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Dipole selection rules for the hexagonal-close-packed lattice

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Complete tables of optical dipole selection rules for Bloch states in the hexagonal-close-packed lattice are given for symmetry lines and symmetry points in the Brillouin zone. Included are both single and double group representations.

It has long been known that a knowledge of optical dipole selection rules is useful in interpreting optical spectra and other photoexcitative processes in solids. The recent prolific growth of angle-resolving photoelectron spectroscopy calls attention to the fact that selection rules for optical dipole transitions are necessary for correct assignment of structures in experimental spectra to calculated energy bands. In the case of symmorphic space groups (e.g., those with fcc and bcc lattices and many others), the appropriate selection rules are easily derived. In the case of the nonsymmorphic groups (e.g., hcp and diamond among others), the method is not as obvious, mainly because one cannot find irreducible representations to some of the factor groups G_K/T_K of the space group G_K which have as basis functions components of the polar vector $\vec{r}$. T_K is the translation group in three dimensions, and we take K to run over symmetrical points in the Brillouin zone.

Selection rules for the hexagonal-close-packed (hcp) lattice structure are not widely known. The purpose here is to present the optical dipole selection rules for all symmetry lines and points. We note that the general methods of computing selection rules for nonsymmorphic groups have been developed and applied to the diamond lattice.[1,2] The method has been elucidated in the book by Cornwell,[3] and is applied here. Actually, the optical dipole selection rules for the hcp lattice at the symmetry points Γ, A, L, M, H, and K were previously published by Cornwell.[4] We include the selection rules for those points in order to present a complete set.

The direct optical dipole selection rules for the hcp lattice are given in Table I. The notations for the single groups and the Brillouin-zone orientation are those of Herring.[5] The notations for the double

TABLE I. The direct optical dipole selection rules for the hcp lattice. When double group representations are time-reversal degenerate, they are not separated in the tables but are joined by a plus (+) sign. Note that in Herring's figure for the Brillouin zone, $\Gamma-T-K$ is the k_x axis, $\Gamma-\Sigma-M$ is the k_y axis, and $\Gamma-\Delta-A$ is the k_z axis. S, S', and T' are parallel to the k_x axis, R is parallel to the k_y axis, and U is parallel to the Z axis.

	$\Gamma_1^\pm$	$\Gamma_2^\pm$	$\Gamma_3^\pm$	$\Gamma_4^\pm$	$\Gamma_5^\pm$	$\Gamma_6^\pm$	$\Gamma_7^\pm$	$\Gamma_8^\pm$	$\Gamma_9^\pm$
x, y	$\Gamma_6^\mp$	$\Gamma_6^\mp$	$\Gamma_5^\mp$	$\Gamma_5^\mp$	$\Gamma_3^\mp, \Gamma_4^\mp, \Gamma_6^\mp$	$\Gamma_1^\mp, \Gamma_2^\mp, \Gamma_5^\mp$	$\Gamma_7^\mp, \Gamma_9^\mp$	$\Gamma_8^\mp, \Gamma_9^\mp$	$\Gamma_7^\mp, \Gamma_8^\mp$
z	$\Gamma_2^\mp$	$\Gamma_1^\mp$	$\Gamma_4^\mp$	$\Gamma_3^\mp$	$\Gamma_5^\mp$	$\Gamma_6^\mp$	$\Gamma_7^\mp$	$\Gamma_8^\mp$	$\Gamma_9^\mp$

	A_1	A_2	A_3	A_4+A_5	A_6
x, y	A_3	A_3	A_1, A_2, A_3	A_6	A_4+A_5, A_6
z	A_1	A_2	A_3	A_4+A_5	A_6

	Δ_1	Δ_2	Δ_3	Δ_4	Δ_5	Δ_6	Δ_7	Δ_8	Δ_9
x, y	Δ_6	Δ_5	Δ_6	Δ_5	$\Delta_2, \Delta_4, \Delta_6$	$\Delta_1, \Delta_3, \Delta_5$	Δ_7, Δ_9	Δ_8, Δ_9	Δ_7, Δ_8
z	Δ_1	Δ_2	Δ_3	Δ_4	Δ_5	Δ_6	Δ_7	Δ_8	Δ_9

TABLE I (*Continued*).

	$M_1^{\pm}$	$M_2^{\pm}$	$M_3^{\pm}$	$M_4^{\pm}$	$M_5^{\pm}$
x	$M_3^{\mp}$	$M_4^{\mp}$	$M_1^{\mp}$	$M_2^{\mp}$	$M_5^{\mp}$
y	$M_2^{\mp}$	$M_1^{\mp}$	$M_4^{\mp}$	$M_3^{\mp}$	$M_5^{\mp}$
z	$M_4^{\mp}$	$M_3^{\mp}$	$M_2^{\mp}$	$M_1^{\mp}$	$M_5^{\mp}$

	L_1	L_2	L_3	L_4
x	L_2	L_1	L_3	L_4
y, z	L_1	L_2	L_4	L_3

	U_1	U_2	U_3	U_4	U_5
x	U_3	U_4	U_1	U_2	U_5
y	U_2	U_1	U_4	U_3	U_5
z	U_1	U_2	U_3	U_4	U_5

	R_1	R_2	R_3	R_4	R_5	Σ_1	Σ_2	Σ_3	Σ_4	Σ_5
x	R_4	R_3	R_2	R_1	R_5	Σ_4	Σ_3	Σ_2	Σ_1	Σ_5
y	R_1	R_2	R_3	R_4	R_5	Σ_1	Σ_2	Σ_3	Σ_4	Σ_5
z	R_3	R_4	R_1	R_2	R_5	Σ_3	Σ_4	Σ_1	Σ_2	Σ_5

	H_1	H_2	H_3	H_4+H_6	H_5+H_7	H_8	H_9
x, y	H_2, H_3	H_1, H_3	H_1, H_2	H_9	H_8	H_5+H_7, H_8	H_4+H_6, H_9
z	H_1	H_3	H_2	H_5+H_7	H_4+H_6	H_9	H_8

	K_1	K_2	K_3	K_4	K_5	K_6	K_7	K_8	K_9
x, y	K_5	K_6	K_5	K_6	K_1, K_3, K_5	K_2, K_4, K_6	K_8, K_9	K_7, K_9	K_7, K_8
z	K_4	K_3	K_2	K_1	K_6	K_5	K_8	K_7	K_9

	P_1	P_2	P_3	P_4+P_5	P_6
x, y	P_3	P_3	P_1, P_2, P_3	P_6	P_4+P_5, P_6
z	P_1	P_2	P_3	P_4+P_5	P_6

	S_1	S_2+S_5	S_3+S_4	(Applies to S' as well)
x, y	S_1	S_2+S_5	S_3+S_4	
z	S_1	S_3+S_4	S_2+S_5	

	T_1	T_2	T_3	T_4	T_5	(Applies to T' as well)
x	T_1	T_2	T_3	T_4	T_5	
y	T_4	T_3	T_2	T_1	T_5	
z	T_3	T_4	T_1	T_2	T_5	

groups are those of Elliott,[6] following the corrections given by Cornwell[4]:

$$\Gamma_5^{\pm} \times D_{1/2} = \Gamma_8^{\pm} + \Gamma_9^{\pm} \quad , \quad \Gamma_6^{\pm} \times D_{1/2} = \Gamma_7^{\pm} + \Gamma_9^{\pm} \quad .$$

The selection rules for direct optical transitions are given by symmetry point or line. The polarization is given at the left side and the symmetry of the initial *(or* final) state is given at the top of each subtable. The bodies contain the allowed final *(or* initial) state for each polarization (resolved into the maximal number of separable components). The extra irreducible representations for the double groups are set off on the right-hand side in each subtable by extra spaces.

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