Table 2.5.3.3. *Diffraction point-group tables, giving whole-pattern and central-beam pattern symmetries in terms of BESR diffraction-group symbols and diperiodic group symbols*

I	II	III	IV	V	
				Cubic point groups	
Whole pattern	Bright field (central beam)	BESR group	Diperiodic group (point group)	[100]	[110]
1	1	1	1		
1	2	$\underline{1}_R$	m'		
2	2	2	2		
1	1	$^*2_R$	$\bar{1}'$		
2	2	$^*\underline{21}_R$	$2/m'$		
1	m	m_R	$2'$		23
m	m	m	m		
m	$2mm$	$\underline{m1}_R$	$2'mm'$		$\bar{4}3m$
2	$2mm$	$2m_Rm_R$	$2'2'2$	23	432
$2mm$	$2mm$	$2mm$	$mm2$		
m	m	$^*2_Rmm_R$	$2'/m$		$m\bar{3}$
$2mm$	$2mm$	$^*\underline{2mm1}_R$	mmm'	$m\bar{3}$	$m\bar{3}m$
4	4	4	4		
2	4	4_R	$\bar{4}'$		
4	4	$^*\underline{41}_R$	$4/m'$		
4	$4mm$	$4m_Rm_R$	$42'2'$	$\bar{4}32$	
$4mm$	$4mm$	$4mm$	$4mm$		
$2mm$	$4mm$	4_Rmm_R	$\bar{4}'m2'$	$\bar{4}3m$	
$4mm$	$4mm$	$^*\underline{4mm1}_R$	$4/m'mm$	$m\bar{3}m$	
3	3	3	3		
3	6	$\underline{31}_R$	$\bar{6}'$		
3	$3m$	$3m_R$	$32'$		
$3m$	$3m$	$3m$	$3m$		
$3m$	$6mm$	$\underline{3m1}_R$	$\bar{6}'m2'$		
6	6	6	6		
3	3	$^*6_R$	$\bar{3}'$		
6	6	$^*\underline{61}_R$	$6/m'$		
6	$6mm$	$6m_Rm_R$	$62'2'$		
$6mm$	$6mm$	$6mm$	$6mm$		
$3m$	$3m$	$^*6_Rmm_R$	$\bar{3}'m$		
$6mm$	$6mm$	$^*\underline{6mm1}_R$	$6/m'mm$		

Inspection of columns I and II shows that 11 of the 31 diffraction groups can be determined from a knowledge of the whole pattern and bright-field (central-beam disc) point symmetries alone. The remaining 10 pairs of groups need additional observation of the dark-field pattern for their resolution. Disc symmetries 1_R, m_R (Fig. 2.5.3.2; Table 2.5.3.2) are sought (*a*) in general zero-layer discs and (*b*) in discs having an m_R line perpendicular to a proposed twofold axis, respectively; the $\pm H$ test is applied for centrosymmetry, to complete the classification.

Column IV gives the equivalent diperiodic point-group symbol, which, unprimed, gives the corresponding three-dimensional symbol. This will always refer to a non-cubic point group. Column V gives the additional cubic point-group information indicating, where appropriate, how to translate the diffraction symmetry into [100] or [110] cubic settings, respectively.

Of the groups listed in column III, those representing the projection group of their class are underlined. These groups all contain 1_R, the BESR symbol for m'. When the projection approximation is applicable, only those groups underlined will apply. The effect of this approximation is to add a horizontal mirror plane to the symmetry group.

Table 2.5.3.4. This lists possible space groups for each of the classified zero-layer CBED symmetries. Since the latter constitute the 80 diperiodic groups, it is first necessary to index the pattern in diperiodic nomenclature; the set of possible space groups is then given by the table.

A basic requirement for diperiodic group nomenclature has been that of compatibility with *IT* A and I. This has been met by the recent Pond & Vlachavas (1983) tabulation. For example, DG: $(^*)pban'$, where * indicates centrosymmetry, becomes space group *Pban* when, in Seitz matrix description, the former group matrix is multiplied by the third primitive translation, a_3. Furthermore, in textual reference the prime can be optionally omitted, since the lower-case lattice symbol is sufficient indication of a two-dimensional periodicity (as *pban*).

The three sections of Table 2.5.3.4 are:

I. Point-group entries, given in H–M and BESR symbols.

II. Pattern symmetries, in diperiodic nomenclature, have three subdivisions: (i) symmorphic groups: patterns without zero-layer absences or extinctions. Non-symmorphic groups are then given in two categories: (ii) patterns with zero-layer GS bands, and (iii) patterns with zero-layer absences resulting from a horizontal glide plane; where the pattern *also* contains dynamic extinctions (GS bands) and so is listed in column (ii), the column (iii) listing is given in parentheses.

The 'short' (Pond & Vlachavas) symbol has proved an adequate description for all but nine groups for which the screw-axis content was needed: here $(2'_1)$, or $(2'_12'_1)$, have been added to the symbol.

III. Space-group entries are given in terms of *IT* A numbers. The first column of each row gives the same-name space group as illustrated by the example $pban' \rightarrow Pban$ above. The groups following in the same row (which have the same zero-layer symmetry) complete an exhaustive listing of the II*b* subgroups, given in *IT* A. Cubic space groups are underlined for the sake of clarity; hence, those giving rise to the zero-layer symmetry of the diffraction group in the [100] (cyclic) setting have a single underline: these are type I minimal supergroups in *IT* A nomenclature. The cubic groups are also given in the [110] setting, in underlined italics, since this is a commonly encountered high-symmetry setting. (*Note*: these then are no longer *minimal* supergroups and the relationship has to be found through a series of *IT* A listings.)

The table relates to maximal-symmetry settings. For monoclinic and orthorhombic systems there are three equally valid settings. For monoclinic groups, the oblique and rectangular settings appear separately; where rectangular *C*-centred groups appear in a second setting this is indicated by superscript '2'. For orthorhombic groups, superscripts correspond to the 'incident-beam' system adopted in Table 2.5.3.5, as follows: no superscript: [001] beam direction; superscript 1: [100] beam direction; superscript 2: [010] beam direction. The cubic system is treated specially as described above.

Table 2.5.3.5. This lists conditions for observation of GS bands for the 137 space groups exhibiting these extinctions. These are entered as '*G*', '*S*', or '*GS*', indicating whether a glide plane, screw axis, or both is responsible for the GS band. All three possibilities will lead to a glide line (and hence to both extinction bands) in projection, and one of the procedures (*a*), (*b*), or (*c*) of Section 2.5.3.3(iv) above is needed to complete the three-dimensional interpretation. In addition, the presence of horizontal glide planes, which result in systematic absences in these particular cases in the zero-layer pattern, is indicated by the symbol '–'. Where these occur at the site of prospective '*G*' or '*S*' bands from other glide or

references