1, Σ_2	T_1, T_2

	Σ	T'
M_1	Σ_1	T_1'
M_2	Σ_2	T_1'
M_3	Σ_2	T_2'
M_4	Σ_1	T_2'

	T	T'
K_1	T_1	T_1'
K_2	T_2	T_2'
K_3	T_1, T_2	T_1', T_2'