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1998 J. Phys. A: Math. Gen. 31 3625

(http://iopscience.iop.org/0305-4470/31/15/023)

J. Phys. A: Math. Gen. **31** (1998) 3625–3648. Printed in the UK PII: S0305-4470(98)87096-0

Irreducible representations of diperiodic groups

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Received 26 August 1997, in final form 21 November 1997

Abstract. The irreducible representations of all of the 80 diperiodic groups, being the symmetries of the systems translationally periodical in two directions, are calculated. To this end, each of these groups is factorized as the product of a generalized translational group and an axial point group. The results are presented in the form of the tables, containing the matrices of the irreducible representations of the generators of the groups. General properties and some physical applications (degeneracy and topology of the energy bands, selection rules, etc) are discussed.

1. Introduction

The diperiodic groups [1, 2] are the symmetry groups of the systems with translational periodicity in two directions. Thin layers and multilayers are the obvious examples of such systems. The interest in the diperiodic structures increased after it was observed that the CuO_2 layers are responsible for the high-temperature superconductivity [4], and that the main effects (including superconductivity and the unusual conducting properties above T_c) are present even if there is no periodicity in the direction orthogonal onto conducting block.

There are 80 diperiodic groups; 17 of them are planar, i.e. describe the symmetry of the strictly two-dimensional (2D) systems. All of them are subgroups of the three-dimensional (3D) space groups; this correspondence (involving additional conventions to reduce the nonuniqueness—for each space group a number of diperiodic subgroups can be found, while each diperiodic group is subgroup in various space groups) has been determined [2, 3]. The orbits and stabilizers of the diperiodic groups are known [1]. In contrast, there is no general tabulation of the irreducible representations (irrs), beyond the more specialized tables of Hatch and Stokes [3] (irrs related to the points of symmetry in the Brillouin zone are considered in the context of phase transitions). This may be the reason why the rare usage of the diperiodic groups in the literature (in contrast to the space, the point and the line groups) mostly refers to the IC and Raman spectra, when the irrs of the isogonal point group are effectively employed. In fact, most of the results refer to the phase transitions. Hatch and Stokes also found Molien functions and invariants [3]. The aim of this paper is to fill this gap, and to construct the irrs of all the diperiodic groups, thus enabling extensive treatment of this type of symmetry in the solid-state physics.

In section 3, the specific structural properties of the diperiodic groups are reviewed. These allow the simple construction of the irrs, involving neither projective representations, nor the representations of the space supergroups. The results are given in section 3. Finally,

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0305-4470/98/153625+24$19.50

Table 1. The factorization of the diperiodic groups. For each diperiodic group **Dg**, the holohedry **H**, the isogonal point group **I**, the factorization **PT** and the international symbol according to [1], is given. The last column refers to the table containing the irrs of the group.

Dg	H	I	PT	Int. simb.	Table	Dg	H	I	PT	Int. simb.	Table
1	$\mathbf{C}_{2h}$	$\mathbf{C}_1$	$\mathbf{T}$	p1	2	41	$\mathbf{D}_{2h}$	$\mathbf{D}_{2h}$	$\mathbf{C}_{2v}\mathbf{T}_h$	$\mathrm{p}\frac{2}{a}\frac{2_1}{m}\frac{2}{m}$	11
2		$\mathbf{S}_2$	$\mathbf{S}_2\mathbf{T}$	$\mathrm{p}\bar{1}$	3	42		$\mathbf{D}_{2h}$	$\mathbf{D}_{1d}\mathbf{T}'_h$	$\mathrm{p}\frac{2}{n}\frac{2}{m}\frac{2_1}{a}$	17
3		$\mathbf{C}_2$	$\mathbf{C}_2\mathbf{T}$	p211	3	43		$\mathbf{D}_{2h}$	$\mathbf{D}_1 2_1 T_h$	$\mathrm{p}\frac{2}{a}\frac{2}{b}\frac{2_1}{a}$	12
4		$\mathbf{C}_{1h}$	$\mathbf{C}_{1h}\mathbf{T}$	pm11	2	44		$\mathbf{D}_{2h}$	$\mathbf{C}_{2h}\mathbf{T}'_v$	$\mathrm{p}\frac{2}{m}\frac{2_1}{b}\frac{2_1}{a}$	15
5		$\mathbf{C}_{1h}$	$\mathbf{T}_h$	pb11	2	45		$\mathbf{D}_{2h}$	$\mathbf{C}_2 2_1 T_h$	$\mathrm{p}\frac{2}{a}\frac{2_1}{b}\frac{2_1}{m}$	10
6		$\mathbf{C}_{2h}$	$\mathbf{C}_{2h}\mathbf{T}$	$\mathrm{p}\frac{2}{m}11$	3	46		$\mathbf{D}_{2h}$	$\mathbf{C}_{2v}\mathbf{T}'_h$	$\mathrm{p}\frac{2}{n}\frac{2_1}{m}\frac{2_1}{m}$	17
7		$\mathbf{C}_{2h}$	$\mathbf{C}_2\mathbf{T}_h$	$\mathrm{p}\frac{2}{b}11$	4	47		$\mathbf{D}_{2h}$	$\mathbf{D}_{2h}\mathbf{T}'$	$\mathrm{c}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	14
8	$\mathbf{D}_{2h}$	$\mathbf{D}_1$	$\mathbf{D}_1\mathbf{T}$	p112	5	48		$\mathbf{D}_{2h}$	$\mathbf{C}_{2v}\mathbf{T}'_h$	$\mathrm{c}\frac{2}{a}\frac{2}{m}\frac{2}{m}$	18
9		$\mathbf{D}_1$	$\mathbf{2}_1$	$\mathrm{p}112_1$	7	49	$\mathbf{D}_{4h}$	$\mathbf{C}_4$	$\mathbf{C}_4\mathbf{T}$	p4	19
10		$\mathbf{D}_1$	$\mathbf{D}_1\mathbf{T}'$	c112	13	50		$\mathbf{S}_4$	$\mathbf{S}_4\mathbf{T}$	$\mathrm{p}\bar{4}$	19
11		$\mathbf{C}_{1v}$	$\mathbf{C}_{1v}\mathbf{T}$	p11m	5	51		$\mathbf{C}_{4h}$	$\mathbf{C}_{4h}\mathbf{T}$	p4/m	19
12		$\mathbf{C}_{1v}$	$\mathbf{T}_v$	p11a	7	52		$\mathbf{C}_{4h}$	$\mathbf{C}_4\mathbf{T}'_h$	p4/n	20
13		$\mathbf{C}_{1v}$	$\mathbf{C}_{1v}\mathbf{T}'$	c11m	13	53		$\mathbf{D}_4$	$\mathbf{D}_4\mathbf{T}$	p422	21
14		$\mathbf{D}_{1d}$	$\mathbf{D}_{1d}\mathbf{T}$	$\mathrm{p}11\frac{2}{m}$	6	54		$\mathbf{D}_4$	$\mathbf{C}_4\mathbf{2}'_1$	$\mathrm{p}42_12$	14
15		$\mathbf{D}_{1d}$	$\mathbf{S}_2\mathbf{2}_1$	$\mathrm{p}11\frac{2_1}{m}$	8	55		$\mathbf{C}_{4v}$	$\mathbf{C}_{4v}\mathbf{T}$	p4mm	21
16		$\mathbf{D}_{1d}$	$\mathbf{D}_{1d}\mathbf{T}'$	$\mathrm{c}11\frac{2}{m}$	14	56		$\mathbf{C}_{4v}$	$\mathbf{C}_4\mathbf{T}'_v$	p4bm	14
17		$\mathbf{D}_{1d}$	$\mathbf{S}_2\mathbf{T}_v$	$\mathrm{p}11\frac{2}{a}$	8	57		$\mathbf{D}_{2d}$	$\mathbf{D}_{2d}\mathbf{T}$	$\mathrm{p}\bar{4}2\mathrm{m}$	21
18		$\mathbf{D}_{1d}$	$\mathbf{S}_2\mathbf{T}'_v$	$\mathrm{p}11\frac{2_1}{a}$	15	58		$\mathbf{D}_{2d}$	$\mathbf{S}_4\mathbf{2}'_1$	$\mathrm{p}\bar{4}2_1\mathrm{m}$	14
19		$\mathbf{D}_2$	$\mathbf{D}_2\mathbf{T}$	p222	6	59		$\mathbf{D}_{2d}$	$\mathbf{D}_{2d}\mathbf{T}$	$\mathrm{p}\bar{4}\mathrm{m}2$	21
20		$\mathbf{D}_2$	$\mathbf{C}_2\mathbf{2}_1$	$\mathrm{p}222_1$	8	60		$\mathbf{D}_{2d}$	$\mathbf{S}_4\mathbf{T}'_v$	$\mathrm{p}\bar{4}\mathrm{b}2$	14
21		$\mathbf{D}_2$	$\mathbf{C}_2\mathbf{2}'_1$	$\mathrm{p}22_12_1$	15	61		$\mathbf{D}_{4h}$	$\mathbf{D}_{4h}\mathbf{T}$	$\mathrm{p}\frac{4}{m}\frac{2}{m}\frac{2}{m}$	21
22		$\mathbf{D}_2$	$\mathbf{D}_2\mathbf{T}'$	c222	14	62		$\mathbf{D}_{4h}$	$\mathbf{D}_{2d}\mathbf{T}'_h$	$\mathrm{p}\frac{4}{n}\frac{2}{b}\frac{2}{m}$	14
23		$\mathbf{C}_{2v}$	$\mathbf{C}_{2v}\mathbf{T}$	p2mm	6	63		$\mathbf{D}_{4h}$	$\mathbf{C}_{4h}\mathbf{T}'_v$	$\mathrm{p}\frac{4}{m}\frac{2_1}{b}\frac{2}{m}$	14
24		$\mathbf{D}_{1h}$	$\mathbf{D}_{1h}\mathbf{T}$	pmm2	5	64		$\mathbf{D}_{4h}$	$\mathbf{D}_{2d}\mathbf{T}'_h$	$\mathrm{p}\frac{4}{n}\frac{2_1}{m}\frac{2}{m}$	14
25		$\mathbf{D}_{1h}$	$\mathbf{C}_{1h}\mathbf{2}_1$	$\mathrm{pm}2_1\mathrm{a}$	7	65	$\mathbf{D}_{6h}$	$\mathbf{C}_3$	$\mathbf{C}_3\mathbf{T}$	p3	7
26		$\mathbf{D}_{1h}$	$\mathbf{C}_{1v}\mathbf{2}_1$	$\mathrm{pbm}2_1$	7	66		$\mathbf{S}_6$	$\mathbf{S}_6\mathbf{T}$	$\mathrm{p}\bar{3}$	27
27		$\mathbf{D}_{1h}$	$\mathbf{D}_1\mathbf{T}_v$	pbb2	7	67		$\mathbf{D}_3$	$\mathbf{D}_3\mathbf{T}$	p312	26
28		$\mathbf{C}_{2v}$	$\mathbf{C}_2\mathbf{T}_v$	p2ma	8	68		$\mathbf{D}_3$	$\mathbf{D}_3\mathbf{T}$	p321	25
29		$\mathbf{D}_{1h}$	$\mathbf{D}_1\mathbf{T}_h$	pam2	9	69		$\mathbf{C}_{3v}$	$\mathbf{C}_{3v}\mathbf{T}$	p3m1	26
30		$\mathbf{D}_{1h}$	2_1T_h	$\mathrm{pab}2_1$	9	70		$\mathbf{C}_{3v}$	$\mathbf{C}_{3v}\mathbf{T}$	p31m	25
31		$\mathbf{D}_{1h}$	$\mathbf{D}_1\mathbf{T}'_h$	pnb2	13	71		$\mathbf{D}_{3d}$	$\mathbf{D}_{3d}\mathbf{T}$	$\mathrm{p}\bar{3}1\frac{2}{m}$	28
32		$\mathbf{D}_{1h}$	$\mathbf{C}_{1v}\mathbf{T}'_h$	$\mathrm{p\ nm}2_1$	13	72		$\mathbf{D}_{3d}$	$\mathbf{D}_{3d}\mathbf{T}$	$\mathrm{p}\bar{3}\frac{2}{m}1$	28
33		$\mathbf{C}_{2v}$	$\mathbf{C}_2\mathbf{T}'_v$	p2ba	15	73		$\mathbf{C}_6$	$\mathbf{C}_6\mathbf{T}$	p6	27
34		$\mathbf{C}_{2v}$	$\mathbf{C}_{2v}\mathbf{T}'$	c2mm	14	74		$\mathbf{C}_{3h}$	$\mathbf{C}_{3h}\mathbf{T}$	$\mathrm{p}\bar{6}$	7
35		$\mathbf{D}_{1h}$	$\mathbf{D}_{1h}\mathbf{T}'$	cmm2	13	75		$\mathbf{C}_{6h}$	$\mathbf{C}_{6h}\mathbf{T}$	p6/m	27
36		$\mathbf{D}_{1h}$	$\mathbf{D}_1\mathbf{T}'_h$	cam2	16	76		$\mathbf{D}_6$	$\mathbf{D}_6\mathbf{T}$	p622	28
37		$\mathbf{D}_{2h}$	$\mathbf{D}_{2h}\mathbf{T}$	$\mathrm{p}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	6	77		$\mathbf{C}_{6v}$	$\mathbf{C}_{6v}\mathbf{T}$	p6mm	28
38		$\mathbf{D}_{2h}$	$\mathbf{D}_2\mathbf{T}_h$	$\mathrm{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}$	11	78		$\mathbf{D}_{3h}$	$\mathbf{D}_{3h}\mathbf{T}$	$\mathrm{p}\bar{6}\mathrm{m}2$	26
39		$\mathbf{D}_{2h}$	$\mathbf{D}_2\mathbf{T}'_h$	$\mathrm{p}\frac{2}{n}\frac{2}{b}\frac{2}{a}$	17	79		$\mathbf{D}_{3h}$	$\mathbf{D}_{3h}\mathbf{T}$	$\mathrm{p}\bar{6}2\mathrm{m}$	25
40		$\mathbf{D}_{2h}$	$\mathbf{C}_{2h}\mathbf{T}_v$	$\mathrm{p}\frac{2}{m}\frac{2_1}{m}\frac{2}{a}$	8	80		$\mathbf{D}_{6h}$	$\mathbf{D}_{6h}\mathbf{T}$	$\mathrm{p}\frac{6}{m}\frac{2}{m}\frac{2}{m}$	28

in section 4 concluding remarks summarize some general properties of the irrs in view of their physical applications.

2. Group structure and construction of irrs

Each diperiodic group **Dg** can be factorized as a weak direct product of the generalized translational group **Z** and the axial point group **P** : $\mathbf{Dg} = \mathbf{ZP}$. This is analogous to the line

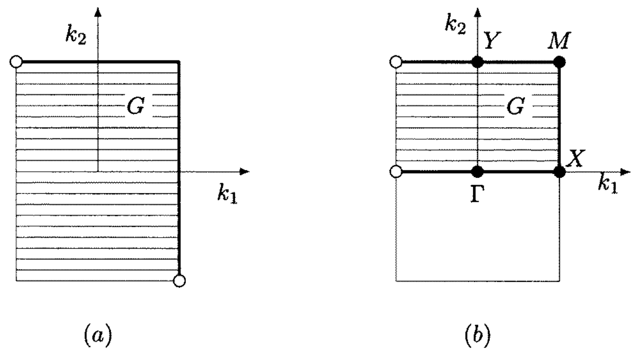

Figure 1. The irreducible domains of the Brillouin zone for the oblique diperiodic groups. The coordinates of the special points (full circles) are: $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$ and $M = (\pi, \pi)$. The coordinate lines k_1 and k_2 are allowed not to be orthogonal.

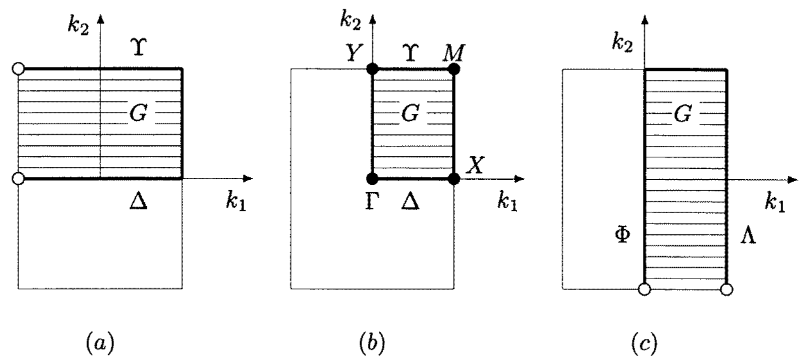

Figure 2. The irreducible domains of the Brillouin zone for the rectangular diperiodic groups. The different special points (full circles) are $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$ and $M = (\pi, \pi)$, while the special lines are $\Delta = (k, 0)$, $\Upsilon = (k, \pi)$, $\Phi = (0, k)$, $\Upsilon = (\pi, k)$, $\Sigma = (k, k)$ and $\Sigma' = (-k, k)$.

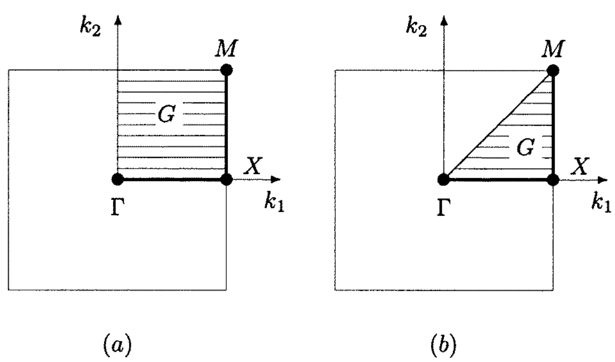

Figure 3. The irreducible domains of the Brillouin zone for the square diperiodic groups. The special points (full circles) are $\Gamma = (0, 0)$, $X = (\pi, 0)$ and $M = (\pi, \pi)$, while the special lines are $\Delta = (k, 0)$, $\Lambda = (\pi, k)$ and $\sigma = (k, k)$, with $k \in (0, \pi)$.

groups [5], except that the generalized translational group, **Z**, is 2D, since it describes the periodical arrangement of the elementary motifs along two independent directions (these two

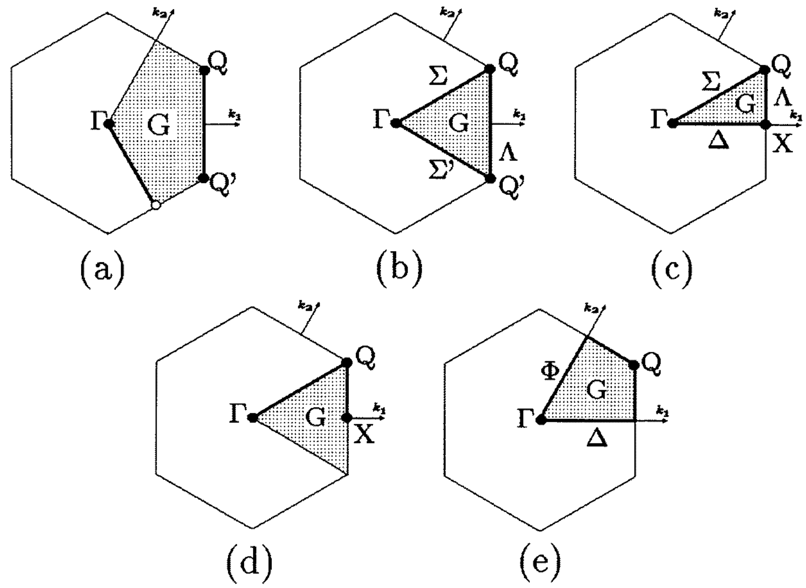

Figure 4. The irreducible domains of the Brillouin zone for the hexagonal diperiodic groups. The special points (full circles) are $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Q = (\frac{2\pi}{3}, \frac{2\pi}{3})$ and $Q' = (\frac{4\pi}{3}, -\frac{2\pi}{3})$, while the special lines are $\Delta = (k, 0)$ (for $k \in (0, \pi)$), $\Phi = (0, k)$ (for $k \in (0, \pi)$), $\Sigma = (k, k)$ (for $k \in (0, \frac{2\pi}{3})$), $\Sigma' = (k, -\frac{k}{2})$ (for $k \in (0, \frac{4\pi}{3})$) and $\Lambda = (k, 2\pi - 2k)$ (where $k \in (\frac{2\pi}{3}, \pi)$ for the groups with the principle axis of the order 6, and $k \in (\frac{2\pi}{3}, \frac{4\pi}{3})$ for the groups principle axis of the order 3).

directions are assumed to be in the xy-plane). Therefore, **Z** can be formed of the generalized one-dimensional (1D) translational groups leaving the xy-plane invariant. There are only four generalized 1D translational groups satisfying this condition:

(1) pure translational group T along an axis in the plane,

(2) screw axis group 2_1 with the C_2 axis in the plane,

(3) glide plane group T_h of the horizontal, xy, glide plane,

(4) glide plane group T_v of the vertical glide plane (containing z-axis).

All these groups are infinite cyclic groups. The first of them is generated by pure translation; as for the remaining three groups, pure translations are the index-2 subgroup generated by the square of the generator of the glide plane or the screw axis. The generalized 2D translational groups are direct or weak direct products of the listed four 1D generalized translations:

(1) The pure 2D translational group **T** is the direct product of the two 1D translational groups T along independent directions, with, in general, different translational periods and an arbitrary angle between the translational directions.

(2) The horizontal 2D glide plane group $\mathbf{T}_h = TT_h$; translational periods of T and T_h may be different, and their directions form an arbitrary angle.

(3) The 2D screw axis group $\mathbf{2}_1 = T2_1$ (horizontal screw axis).

(4) The vertical 2D glide plane group $\mathbf{T}_v = TT_v$ (vertical glide plane).

(5) The product 2_1T_h of the groups 2_1 and T_h generated by $(U_x|\frac{1}{2}\,0)$ and $(\sigma_h|0\,\frac{1}{2})$.

In the last three cases the screw axis (glide plane) can be chosen in the direction orthogonal to the translations of the group T or T_h, while the translational periods of the groups T and T_h are not related to those of 2_1 (respectively T_v).

Table 2. The irrs of the oblique 2D translational group $\mathbf{Dg}1 = \mathbf{T} = \mathrm{gr}\{(I|1\,0), (I|0\,1)\}$ and the oblique generalized 2D translational groups $\mathbf{Dg}4 = \mathbf{C}_{1h}\mathbf{T} = \mathrm{gr}\{\sigma_h, (I|1\,0), (I|0\,1)\}$ and $\mathbf{Dg}5 = \mathbf{T}_h = \mathrm{gr}\{(I|1\,0), (\sigma_h|0\,\frac{1}{2})\}$. The Brillouin zone, being the irreducible domain, is shown in figure 1(*a*).

Irr	D	σ_h	$(I\|1\,0)$	$(I\|0\,1)$	$(\sigma_h\|0\frac{1}{2})$
${}_kG^{\pm}$	1	±1	$\mathrm{e}^{\mathrm{i}k_1}$	$\mathrm{e}^{\mathrm{i}k_2}$	$\pm\mathrm{e}^{\mathrm{i}\frac{k_2}{2}}$

Table 3. The irrs of the oblique diperiodic groups $\mathbf{Dg}2 = \mathbf{S}_2\mathbf{T} = \mathrm{gr}\{C_2\sigma_h, (I|1\,0), (I|0\,1)\}$, $\mathbf{Dg}3 = \mathbf{C}_2\mathbf{T} = \mathrm{gr}\{C_2, (I|1\,0), (I|0\,1)\}$ and $\mathbf{Dg}6 = \mathbf{C}_{2h}\mathbf{T} = \mathrm{gr}\{C_2, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the elements $C_2\sigma_h$ or C_2 from the irrs of the groups **Dg**1 and **Dg**4 (table 2). The quasiangular momentum m takes on the values 0 and 1. The irreducible domain is presented in figure 1(*b*).

Irr	D	C_2 or $C_2\sigma_h$	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
$\Gamma_m^{\pm}$	1	$(-1)^m$	±1	1	1
$\mathrm{X}_m^{\pm}$	1	$(-1)^m$	±1	-1	1
$\mathrm{Y}_m^{\pm}$	1	$(-1)^m$	±1	1	-1
$\mathrm{M}_m^{\pm}$	1	$(-1)^m$	±1	-1	-1
${}_kG^{\pm}$	2	A_2	$\pm I_2$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k_1} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k_1}\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k_2} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k_2}\end{pmatrix}$

Table 4. The irrs of the oblique diperiodic group $\mathbf{Dg}7 = \mathbf{C}_2\mathbf{T}_h = \mathrm{gr}\{C_2, (I|1\,0), (\sigma_h|0\,\frac{1}{2})\}$ induced by the element $(\sigma_h|0\frac{1}{2})$ from the irrs of the group **Dg**3 (table 3). The quasiangular momentum m takes on the values 0 and 1. The irreducible domain is presented in figure 1(*b*).

Irr	D	C_2	$(\sigma_h\|0\,\frac{1}{2})$	$(I\|1\,0)$
$\Gamma_m^{\pm}$	1	$(-1)^m$	±1	1
$\mathrm{X}_m^{\pm}$	1	$(-1)^m$	±1	-1
Y	2	A_2	$\begin{pmatrix}\mathrm{i} & 0\\ 0 & -\mathrm{i}\end{pmatrix}$	I_2
M	2	A_2	$\begin{pmatrix}-\mathrm{i} & 0\\ 0 & \mathrm{i}\end{pmatrix}$	$-I_2$
${}_kG^{\pm}$	2	A_2	$\pm\begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{k_2}{2}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k_2}{2}}\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k_1} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k_1}\end{pmatrix}$

These five 2D generalized translational groups form the lattices classified according to the four holohedries: the oblique (holohedry $\mathbf{C}_{2h}$; arbitrary angle between the translational directions, with different periods), the rectangular ($\mathbf{D}_{2h}$; orthogonal translational directions with different periods), the square one ($\mathbf{D}_{4h}$; orthogonal translational directions and equal periods) and the hexagonal one ($\mathbf{D}_{6h}$; the angle $2\pi/3$ between the translational directions with the equal periods) [2]. If together with the primitive rectangular translations $\boldsymbol{a}$ and $\boldsymbol{b}$, the lattice contains the vector $\frac{1}{2}(\boldsymbol{a}+\boldsymbol{b})$, it is called the centred rectangular, to differ from the primitive ones (these generalized translational groups are emphasized by primes in the text).

Depending on the type of the lattice, various orthogonal symmetries can be involved. They combine into the point factors, being the axial point groups, [6], leaving the z-axis invariant. Since the crystallographic conditions on the order of the principal axis of rotation must be imposed (analogously to the space groups, but in the contrast to the line groups), the

Table 5. The irrs of the rectangular primitive diperiodic groups **Dg**8 = $\mathbf{D}_1\mathbf{T}$ = gr$\{U_x, (I|1\,0), (I|0\,1)\}$, **Dg**11 = $\mathbf{C}_{1v}\mathbf{T}$ = gr$\{\sigma_x, (I|1\,0), (I|0\,1)\}$ and **Dg**24 = $\mathbf{D}_{1h}\mathbf{T}$ = gr$\{U_x, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the elements U_x and σ_x from the irrs of the groups **Dg**1 and **Dg**4 (table 2). The irreducible domain is presented in figure 2(*a*).

Irr	D	σ_x or U_x	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
${}^v_k\Delta^\pm$	1	$(-1)^v$	± 1	e^{ik}	1
${}^v_k\Upsilon^\pm$	1	$(-1)^v$	± 1	e^{ik}	-1
${}_kG^\pm$	2	A_2	$\pm I_2$	$e^{ik_x} I_2$	$\begin{pmatrix} e^{ik_y} & 0 \\ 0 & e^{-ik_y} \end{pmatrix}$

Table 6. The irrs of the rectangular primitive diperiodic groups **Dg**14 = $\mathbf{D}_{1d}\mathbf{T}$ = gr$\{C_2\sigma_h, \sigma_x, (I|1\,0), (I|0\,1)\}$, **Dg**19 = $\mathbf{D}_2\mathbf{T}$ = gr$\{C_2, U_x, (I|1\,0), (I|0\,1)\}$, **Dg**23 = $\mathbf{C}_{2v}\mathbf{T}$ = gr$\{C_2, \sigma_x, (I|1\,0), (I|0\,1)\}$ and **Dg**37 = $\mathbf{D}_{2h}\mathbf{T}$ = gr$\{C_2, U_x, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the elements U_x and σ_x from the irrs of the groups **Dg**2, **Dg**3 and **Dg**6 (table 3). The irreducible domain is presented in figure 2(*b*). The quasi angular momentum m takes on the values 0 and 1. Here, $K_2 = \mathrm{diag}\,(e^{ik_x}, e^{-ik_x})$.

Irr	D	C_2 or $C_2\sigma_h$	σ_x or U_x	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
${}^v\Gamma^\pm_m$	1	$(-1)^m$	$(-1)^v$	± 1	1	1
${}^vX^\pm_m$	1	$(-1)^m$	$(-1)^v$	± 1	-1	1
${}^vY^\pm_m$	1	$(-1)^m$	$(-1)^v$	± 1	1	-1
${}^vM^\pm_m$	1	$(-1)^m$	$(-1)^v$	± 1	-1	-1
${}^v_k\Delta^\pm$	2	A_2	$(-1)^v I_2$	$\pm I_2$	$\begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}$	I_2
${}^v_k\Upsilon^\pm$	2	A_2	$(-1)^v I_2$	$\pm I_2$	$\begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}$	$-I_2$
${}^v_k\Phi^\pm$	2	A_2	$(-1)^v A_2$	$\pm I_2$	I_2	$\begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}$
${}^v_k\Lambda^\pm$	2	A_2	$(-1)^v A_2$	$\pm I_2$	$-I_2$	$\begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}$
${}_kG^\pm$	4	$\begin{pmatrix} A_2 & 0 \\ 0 & A_2 \end{pmatrix}$	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\pm I_4$	$\begin{pmatrix} K_2 & 0 \\ 0 & K_2 \end{pmatrix}$	$\begin{pmatrix} e^{ik_y} & 0 & 0 \\ 0 & e^{-ik_y} I_2 & 0 \\ 0 & 0 & e^{ik_y} \end{pmatrix}$

possible point factors are: $\mathbf{C}_n$, $\mathbf{C}_{nv}$, $\mathbf{C}_{nh}$, $\mathbf{D}_n$, and $\mathbf{D}_{nh}$ for $n = 1, 2, 3, 4$ and 6; $\mathbf{D}_{nd}$ and $\mathbf{S}_{2n}$ for $n = 1$, 2 and 3. These are also the possible isogonal point groups, which are obtained by adding the orthogonal part of the generalized translational generators to the point factor (thus the point factor **P** is either the isogonal point group, or its index-2 subgroup). The list of all diperiodic groups (in the numerical, [1], and international notation), factorized in the described form **PZ**, is given in table 1.

The factorization is utilized in the construction of the irrs. First, it immediately gives the generators of the diperiodic groups: two generators for the generalized translational factor, **Z**, and at most three additional generators of the point factor **P**. Since the representation of a group is completely determined by the matrices representing the generators, the irrs of the diperiodic groups are tabulated in the next section by giving at most five matrices. Further, the factorization straightforwardly gives an optimal method for the construction of irrs. Namely, it enables us to classify the groups into the chains, so that each member of a chain is an index-2 subgroup of the next one. This is necessary in order to apply, whenever it is

Table 7. The irrs of the rectangular primitive diperiodic groups **Dg**9 = $\mathbf{2}_1$ = gr$\{(I|1\,0),(U_y|0\,\frac{1}{2})\}$, **Dg**12 = $\mathbf{T}_v$ = gr$\{(I|1\,0),(\sigma_y|0\,\frac{1}{2})\}$, **Dg**25 = $\mathbf{C}_{1h}\mathbf{2}_1$ = gr$\{\sigma_h,(I|1\,0),(U_y|0\,\frac{1}{2})\}$, **Dg**26 = $\mathbf{C}_{1v}\mathbf{2}_1$ = gr$\{\sigma_y,(I|1\,0),(U_y|0\,\frac{1}{2})\}$ and **Dg**27 = $\mathbf{D}_1\mathbf{T}_v$ = gr$\{U_y,(I|1\,0),(\sigma_y|0\,\frac{1}{2})\}$. The irrs of the first three groups are induced by the elements $(U_y|0\,\frac{1}{2})$ and $(\sigma_y|0\,\frac{1}{2})$ from the groups **Dg**1 and **Dg**4 (table 2), while the irrs of **Dg**26 and **Dg**27 are induced by the elements σ_y and U_y from the irrs of the groups **Dg**9 and **Dg**12. The irreducible domain is presented in figure 2(*c*).

Irr	D	σ_h	σ_y or U_y	$(\sigma_y|0\,\frac{1}{2})$ or $(U_y|0\,\frac{1}{2})$	$(I|1\,0)$
${}^{v}_{k}\Phi^{\pm}$	1	±1	$(-1)^{v_1}$	$(-1)^{v}\mathrm{e}^{\mathrm{i}\frac{k}{2}}$	1
${}^{v}_{k}\Lambda^{\pm}$	1	±1	$(-1)^{v_1}$	$(-1)^{v}\mathrm{e}^{\mathrm{i}\frac{k}{2}}$	-1
${}_{\boldsymbol{k}}G^{\pm}$	2	$\pm I_2$	$(-1)^{v}\begin{pmatrix}0 & \mathrm{e}^{\mathrm{i}\frac{k_y}{2}}\\ \mathrm{e}^{-\mathrm{i}\frac{k_y}{2}} & 0\end{pmatrix}$	$\begin{pmatrix}0 & \mathrm{e}^{\mathrm{i}k_y}\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k_x} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k_x}\end{pmatrix}$

Table 8. The irrs of the rectangular primitive diperiodic groups **Dg**15 = $\mathbf{S}_2\mathbf{2}_1$ = gr$\{C_2\sigma_h,(I|1\,0),(U_y|0\,\frac{1}{2})\}$, **Dg**17 = $\mathbf{S}_2\mathbf{T}_v$ = gr$\{C_2\sigma_h,(I|1\,0),(\sigma_y|0\,\frac{1}{2})\}$, **Dg**20 = $\mathbf{C}_2\mathbf{2}_1$ = gr$\{C_2,(I|1\,0),(U_y|0\,\frac{1}{2})\}$, **Dg**28 = $\mathbf{C}_2\mathbf{T}_v$ = gr$\{C_2,(I|1\,0),(\sigma_y|0\,\frac{1}{2})\}$ and **Dg**40 = $\mathbf{C}_{2h}\mathbf{T}_v$ = gr$\{C_2,\sigma_h,(I|1\,0),(\sigma_y|0\,\frac{1}{2})\}$ induced by the element C_2 or $\sigma_h C_2$ from the irrs of the groups **Dg**9, **Dg**12 and **Dg**25 (table 7). The irreducible domain is presented in figure 2(*b*). The quasiangular momentum m takes on the values 0 and 1. Here, $L_2=\begin{pmatrix}0 & \mathrm{e}^{\mathrm{i}k_y}\\ 1 & 0\end{pmatrix}$.

Irr	D	C_2 or $C_2\sigma_h$	σ_h	$(\sigma_y|0\,\frac{1}{2})$ or $(U_y|0\,\frac{1}{2})$	$(I|1\,0)$
${}^{v}\Gamma^{\pm}_{m}$	1	$(-1)^m$	±1	$(-1)^v$	1
${}^{v}X^{\pm}_{m}$	1	$(-1)^m$	±1	$(-1)^v$	-1
$Y^{\pm}$	2	A_2	$\pm I_2$	$\begin{pmatrix}\mathrm{i} & 0\\ 0 & -\mathrm{i}\end{pmatrix}$	I_2
$M^{\pm}$	2	A_2	$\pm I_2$	$\begin{pmatrix}\mathrm{i} & 0\\ 0 & -\mathrm{i}\end{pmatrix}$	$-I_2$
${}^{v}_{k}\Phi^{\pm}$	2	A_2	$\pm I_2$	$(-1)^v\begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}}\end{pmatrix}$	I_2
${}^{v}_{k}\Lambda^{\pm}$	2	A_2	$\pm I_2$	$(-1)^v\begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}}\end{pmatrix}$	$-I_2$
${}_{k}\Delta^{\pm}_{m}$	2	$(-1)^m A_2$	$\pm I_2$	A_2	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k}\end{pmatrix}$
${}_{k}\Upsilon^{\pm}_{m}$	2	$(-1)^m A_2$	$\pm I_2$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k}\end{pmatrix}$
${}_{\boldsymbol{k}}G^{\pm}$	4	$\begin{pmatrix}0 & I_2\\ I_2 & 0\end{pmatrix}$	$\pm I_4$	$\begin{pmatrix}L_2 & 0\\ 0 & L_2^{-1}\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k_x} & 0 & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k_x}I_2 & 0\\ 0 & 0 & \mathrm{e}^{\mathrm{i}k_x}\end{pmatrix}$

possible, the simplest method of construction—the induction from the index-2 subgroup, [7]. The starting group in each chain is either with known irrs (i.e. it belongs to some other chain), or it is the direct or the semidirect product of its two Abelian subgroups, with the elaborated techniques of the construction of irrs [8, 7]. Hence, depending on the structure of the diperiodic group, one of these three methods of constructing their irrs is applied. Some necessary details about these methods are briefly sketched in the appendix.

Table 9. The irrs of the rectangular primitive diperiodic groups **Dg**29 = $\mathbf{D}_1\mathbf{T}_h$ = gr$\{U_x, (I|1\,0), (\sigma_h|0\,\frac{1}{2})\}$ and **Dg**30 = 2_1T_h = gr$\{(U_x|\frac{1}{2}\,0), (\sigma_h|0\,\frac{1}{2})\}$ induced by the elements $(U_x|\frac{1}{2}\,0)$ and U_x from the irrs of the group **Dg**5 (table 2). The irreducible domain is presented in figure 2(*a*).

Irr	D	U_x	$(U_x\|\frac{1}{2}\,0)$	$(\sigma_h\|0\,\frac{1}{2})$	$(I\|1\,0)$
${}^{v}_{k}\Delta^{\pm}$	1	$(-1)^v$	$(-1)^v e^{i\frac{k}{2}}$	± 1	e^{ik}
${}_{k}\Upsilon$	2	A_2	$\begin{pmatrix} 0 & e^{ik} \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$e^{ik} I_2$
${}_{\boldsymbol{k}}G^{\pm}$	2	A_2	$\begin{pmatrix} 0 & e^{ik_x} \\ 1 & 0 \end{pmatrix}$	$\pm\begin{pmatrix} e^{i\frac{k_y}{2}} & 0 \\ 0 & e^{-i\frac{k_y}{2}} \end{pmatrix}$	$e^{ik_x} I_2$

Table 10. The irrs of the rectangular primitive diperiodic group **Dg**45 = $\mathbf{C}_2 2_1 T_h$ = gr$\{C_2, (U_x|\frac{1}{2}\,0), (\sigma_h|0\,\frac{1}{2})\}$ induced by the element C_2 from the group **Dg**30 (table 9). The irreducible domain is presented in figure 2(*b*). The quasi angular momentum m takes on the values 0 and 1. Here, $L_2(k) = \begin{pmatrix} 0 & e^{ik} \\ 1 & 0 \end{pmatrix}$ and $K_2 = \mathrm{diag}\,(e^{i\frac{k_y}{2}}, e^{-i\frac{k_y}{2}})$.

Irr	D	C_2	$(U_x\|\frac{1}{2}\,0)$	$(\sigma_h\|0\,\frac{1}{2})$
${}^{v}\Gamma^{\pm}_{m}$	1	$(-1)^m$	$(-1)^v$	± 1
$X^{\pm}$	2	A_2	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\pm I_2$
Y_m	2	$(-1)^m A_2$	A_2	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$
M_m	2	$(-1)^m A_2$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$
${}^{v}_{k}\Delta^{\pm}$	2	A_2	$(-1)^v \begin{pmatrix} e^{i\frac{k}{2}} & 0 \\ 0 & e^{-i\frac{k}{2}} \end{pmatrix}$	$\pm I_2$
${}_{k}\Lambda^{\pm}_{m}$	2	$(-1)^m A_2$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\pm\begin{pmatrix} e^{i\frac{k}{2}} & 0 \\ 0 & e^{-i\frac{k}{2}} \end{pmatrix}$
${}_{k}\Phi^{\pm}_{m}$	2	$(-1)^m A_2$	A_2	$\pm\begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}$
${}_{k}\Upsilon$	4	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} L_2(k) & 0 \\ 0 & L_2(k)^{-1} \end{pmatrix}$	$\begin{pmatrix} i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}$
${}_{\boldsymbol{k}}G^{\pm}$	4	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} L_2(k_x) & 0 \\ 0 & L_2(k_x)^{-1} \end{pmatrix}$	$\pm\begin{pmatrix} K_2 & 0 \\ 0 & K_2^{*} \end{pmatrix}$

3. The irreducible representations (irrs)

In this section, the irrs of the diperiodic groups are tabulated. Most of the tables present the irrs of several diperiodic groups. If the group **Dg** is generated by the set $\{g_1, g_2, \ldots\}$, this is denoted in the caption as **Dg** = gr$\{g_1, g_2, \ldots\}$. The symbols of the generators are: C_n is the rotation for $2\pi/n$ around the z-axis, σ_h is the horizontal mirror plane, while σ_x, σ_y and σ are the vertical mirror planes containing the x-axis, y-axis and the axis $x = y$, respectively; rotations for π around x-axis, y-axis and the line $x = y$ are denoted by U_x, U_y and U. The Koster–Seitz notation is used for the generators of the generalized translations: $(A|xy)$ is the orthogonal transformation A followed by the translations for x and y along

Table 11. The irrs of the rectangular primitive diperiodic groups **Dg**38 $= \mathbf{D}_2\mathbf{T}_h = \mathrm{gr}\{C_2, U_y, (I|1\,0), (\sigma_h|0\,\frac{1}{2})\}$ and **Dg**41 $= \mathbf{C}_{2v}\mathbf{T}_h = \mathrm{gr}\{C_2, \sigma_y, (I|1\,0), (\sigma_h|0\,\frac{1}{2})\}$ induced by the element U_y or σ_y from the irrs of the group **Dg**7 (table 4). The irreducible domain is presented in figure 2(*b*). The quasi angular momentum m takes on the values 0 and 1. Here, $K_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}\frac{k_y}{2}}, \mathrm{e}^{-\mathrm{i}\frac{k_y}{2}})$.

Irr	D	C_2	σ_y or U_y	$(\sigma_h\|0\frac{1}{2})$	$(I\|1\,0)$
${}^{v}\Gamma_m^{\pm}$	1	$(-1)^m$	$(-1)^v$	± 1	1
${}^{v}X_m^{\pm}$	1	$(-1)^m$	$(-1)^v$	± 1	-1
${}^{v}Y_{(0,1)}$	2	A_2	$(-1)^v I_2$	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	I_2
${}^{v}M_{(0,1)}$	2	A_2	$(-1)^v I_2$	$\begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix}$	$-I_2$
${}_k^v\Delta^{\pm}$	2	A_2	$(-1)^v A_2$	$\pm I_2$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}k} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k} \end{pmatrix}$
${}_k^v\Phi^{\pm}$	2	A_2	$(-1)^v I_2$	$\pm\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} \end{pmatrix}$	I_2
${}_k^v\Lambda^{\pm}$	2	A_2	$(-1)^v I_2$	$\pm\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} \end{pmatrix}$	$-I_2$
${}_k\Upsilon$	4	$\begin{pmatrix} A_2 & 0 \\ 0 & A_2 \end{pmatrix}$	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} \mathrm{i} & 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 & 0 \\ 0 & 0 & \mathrm{i} & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{pmatrix}$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}k} & 0 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k} I_2 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}k} \end{pmatrix}$
${}_{\mathbf{k}}G^{\pm}$	4	$\begin{pmatrix} A_2 & 0 \\ 0 & A_2 \end{pmatrix}$	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\pm\begin{pmatrix} K_2 & 0 \\ 0 & K_2 \end{pmatrix}$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}k_x} & 0 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k_x} I_2 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}k_x} \end{pmatrix}$

the corresponding directions.

To find the representations of the group **Dg**, only the matrices corresponding to these generators are to be taken. Each row of a table gives one or more irrs of the groups enumerated in the caption. In the first column, the symbol of the representation is indicated, and its dimension follows in column 2. The matrices of the generators are listed in the remaining columns. Some additional explanations, given in the captions of the tables, are necessary to describe the specific notion and the range of the quantum numbers.

The general label of the representation, ${}_k^{v,t}D_m^{\pm}$, emphasizes the symmetry-based quantum numbers of the corresponding states. The left subscript **k** is the wavevector, taking the values from the irreducible (basic) domain of the Brillouin zone (shaded part in the figures). The Brillouin zones are chosen as the oblique, rectangular, square and hexagonal. There are eight types of the irreducible domains [9], drawn in figures 1–4, and each table refers to one of these domains, specified in the caption. It is either the whole Brillouin zone, or the part of it ($\frac{1}{2}$, $\frac{1}{3}$, $\frac{1}{4}$, $\frac{1}{6}$, $\frac{1}{8}$, $\frac{1}{12}$). Only the heavy lines and the full curves at the boundary of the basic domain belong to the domain (when necessary, the empty circles specify the boundary points excluded from the domain). If the boundary point or line is special, i.e. with the representations differing from those in the adjacent points, it is additionally labelled at the corresponding figure. The basic symbol, D, specifies the type of the position in the zone: G stands for the general interior point of the domain, $\boldsymbol{k} = (k_1, k_2)$, while the other letters denote the special points (Γ, X, Y, M, Q and Q') and the special lines (Δ, Λ, Σ, Σ', Υ and Φ). Note that the translational periods are used as the unit lengths along the corresponding directions.

The components k_1 and k_2 of the quasimomentum vector $\boldsymbol{k}$ are conjugated to the

Table 12. The irrs of the rectangular primitive diperiodic group $\mathbf{Dg}43 = \mathbf{D}_1 2_1 T_h = \mathrm{gr}\{U_y, (U_x|\frac{1}{2}\,0), (\sigma_h|0\,\frac{1}{2})\}$ induced by the element U_y from the irrs of the group $\mathbf{Dg}30$ (table 9). The irreducible domain is presented in figure 2(*b*). Here, $L_2(k) = \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}k} \\ 1 & 0 \end{pmatrix}$ and $K_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}\frac{k_y}{2}}, \mathrm{e}^{-\mathrm{i}\frac{k_y}{2}})$.

Irr	D	U_y	$(U_x\|\frac{1}{2}\,0)$	$(\sigma_h\|0\,\frac{1}{2})$
${}^v\Gamma^{\pm}$	1	$(-1)^{v_y}$	$(-1)^{v_x}$	± 1
$X^{\pm}$	2	A_2	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	$\pm I_2$
${}^vY$	2	$(-1)^v I_2$	A_2	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$
${}^vM$	2	$(-1)^v \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$
${}^v_k\Delta^{\pm}$	2	A_2	$(-1)^v \begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} \end{pmatrix}$	$\pm I_2$
${}^v_k\Phi^{\pm}$	2	$(-1)^v I_2$	A_2	$\pm \begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} \end{pmatrix}$
${}^v_k\Lambda^{\pm}$	2	$(-1)^v \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\pm \begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} \end{pmatrix}$
${}_k\Upsilon$	4	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} L_2(k) & 0 \\ 0 & L_2(k)^{-1} \end{pmatrix}$	$\begin{pmatrix} \mathrm{i} & 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 & 0 \\ 0 & 0 & \mathrm{i} & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{pmatrix}$
${}_kG^{\pm}$	4	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} L_2(k_x) & 0 \\ 0 & L_2(k_x)^{-1} \end{pmatrix}$	$\pm \begin{pmatrix} K_2 & 0 \\ 0 & K_2 \end{pmatrix}$

Table 13. The irrs of the rectangular centered diperiodic groups $\mathbf{Dg}10 = \mathbf{D}_1\mathbf{T}' = \mathrm{gr}\{U_x, (I|1\,0), (I|\frac{1}{2}\,\frac{1}{2})\}$, $\mathbf{Dg}13 = \mathbf{C}_{1v}\mathbf{T}' = \mathrm{gr}\{\sigma_x, (I|1\,0), (I|\frac{1}{2}\,\frac{1}{2})\}$, $\mathbf{Dg}35 = \mathbf{D}_{1h}\mathbf{T}' = \mathrm{gr}\{U_x, \sigma_h, (I|1\,0), (I|\frac{1}{2}\,\frac{1}{2})\}$ and the rectangular primitive diperiodic groups $\mathbf{Dg}31 = \mathbf{D}_1\mathbf{T}'_h = \mathrm{gr}\{U_x, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$, $\mathbf{Dg}32 = \mathbf{C}_{1v}\mathbf{T}'_h = \mathrm{gr}\{\sigma_x, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$, induced by the elements $(I|\frac{1}{2}\,\frac{1}{2})$ and $(\sigma_h|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the groups $\mathbf{Dg}8$, $\mathbf{Dg}11$ and $\mathbf{Dg}24$ (table 5). The irreducible domain is presented in figure 2(*a*).

Irr	D	σ_x or U_x	σ_h	$(I\|1\,0)$	$(I\|\frac{1}{2}\,\frac{1}{2})$	$(\sigma_h\|\frac{1}{2}\,\frac{1}{2})$
${}^{v,t}_k\Delta^{\pm}$	1	(-1)^v	± 1	$\mathrm{e}^{\mathrm{i}k}$	$(-1)^t \mathrm{e}^{\mathrm{i}\frac{k}{2}}$	$\pm \mathrm{e}^{\mathrm{i}\frac{k}{2}}$
${}_k\Upsilon^{\pm}$	2	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\pm I_2$	$\mathrm{e}^{\mathrm{i}k} I_2$	$\begin{pmatrix} 0 & -\mathrm{e}^{\mathrm{i}k} \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -\mathrm{e}^{\mathrm{i}k} \\ 1 & 0 \end{pmatrix}$
${}^t_kG^{\pm}$	2	A_2	$\pm I_2$	$\mathrm{e}^{\mathrm{i}k_x} I_2$	$(-1)^t \begin{pmatrix} \mathrm{e}^{\frac{\mathrm{i}}{2}(k_x+k_y)} & 0 \\ 0 & \mathrm{e}^{\frac{\mathrm{i}}{2}(k_x-k_y)} \end{pmatrix}$	$\pm \begin{pmatrix} \mathrm{e}^{\frac{\mathrm{i}}{2}(k_x+k_y)} & 0 \\ 0 & \mathrm{e}^{\frac{\mathrm{i}}{2}(k_x-k_y)} \end{pmatrix}$

translational directions of the 2D generalized translational group. For rectangular and square diperiodic groups, k_1 and k_2 are the Cartesian coordinates k_x and k_y, respectively. The right subscript m is the quasiangular momentum; it takes on the integer values specified in the table captions. The quantum numbers v and t take on the values 0 and 1. The first one is the parity of the mirror symmetry in the vertical planes, or of the rotation for π around the horizontal axes. The second one, t, refers to the rectangular centred groups only, being related to the element $(I|\frac{1}{2}\frac{1}{2})$. The $\pm$ signs are reserved for the symmetry of the horizontal plane σ_h, or of the glide plane $(\sigma_h|\frac{1}{2}\frac{1}{2})$.

Table 14. The irrs of the rectangular centered diperiodic groups **Dg**16 = $\mathbf{D}_{1d}\mathbf{T}'$ = gr$\{C_2\sigma_h, \sigma_x, (I|1\,0), (I|\frac{1}{2}\,\frac{1}{2})\}$, **Dg**22 = $\mathbf{D}_2\mathbf{T}'$ = gr$\{C_2, U_x, (I|1\,0), (I|\frac{1}{2}\,\frac{1}{2})\}$, **Dg**34 = $\mathbf{C}_{2v}\mathbf{T}'$ = gr$\{C_2, \sigma_x, (I|1\,0), (I|\frac{1}{2}\,\frac{1}{2})\}$ and **Dg**47 = $\mathbf{D}_{2h}\mathbf{T}'$ = gr$\{C_2, U_x, \sigma_h, (I|1\,0), (I|\frac{1}{2}\,\frac{1}{2})\}$ induced by the element $(I|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the groups **Dg**14, **Dg**19, **Dg**23 and **Dg**37 (table 6). The irreducible domain is presented in figure 2(*b*). The quasiangular momentum takes on the values 0 and 1. Here, $K_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k_x}, \mathrm{e}^{-\mathrm{i}k_x})$, $L_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{-\mathrm{i}k})$ and $K_4 = \mathrm{diag}\,(\mathrm{e}^{\frac{\mathrm{i}}{2}(k_x+k_y)}, \mathrm{e}^{-\frac{\mathrm{i}}{2}(k_x+k_y)}, \mathrm{e}^{\frac{\mathrm{i}}{2}(k_x-k_y)}, \mathrm{e}^{-\frac{\mathrm{i}}{2}(k_x-k_y)})$.

Irr	D	C_2 or $C_2\sigma_h$	σ_x or U_x	σ_h	$(I\|1\,0)$	$(I\|\frac{1}{2}\,\frac{1}{2})$
${}^{v,t}\Gamma_m^{\pm}$	1	$(-1)^m$	$(-1)^v$	± 1	1	$(-1)^t$
${}^{v}X_{(0,1)}^{\pm}$	2	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$(-1)^v I_2$	$\pm I_2$	$-I_2$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$
${}^{v}Y^{\pm}$	2	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$(-1)^v \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$\pm I_2$	I_2	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$
$M_m^{\pm}$	2	$(-1)^m I_2$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$\pm I_2$	$-I_2$	A_2
${}^{v,t}_{k}\Delta^{\pm}$	2	A_2	$(-1)^v I_2$	$\pm I_2$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k}\end{pmatrix}$	$(-1)^t \begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}}\end{pmatrix}$
${}^{v,t}_{k}\Phi^{\pm}$	2	A_2	$(-1)^v A_2$	$\pm I_2$	I_2	$(-1)^t \begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}}\end{pmatrix}$
${}_{k}\Upsilon^{\pm}$	4	$\begin{pmatrix}A_2 & 0 & 0\\ 0 & 0 & -\mathrm{e}^{-\mathrm{i}k}\\ 0 & -\mathrm{e}^{\mathrm{i}k} & 0\end{pmatrix}$	$\begin{pmatrix}I_2 & 0\\ 0 & -I_2\end{pmatrix}$	$\pm I_4$	$\begin{pmatrix}L_2 & 0\\ 0 & L_2\end{pmatrix}$	$\begin{pmatrix}0 & -L_2\\ I_2 & 0\end{pmatrix}$
${}_{k}\Lambda^{\pm}$	4	$\begin{pmatrix}A_2 & 0 & 0\\ 0 & 0 & -\mathrm{e}^{-\mathrm{i}k}\\ 0 & -\mathrm{e}^{\mathrm{i}k} & 0\end{pmatrix}$	$\begin{pmatrix}A_2 & 0 & 0\\ 0 & 0 & \mathrm{e}^{-\mathrm{i}k}\\ 0 & \mathrm{e}^{\mathrm{i}k} & 0\end{pmatrix}$	$\pm I_4$	$-I_4$	$\begin{pmatrix}0 & -L_2\\ I_2 & 0\end{pmatrix}$
${}^{t}_{\boldsymbol{k}}G^{\pm}$	4	$\begin{pmatrix}A_2 & 0\\ 0 & A_2\end{pmatrix}$	$\begin{pmatrix}0 & I_2\\ I_2 & 0\end{pmatrix}$	$\pm I_4$	$\begin{pmatrix}K_2 & 0\\ 0 & K_2\end{pmatrix}$	$(-1)^t K_4$

The method of construction of the irrs is indicated in the caption. As a rule, the irrs of the translational subgroup are found first, then the rotations around z-axis are included (the translations being an Abelian invariant subgroup). This group and its irrs are the starting point for the chain of successive inductions (from the index-2 subgroup) procedures, until the whole group being incorporated.

Some abbreviations, necessary to make the tables clear, are listed separately for each type of groups. Throughout the text, the n-dimensional identity matrix is denoted by I_n, while A_n stands for the off-diagonal matrix $A_n = \mathrm{offdiag}\,(\underbrace{1, \ldots, 1}_{n})$.

3.1. The irrs of the oblique groups

The diperiodic groups with the primitive translations making an arbitrary angle are **Dg**1–**Dg**7. Their irrs are listed in tables 2–4. Since the groups with different angles between the translational periods are isomorphic, their representations are the same; therefore, although in figure 1, the rectangular irreducible domains are depicted, suitable for the construction of the irrs of other groups, the figures refer equally well to the most general case. The diperiodic groups **Dg**1, **Dg**4 and **Dg**5 are the direct products and their irrs are obtained as the products of the relevant subgroup irrs.

Table 15. The irrs of the rectangular primitive diperiodic groups **Dg**18 = $\mathbf{S}_2\mathbf{T}'_v$ = gr$\{C_2\sigma_h, (I|1\,0), (\sigma_y|\frac{1}{2}\,\frac{1}{2})\}$, **Dg**21 = $\mathbf{C}_2\mathbf{2}'_1$ = gr$\{C_2, (I|1\,0), (U_y|\frac{1}{2}\,\frac{1}{2})\}$, **Dg**33 = $\mathbf{C}_2\mathbf{T}'_v$ = gr$\{C_2, (I|1\,0), (\sigma_y|\frac{1}{2}\,\frac{1}{2})\}$ and **Dg**44 = $\mathbf{C}_{2h}\mathbf{T}'_v$ = gr$\{C_2, \sigma_h, (I|1\,0), (\sigma_y|\frac{1}{2}\,\frac{1}{2})\}$ induced by the elements $(\sigma_y|\frac{1}{2}\,\frac{1}{2})$ and $(U_y|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the groups **Dg**2, **Dg**3 and **Dg**6 (table 3). The irreducible domain is presented in figure 2(*b*). The quasiangular momentum m takes on the values 0 and 1.

Irr	D	C_2 or $C_2\sigma_h$	σ_h	$(\sigma_y\|\frac{1}{2}\,\frac{1}{2})$ or $(U_y\|\frac{1}{2}\,\frac{1}{2})$	$(I\|1\,0)$
${}^v\Gamma_m^{\pm}$	1	$(-1)^m$	± 1	$(-1)^v$	1
${}^vM_m^{\pm}$	1	$(-1)^m$	± 1	$(-1)^v$	-1
$X^{\pm}$	2	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\pm I_2$	A_2	$-I_2$
$Y^{\pm}$	2	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\pm I_2$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	I_2
${}_k^v\Delta^{\pm}$	2	A_2	$\pm I_2$	$(-1)^v \begin{pmatrix} 0 & e^{-i\frac{k}{2}} \\ e^{i\frac{k}{2}} & 0 \end{pmatrix}$	$\begin{pmatrix} e^{ik_x} & 0 \\ 0 & e^{-ik_x} \end{pmatrix}$
${}_k^v\Upsilon^{\pm}$	2	A_2	$\pm I_2$	$(-1)^v \begin{pmatrix} 0 & e^{-i\frac{k}{2}} \\ -e^{i\frac{k}{2}} & 0 \end{pmatrix}$	$\begin{pmatrix} e^{ik_x} & 0 \\ 0 & e^{-ik_x} \end{pmatrix}$
${}_k^v\Phi^{\pm}$	2	A_2	$\pm I_2$	$(-1)^v \begin{pmatrix} e^{i\frac{k}{2}} & 0 \\ 0 & e^{-i\frac{k}{2}} \end{pmatrix}$	I_2
${}_k^v\Lambda^{\pm}$	2	A_2	$\pm I_2$	$(-1)^v \begin{pmatrix} e^{i\frac{k}{2}} & 0 \\ 0 & -e^{-i\frac{k}{2}} \end{pmatrix}$	$-I_2$
${}_kG^{\pm}$	4	$\begin{pmatrix} A_2 & 0 & 0 \\ 0 & 0 & e^{i(k_x-k_y)} \\ 0 & e^{-i(k_x-k_y)} & 0 \end{pmatrix}$	$\pm I_4$	$\begin{pmatrix} 0 & e^{ik_y} & 0 \\ 0 & 0 & e^{-ik_y} \\ I_2 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} e^{ik_x} & 0 & 0 \\ 0 & e^{-ik_x} I_2 & 0 \\ 0 & 0 & e^{ik_x} \end{pmatrix}$

Table 16. The irrs of the rectangular centered diperiodic group **Dg**36 = $\mathbf{D}_1\mathbf{T}_h$ = gr$\{U_y, (I|\frac{1}{2}\,\frac{1}{2}), (\sigma_h|0\,\frac{1}{2})\}$ induced by the elements U_y and $(I|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the group **Dg**5 (table 2). The irreducible domain is presented in figure 2(*c*).

Irr	D	U_y	$(\sigma_h\|0\,\frac{1}{2})$	$(I\|\frac{1}{2}\,\frac{1}{2})$
${}_k^{v,t}\Phi^{\pm}$	1	$(-1)^v$	$\pm e^{i\frac{k_y}{2}}$	$(-1)^t e^{i\frac{k}{2}}$
${}_k\Lambda^{\pm}$	2	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\pm e^{i\frac{k}{2}} I_2$	$\begin{pmatrix} 0 & -e^{ik} \\ 1 & 0 \end{pmatrix}$
${}_k^tG^{\pm}$	2	A_2	$\pm e^{i\frac{k_y}{2}} I_2$	$(-1)^t \begin{pmatrix} e^{\frac{i}{2}(k_x+k_y)} & 0 \\ 0 & e^{-\frac{i}{2}(k_x-k_y)} \end{pmatrix}$

3.2. The irrs of the rectangular groups

The groups **Dg**8–**Dg**48 are rectangular. Among these 41 groups there are 23 with the primitive and 18 with the centred lattice. The irreducible domains are given in figure 2. The irrs are induced from the irrs of the oblique groups with the rectangular translational directions. First, the irrs of the rectangular primitive groups are obtained and afterwards the induction by the nonsymorphic generators $(I|\frac{1}{2}\,\frac{1}{2})$, $(\sigma_h|\frac{1}{2}\,\frac{1}{2})$, $(\sigma|\frac{1}{2}\,\frac{1}{2})$ and $(U|\frac{1}{2}\,\frac{1}{2})$ gives the irrs of the rectangular centred groups.

3.3. The irrs of the square groups

The irrs of the square diperiodic groups **Dg**49–**Dg**64 are presented in tables 19–23 and the corresponding irreducible domains of the Brillouin zone are given in figure 3.

Table 17. The irrs of the rectangular primitive diperiodic groups **Dg**39 = $\mathbf{D}_2\mathbf{T}'_h$ = gr$\{C_2, U_x, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$, **Dg**42 = $\mathbf{D}_{1d}\mathbf{T}'_h$ = gr$\{C_2\sigma_h, U_x, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$ and **Dg**46 = $\mathbf{C}_{2v}\mathbf{T}'_h$ = gr$\{C_2, \sigma_x, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$ induced by the element $(\sigma_h|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the groups **Dg**19, **Dg**14 and **Dg**23, respectively (table 6). The irreducible domain is presented in figure 2(*b*). The angular momentum m takes on the values 0 and 1. Here, $K_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}\frac{k}{2}}, \mathrm{e}^{-\mathrm{i}\frac{k}{2}})$, $L_2(k) = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{-\mathrm{i}k})$ and $K_4 = \mathrm{diag}(\mathrm{e}^{\frac{\mathrm{i}}{2}(k_x+k_y)}, \mathrm{e}^{-\frac{\mathrm{i}}{2}(k_x+k_y)}, \mathrm{e}^{\frac{\mathrm{i}}{2}(k_x-k_y)}, \mathrm{e}^{-\frac{\mathrm{i}}{2}(k_x-k_y)})$.

Irr	D	C_2 or $C_2\sigma_h$	σ_x or U_x	$(\sigma_h\|\frac{1}{2}\,\frac{1}{2})$	$(I\|1\,0)$
${}^v\Gamma_m^\pm$	1	$(-1)^m$	$(-1)^v$	± 1	1
${}^vX_{(1,0)}$	2	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$(-1)^v I_2$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	$-I_2$
${}^vY$	2	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$(-1)^v\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	I_2
M_m	2	$(-1)^m I_2$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	A_2	$-I_2$
${}^v_k\Delta^\pm$	2	A_2	$(-1)^v I_2$	$\pm K_2$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k}\end{pmatrix}$
${}^v_k\Phi^\pm$	2	A_2	$(-1)^v A_2$	$\pm K_2$	I_2
${}_k\Upsilon$	4	$\begin{pmatrix}A_2 & 0 & 0\\ 0 & 0 & -\mathrm{e}^{-\mathrm{i}k}\\ 0 & -\mathrm{e}^{\mathrm{i}k} & 0\end{pmatrix}$	$\begin{pmatrix}I_2 & 0\\ 0 & -I_2\end{pmatrix}$	$\begin{pmatrix}0 & -L_2(k)\\ I_2 & 0\end{pmatrix}$	$\begin{pmatrix}L_2(k) & 0\\ 0 & L_2(k)\end{pmatrix}$
${}_k\Lambda$	4	$\begin{pmatrix}A_2 & 0 & 0\\ 0 & 0 & -\mathrm{e}^{-\mathrm{i}k}\\ 0 & -\mathrm{e}^{\mathrm{i}k} & 0\end{pmatrix}$	$\begin{pmatrix}A_2 & 0 & 0\\ 0 & 0 & \mathrm{e}^{-\mathrm{i}k}\\ 0 & \mathrm{e}^{\mathrm{i}k} & 0\end{pmatrix}$	$\begin{pmatrix}0 & -L_2(k)\\ I_2 & 0\end{pmatrix}$	$-I_4$
${}_kG^\pm$	4	$\begin{pmatrix}A_2 & 0\\ 0 & A_2\end{pmatrix}$	$\begin{pmatrix}0 & I_2\\ I_2 & 0\end{pmatrix}$	$\pm K_4$	$\begin{pmatrix}L_2(k_x) & 0\\ 0 & L_2(k_x)\end{pmatrix}$

The following notation is used:

$$B_4 = \begin{pmatrix}0 & 1\\ I_3 & 0\end{pmatrix} \qquad C_2 = \mathrm{diag}\,(-1, \mathrm{e}^{\mathrm{i}k}) \qquad D_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, -1)$$

$$D_4 = \begin{pmatrix}0 & 0 & 0 & -1\\ \mathrm{e}^{\mathrm{i}k} & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & \mathrm{e}^{-\mathrm{i}k} & 0\end{pmatrix} \qquad E_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}(k_x+k_y)/2}, \mathrm{e}^{\mathrm{i}(k_x-k_y)/2})$$

$$F_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}\frac{k}{2}}, \mathrm{e}^{-\mathrm{i}\frac{k}{2}}) \qquad J_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{-\mathrm{i}k}) \qquad K_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k_x}, \mathrm{e}^{-\mathrm{i}k_y})$$

$$L_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k_y}, \mathrm{e}^{\mathrm{i}k_x}) \qquad P_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, 1) \qquad \text{and} \qquad R_2 = \mathrm{diag}\,(1, \mathrm{e}^{\mathrm{i}k}).$$

3.4. *The irrs of the hexagonal groups*

The irrs of the hexagonal diperiodic groups **Dg**65–**Dg**80 are presented in tables 24–28 and the corresponding irreducible domains of the Brillouin zone are sketched in figure 4. The primitive translations make the angle of $2\pi/3$, while the angle between the basis vectors k_1 and k_2 of the inverse lattice is $\pi/3$.

The following abbreviations are used throughout the tables:

$$B_3 = \begin{pmatrix}0 & 1\\ I_2 & 0\end{pmatrix} \qquad E_3 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}k_1}, \mathrm{e}^{-\mathrm{i}(k_1+k_2)}, \mathrm{e}^{\mathrm{i}k_2}) \qquad J_3 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{\mathrm{i}2k}, \mathrm{e}^{\mathrm{i}k})$$

$$K_2 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}2\frac{\pi}{3}}, \mathrm{e}^{-\mathrm{i}2\frac{\pi}{3}}) \qquad K_3 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{-\mathrm{i}k}, \mathrm{e}^{-2\mathrm{i}k})$$

Table 18. The irrs of the rectangular centered diperiodic group **Dg**48 = $\mathbf{C}_{2v}\mathbf{T}'_h$ = gr$\{C_2, \sigma_y, (I|\frac{1}{2}\,\frac{1}{2}), (\sigma_h|0\,\frac{1}{2})\}$ induced by the element $(I|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the group **Dg**41 (table 11). The irreducible domain is presented in figure 2(*b*). The angular momentum m takes on the values 0 and 1. Here, $K_2(k) = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}\frac{k}{2}}, \mathrm{e}^{-\mathrm{i}\frac{k}{2}})$, $L_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{-\mathrm{i}k})$, $K_4 = \mathrm{diag}\,(\mathrm{e}^{\frac{\mathrm{i}}{2}(k_x+k_y)}, \mathrm{e}^{-\frac{\mathrm{i}}{2}(k_x+k_y)}, \mathrm{e}^{-\frac{\mathrm{i}}{2}(k_x-k_y)}, \mathrm{e}^{\frac{\mathrm{i}}{2}(k_x-k_y)})$ and $L_4 = \mathrm{diag}\,(\mathrm{i}\mathrm{e}^{\frac{\mathrm{i}}{2}k}, -\mathrm{i}\mathrm{e}^{-\frac{\mathrm{i}}{2}k}, \mathrm{i}\mathrm{e}^{-\frac{\mathrm{i}}{2}k}, -\mathrm{i}\mathrm{e}^{\frac{\mathrm{i}}{2}k})$.

Irr	D	C_2	σ_y	$(\sigma_h\|0\,\frac{1}{2})$	$(I\|\frac{1}{2}\,\frac{1}{2})$
${}^{v,t}\Gamma_m^{\pm}$	1	$(-1)^m$	$(-1)^v$	± 1	$(-1)^t$
$X_m^{\pm}$	2	$(-1)^m \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\pm I_2$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
${}^{v,t}Y_{(0,1)}$	2	A_2	$(-1)^v I_2$	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	$(-1)^t \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$
$M_{(0,1)}$	4	$\begin{pmatrix} A_2 & 0 \\ 0 & A_2 \end{pmatrix}$	$\begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$	$\begin{pmatrix} -\mathrm{i} & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & \mathrm{i} \end{pmatrix}$	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$
${}^{v,t}_{k}\Delta^{\pm}$	2	A_2	$(-1)^v A_2$	$\pm I_2$	$(-1)^t K_2(k)$
${}^{v,t}_{k}\Phi^{\pm}$	2	A_2	$(-1)^v I_2$	$\pm K_2(k)$	$(-1)^t K_2(k)$
${}_{k}\Lambda^{\pm}$	4	$\begin{pmatrix} A_2 & 0 & 0 \\ 0 & 0 & -\mathrm{e}^{-\mathrm{i}k} \\ 0 & -\mathrm{e}^{\mathrm{i}k} & 0 \end{pmatrix}$	$\begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$	$\pm \begin{pmatrix} K_2(k) & 0 \\ 0 & K_2(k) \end{pmatrix}$	$\begin{pmatrix} 0 & -L_2 \\ I_2 & 0 \end{pmatrix}$
${}^{t}_{k}\Upsilon$	4	$\begin{pmatrix} A_2 & 0 \\ 0 & A_2 \end{pmatrix}$	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} -\mathrm{i} & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & \mathrm{i} \end{pmatrix}$	$(-1)^t L_4$
${}^{t}_{k}G^{\pm}$	4	$\begin{pmatrix} A_2 & 0 \\ 0 & A_2 \end{pmatrix}$	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\pm \begin{pmatrix} K_2(k_y) & 0 \\ 0 & K_2(k_y) \end{pmatrix}$	$(-1)^t K_4$

Table 19. The irrs of the square diperiodic groups **Dg**49 = $\mathbf{C}_4\mathbf{T}$ = gr$\{C_4, (I|1\,0), (I|0\,1)\}$, **Dg**50 = $\mathbf{S}_4\mathbf{T}$ = gr$\{C_4\sigma_h, (I|1\,0), (I|0\,1)\}$ and **Dg**51 = $\mathbf{C}_{4h}\mathbf{T}$ = gr$\{C_4, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the elements of the groups $\mathbf{C}_4$ and $\mathbf{S}_4$ from the irrs of the groups **Dg**1 and **Dg**4 (table 2). For the $\Gamma_m^{\pm}$ and $\mathrm{M}_m^{\pm}$ the quasiangular momentum m takes on the integer values form the interval $[-1, 2]$, while for the $\mathrm{X}_m^{\pm}$ it takes on the values 0 and 1, only. The irreducible domain of the Brillouin zone is presented in figure 2(*a*).

Irr	D	C_4 or $C_4\sigma_h$	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
$\Gamma_m^{\pm}$	1	i^m	± 1	1	1
$\mathrm{M}_m^{\pm}$	1	i^m	± 1	-1	-1
$\mathrm{X}_m^{\pm}$	2	$\begin{pmatrix} 0 & (-1)^m \\ 1 & 0 \end{pmatrix}$	$\pm I_2$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
${}_{k}G^{\pm}$	4	B_4	$\pm I_4$	$\begin{pmatrix} K_2 & 0 \\ 0 & K_2^* \end{pmatrix}$	$\begin{pmatrix} L_2 & 0 \\ 0 & L_2^* \end{pmatrix}$

$$L_2 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}k_2}, \mathrm{e}^{\mathrm{i}k_1}) \qquad L_3 = \mathrm{diag}(\mathrm{e}^{-\mathrm{i}2k}, \mathrm{e}^{-\mathrm{i}k}, \mathrm{e}^{\mathrm{i}k})$$

$$O_3 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}k_2}, \mathrm{e}^{\mathrm{i}(k_1+k_2)}, \mathrm{e}^{\mathrm{i}k_1}) \qquad P_3 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}k}, 1, \mathrm{e}^{-\mathrm{i}k})$$

$$R_2 = \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}2\frac{\pi}{3}} \\ \mathrm{e}^{\mathrm{i}2\frac{\pi}{3}} & 0 \end{pmatrix} \qquad R_3 = \mathrm{diag}(1, \mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{\mathrm{i}k})$$

and $S_3 = \mathrm{diag}(\mathrm{e}^{\mathrm{i}k_1}, \mathrm{e}^{-\mathrm{i}k_2}, \mathrm{e}^{-\mathrm{i}(k_1+k_2)})$.

Table 20. The irrs of the square diperiodic group $\mathbf{Dg}52 = \mathbf{C}_4\mathbf{T}'_h = \mathrm{gr}\{C_4, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$ induced by the element $(\sigma_h|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the group **Dg**49 (19). For $\Gamma_m^{\pm}$ the quasi angular momentum m takes on the values −1, 0, 1 and 2, and for M_m the possible values are 0 and 1. The irreducible domain of the Brillouin zone is presented in figure 3(*a*).

Irr	D	C_4	$(\sigma_h\|\frac{1}{2}\,\frac{1}{2})$	$(I\|1\,0)$
$\Gamma_m^{\pm}$	1	i^m	± 1	1
M_m	2	$\mathrm{i}^m\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	A_2	$-I_2$
X	4	$\begin{pmatrix}A_2 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & -I_2\\ I_2 & 0\end{pmatrix}$	$\begin{pmatrix}-1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}$
${}_kG^{\pm}$	4	B_4	$\pm\begin{pmatrix}E_2 & 0\\ 0 & E_2^*\end{pmatrix}$	$\begin{pmatrix}K_2 & 0\\ 0 & K_2^*\end{pmatrix}$

Table 21. The irrs of the square diperiodic groups $\mathbf{Dg}53 = \mathbf{D}_4\mathbf{T} = \mathrm{gr}\{C_4, U_x, (I|1\,0), (I|0\,1)\}$, $\mathbf{Dg}55 = \mathbf{C}_{4v}\mathbf{T} = \mathrm{gr}\{C_4, \sigma_x, (I|1\,0), (I|0\,1)\}$, $\mathbf{Dg}57 = \mathbf{D}_{2d}\mathbf{T} = \mathrm{gr}\{C_4\sigma_h, U_x, (I|1\,0), (I|0\,1)\}$, $\mathbf{Dg}59 = \mathbf{D}_{2d}\mathbf{T} = \mathrm{gr}\{C_4\sigma_h, \sigma_x, (I|1\,0), (I|0\,1)\}$ and $\mathbf{Dg}61 = \mathbf{D}_{4h}\mathbf{T} = \mathrm{gr}\{C_4, \sigma_x, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the element U_x and σ_x from the irrs of the groups **Dg**49, **Dg**50 and **Dg**51 (table 19). For ${}^v\Gamma_m^{\pm}$ and ${}^vM_m^{\pm}$ the quasi angular momentum m takes on the values 0 and 2, while for the ${}^vX_m^{\pm}$ it takes on the values 0 and 1. The irreducible domain of the Brillouin zone is presented in figure 3(b).

Irr	D	C_4 or $C_4\sigma_h$	σ_x or U_x	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
${}^v\Gamma_m^{\pm}$	1	i^m	$(-1)^v$	± 1	1	1
${}^vM_m^{\pm}$	1	i^m	$(-1)^v$	± 1	-1	-1
$\Gamma_1^{\pm}$	2	$\begin{pmatrix}\mathrm{i} & 0\\ 0 & -\mathrm{i}\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\pm I_2$	I_2	I_2
$M_1^{\pm}$	2	$\begin{pmatrix}\mathrm{i} & 0\\ 0 & -\mathrm{i}\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\pm I_2$	$-I_2$	$-I_2$
${}^vX_m^{\pm}$	2	$\begin{pmatrix}0 & (-1)^m\\ 1 & 0\end{pmatrix}$	$(-1)^v\begin{pmatrix}1 & 0\\ 0 & (-1)^m\end{pmatrix}$	$\pm I_2$	$\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$
${}_k^v\Sigma^{\pm}$	4	B_4	$(-1)^vA_4$	$\pm I_4$	$\begin{pmatrix}J_2 & 0\\ 0 & J_2^*\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k}I_2 & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k}I_2\end{pmatrix}$
${}_k^v\Delta^{\pm}$	4	B_4	$(-1)^v\begin{pmatrix}1 & 0\\ 0 & A_3\end{pmatrix}$	$\pm I_4$	$\begin{pmatrix}P_2 & 0\\ 0 & P_2^*\end{pmatrix}$	$\begin{pmatrix}R_2 & 0\\ 0 & R_2^*\end{pmatrix}$
${}_k^v\Lambda^{\pm}$	4	B_4	$(-1)^v\begin{pmatrix}A_3 & 0\\ 0 & 1\end{pmatrix}$	$\pm I_4$	$\begin{pmatrix}C_2^* & 0\\ 0 & C_2\end{pmatrix}$	$\begin{pmatrix}D_2 & 0\\ 0 & D_2^*\end{pmatrix}$
${}_kG^{\pm}$	8	$\begin{pmatrix}B_4 & 0\\ 0 & B_4^{-1}\end{pmatrix}$	$\begin{pmatrix}0 & I_4\\ I_4 & 0\end{pmatrix}$	$\pm I_8$	$\begin{pmatrix}K_2 & 0 & 0 & 0\\ 0 & K_2^* & 0 & 0\\ 0 & 0 & K_2 & 0\\ 0 & 0 & 0 & K_2^*\end{pmatrix}$	$\begin{pmatrix}L_2 & 0 & 0 & 0\\ 0 & L_2^* & 0 & 0\\ 0 & 0 & L_2^* & 0\\ 0 & 0 & 0 & L_2\end{pmatrix}$

4. Concluding remarks

Using the factorization (table 1) of the diperiodic groups onto the generalized translational subgroup **Z**, describing the symmetry of the ordering of the elementary motifs, and the axial point group **P**, containing the symmetry of the single motif, the irrs for all of the 80 diperiodic groups are found. They are presented by the matrices of the generators of the groups (tables 2–28).

Table 22. The irrs of the square diperiodic groups $\mathbf{Dg}54 = \mathbf{C}_4\mathbf{2}'_1 = \mathrm{gr}\{C_4, (I|1\,0), (U|\frac{1}{2}\,\frac{1}{2})\}$, $\mathbf{Dg}56 = \mathbf{C}_4\mathbf{T}'_v = \mathrm{gr}\{C_4, (I|1\,0), (\sigma|\frac{1}{2}\,\frac{1}{2})\}$, $\mathbf{Dg}58 = \mathbf{S}_4\mathbf{2}'_1 = \mathrm{gr}\{C_4\sigma_h, (I|1\,0), (U|\frac{1}{2}\,\frac{1}{2})\}$, $\mathbf{Dg}60 = \mathbf{S}_4\mathbf{T}'_v = \mathrm{gr}\{C_4\sigma_h, (I|1\,0), (\sigma|\frac{1}{2}\,\frac{1}{2})\}$ and $\mathbf{Dg}63 = \mathbf{C}_{4h}\mathbf{T}'_v = \mathrm{gr}\{C_4, \sigma_h, (I|1\,0), (\sigma|\frac{1}{2}\,\frac{1}{2})\}$ induced by the elements $(\sigma|\frac{1}{2}\,\frac{1}{2})$ and $(U|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the groups **Dg**49, **Dg**50 and **Dg**51 (table 19). For the irr ${}^{v}\Gamma^{\pm}_{m}$ the quasi angular momentum m takes on the values 0 and 2, while for the irr ${}^{v}M^{\pm}_{m}$ it takes on the values 1 and −1. The irreducible domain of the Brillouin zone is presented in figure 3(*b*). Here, $H_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}(k_x+k_y)}, \mathrm{e}^{\mathrm{i}(k_x-k_y)})$, $O_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{-\mathrm{i}k})$, $S_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k}, 1)$, $N_2 = \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}\frac{k}{2}} \\ \mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0 \end{pmatrix}$, and $C_4 = \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}k_y} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}k_x} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}k_y} \\ \mathrm{e}^{\mathrm{i}k_x} & 0 & 0 & 0 \end{pmatrix}$.

Irr	D	C_4 or $C_4\sigma_h$	σ_h	$(\sigma\|\frac{1}{2}\,\frac{1}{2})$ or $(U\|\frac{1}{2}\,\frac{1}{2})$	$(I\|1\,0)$
${}^{v}\Gamma^{\pm}_{m}$	1	i^m	±1	$(-1)^v$	1
${}^{v}M^{\pm}_{m}$	1	i^m	±1	$(-1)^v$	−1
$\Gamma^{\pm}_{1}$	2	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	$\pm I_2$	A_2	I_2
$M^{\pm}_{0}$	2	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\pm I_2$	A_2	$-I_2$
$X^{\pm}$	4	$\begin{pmatrix} A_2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$	$\pm I_4$	$\begin{pmatrix} 0 & -I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
${}^{v}_{k}\Sigma^{\pm}$	4	B_4	$\pm I_4$	$(-1)^v \begin{pmatrix} \mathrm{e}^{\mathrm{i}k} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}k} & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} O_2 & 0 \\ 0 & O_2^* \end{pmatrix}$
${}^{v}_{k}\Delta^{\pm}$	4	B_4	$\pm I_4$	$(-1)^v \begin{pmatrix} N_2 & 0 \\ 0 & N_2^* \end{pmatrix}$	$\begin{pmatrix} S_2 & 0 \\ 0 & S_2^* \end{pmatrix}$
${}^{v}_{k}\Lambda^{\pm}$	4	B_4	$\pm I_4$	$(-1)^v \begin{pmatrix} 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\frac{k}{2}} \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}\frac{k}{2}} & 0 & 0 \\ -\mathrm{e}^{\mathrm{i}\frac{k}{2}} & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} C_2^* & 0 \\ 0 & C_2 \end{pmatrix}$
${}_{k}G^{\pm}$	8	$\begin{pmatrix} B_4 & 0 \\ 0 & C_4 \end{pmatrix}$	$\pm I_8$	$\begin{pmatrix} 0 & 0 & H_2 & 0 \\ 0 & 0 & 0 & H_2^* \\ I_2 & 0 & 0 & 0 \\ 0 & I_2 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} K_2 & 0 & 0 & 0 \\ 0 & K_2^* & 0 & 0 \\ 0 & 0 & L_2 & 0 \\ 0 & 0 & 0 & L_2^* \end{pmatrix}$

These results enable the full application of symmetry in the studies of the diperiodic physical systems. Although some rare attempts of the symmetry analysis of such systems exist in the literature, they are restricted to the isogonal point groups (IC and Raman spectra, [10], classification of the spin states, [11]), or they use the irrs of the 3D space groups to derive the band representations for a few relevant diperiodic groups, [12]. Also, the relevance of the diperiodic symmetry in the context of the defects at surfaces and interfaces of 3D crystals is notified, [13], but the applications involving the irreducible representations were not available. It is now possible to make some quite general physically relevant conclusions, which are to be mentioned here.

The degeneracy of the quantum levels is equal to the dimension of the corresponding irr. Since the dimension of the irrs is at most 12, this is the maximal orbital degeneracy possible in the diperiodic systems; the other allowed degeneracies are 1, 2, 3, 4, 6 and 8.

The independent good quantum numbers are immediately given by the symbol of the irr. Thus, the diperiodical symmetry generally yields good quantum numbers of quasilinear and quasiangular momenta, and usually one or more types of parities (horizontal and

Table 23. The irrs of the square diperiodic groups $\mathbf{Dg}62 = \mathbf{D}_{2d}\mathbf{T}'_h = \mathrm{gr}\{C_4\sigma_h, U_x, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$ and $\mathbf{Dg}64 = \mathbf{D}_{2d}\mathbf{T}'_h = \mathrm{gr}\{C_4\sigma_h, \sigma_x, (I|1\,0), (\sigma_h|\frac{1}{2}\,\frac{1}{2})\}$ induced by the element $(\sigma_h|\frac{1}{2}\,\frac{1}{2})$ from the irrs of the groups **Dg**57 and **Dg**59 (table 21). The quasiangular momentum m takes on the values 0 and 2. The irreducible domain of the Brillouin zone is presented in figure 3(b). Here, $F_2 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}(k_x-k_y)/2}, \mathrm{e}^{\mathrm{i}(-k_x-k_y)/2})$ and $E_4 = \begin{pmatrix} 0 & 0 & \mathrm{e}^{-\mathrm{i}k} & 0 \\ 0 & -1 & 0 & 0 \\ \mathrm{e}^{\mathrm{i}k} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$.

Irr	D	$C_4\sigma_h$	U_x or σ_x	$(\sigma_h\|\frac{1}{2}\,\frac{1}{2})$	$(I\|1\,0)$
${}^v\Gamma_m^\pm$	1	i^m	$(-1)^v$	± 1	1
$\Gamma_1^\pm$	2	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	A_2	$\pm I_2$	I_2
${}^vM_0$	2	$(-1)^v \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	A_2	$-I_2$
$M_1^\pm$	2	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	A_2	$\pm \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}$	$-I_2$
${}^vX$	4	$\begin{pmatrix} A_2 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$	$(-1)^v \begin{pmatrix} I_3 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -I_2 \\ I_2 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$
${}^v_k\Sigma^\pm$	4	B_4	$(-1)^v A_4$	$\pm \begin{pmatrix} P_2 & 0 \\ 0 & P_2^* \end{pmatrix}$	$\begin{pmatrix} J_2 & 0 \\ 0 & J_2^* \end{pmatrix}$
${}^v_k\Delta^\pm$	4	B_4	$(-1)^v \begin{pmatrix} 1 & 0 \\ 0 & A_3 \end{pmatrix}$	$\pm \begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{k}{2}} I_2 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} I_2 \end{pmatrix}$	$\begin{pmatrix} P_2 & 0 \\ 0 & P_2^* \end{pmatrix}$
${}_k\Lambda$	8	$\begin{pmatrix} B_4 & 0 \\ 0 & D_4 \end{pmatrix}$	$\begin{pmatrix} A_3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & E_4 \end{pmatrix}$	$\begin{pmatrix} 0 & -e^{\mathrm{i}k} & 0 & 0 \\ 0 & 0 & -\mathrm{e}^{-\mathrm{i}k} I_2 & 0 \\ 0 & 0 & 0 & -\mathrm{e}^{\mathrm{i}k} \\ I_4 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} C_2^* & 0 & 0 & 0 \\ 0 & C_2 & 0 & 0 \\ 0 & 0 & C_2^* & 0 \\ 0 & 0 & 0 & C_2 \end{pmatrix}$
${}_kG^\pm$	8	$\begin{pmatrix} B_4 & 0 \\ 0 & B_4^{-1} \end{pmatrix}$	$\begin{pmatrix} 0 & I_4 \\ I_4 & 0 \end{pmatrix}$	$\pm \begin{pmatrix} E_2 & 0 & 0 & 0 \\ 0 & E_2^* & 0 & 0 \\ 0 & 0 & F_2 & 0 \\ 0 & 0 & 0 & F_2^* \end{pmatrix}$	$\begin{pmatrix} K_2 & 0 & 0 & 0 \\ 0 & K_2^* & 0 & 0 \\ 0 & 0 & K_2 & 0 \\ 0 & 0 & 0 & K_2^* \end{pmatrix}$

Table 24. The irrs of the hexagonal diperiodic groups $\mathbf{Dg}65 = \mathbf{C}_3\mathbf{T} = \mathrm{gr}\{C_3, (I|1\,0), (I|0\,1)\}$ and $\mathbf{Dg}74 = \mathbf{C}_{3h}\mathbf{T} = \mathrm{gr}\{C_3, \sigma_h, (I|1\,0), (I|0\,1)\}$, induced by the elements of the axial point group $\mathbf{C}_3$ from the irrs of the diperiodic groups **Dg**1 and **Dg**4 (table 2), respectively. The quasiangular momentum m takes on the values -1, 0 and 1. The irreducible domain of the Brillouin zone is presented in figure 4(a).

Irr	D	C_3	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
$\Gamma_m^\pm$	1	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}m}$	± 1	1	1
$Q_m^\pm$	1	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}m}$	± 1	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}}$	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}}$
$Q'^\pm_m$	1	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}m}$	± 1	$\mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}}$	$\mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}}$
${}_kG^\pm$	3	B_3	$\pm I_3$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}k_1} & 0 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}(k_1+k_2)} & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}k_2} \end{pmatrix}$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}k_2} & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}k_1} & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}(k_1+k_2)} \end{pmatrix}$

vertical mirror planes or rotations for π around horizontal axes). The selection rules related to these quantum numbers reflects the underlying conservation laws; as usual, the

Table 25. The irrs of the hexagonal diperiodic groups **Dg**68 = $\mathbf{D}_3\mathbf{T}$ = gr$\{C_3, U_x, (I|1\,0), (I|0\,1)\}$, **Dg**70 = $\mathbf{C}_{3v}\mathbf{T}$ = gr$\{C_3, \sigma_x, (I|1\,0), (I|0\,1)\}$ and **Dg**79 = $\mathbf{D}_{3h}\mathbf{T}$ = gr$\{C_3, U_x, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the element U_x or σ_x from the irrs of the groups **Dg**65 and **Dg**74 (table 24). The irreducible domain of the Brillouin zone is presented in figure 4(*b*).

Irr	D	C_3	σ_x or U_x	σ_h	$(I|1\,0)$	$(I|0\,1)$
${}^v\Gamma_0^{\pm}$	1	1	$(-1)^v$	±1	1	1
${}^vQ_0^{\pm}$	1	1	$(-1)^v$	±1	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}}$	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}}$
${}^vQ'^{\pm}_0$	1	1	$(-1)^v$	±1	$\mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}}$	$\mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}}$
$\Gamma_1^{\pm}$	2	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}}\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\pm I_2$	I_2	I_2
$Q_1^{\pm}$	2	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}}\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\pm I_2$	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} I_2$	$\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} I_2$
$Q'^{\pm}_1$	2	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}}\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\pm I_2$	$\mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} I_2$	$\mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} I_2$
${}^v_k\Lambda^{\pm}$	3	B_3	$(-1)^v\begin{pmatrix}A_2 & 0\\ 0 & 1\end{pmatrix}$	$\pm I_3$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} I_2 & 0\\ 0 & \mathrm{e}^{-2\mathrm{i}k}\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{-2\mathrm{i}k} & 0\\ 0 & \mathrm{e}^{\mathrm{i}k} I_2\end{pmatrix}$
${}^v_k\Sigma^{\pm}$	3	B_3	$(-1)^v A_3$	$\pm I_3$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} & 0 & 0\\ 0 & \mathrm{e}^{-2\mathrm{i}k} & 0\\ 0 & 0 & \mathrm{e}^{\mathrm{i}k}\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} I_2 & 0\\ 0 & \mathrm{e}^{-2\mathrm{i}k}\end{pmatrix}$
${}^v_k\Sigma'^{\pm}$	3	B_3	$(-1)^v\begin{pmatrix}1 & 0\\ 0 & A_2\end{pmatrix}$	$\pm I_3$	$\begin{pmatrix}\mathrm{e}^{\mathrm{i}k} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}} I_2\end{pmatrix}$	$\begin{pmatrix}\mathrm{e}^{-\mathrm{i}\frac{k}{2}} & 0 & 0\\ 0 & \mathrm{e}^{\mathrm{i}k} & 0\\ 0 & 0 & \mathrm{e}^{-\mathrm{i}\frac{k}{2}}\end{pmatrix}$
${}_{\boldsymbol{k}}G^{\pm}$	6	$\begin{pmatrix}B_3 & 0\\ 0 & B_3^{-1}\end{pmatrix}$	$\begin{pmatrix}0 & I_3\\ I_3 & 0\end{pmatrix}$	$\pm I_6$	$\begin{pmatrix}E_3 & 0\\ 0 & E_3\end{pmatrix}$	$\begin{pmatrix}L_2 & 0 & 0\\ 0 & \mathrm{e}^{-\mathrm{i}(k_1+k_2)} I_2 & 0\\ 0 & 0 & L_2\end{pmatrix}$

linear quasimomenta are conserved or changed for the vector of the inverse lattice (in the umklapp processes), while the quantum number m of the z-component of the angular momenta is conserved up to the order of the principle axis. The precise selection rules for any specific group can be calculated with help of the Clebsch–Gordan coefficients. Similarly, for the other standard applications of the symmetry (independent components of the physical tensors, phase transitions, classification of the vibrational and electronic bands, etc) the particular group must be considered; still, some interesting examples will be briefly discussed here, as a motivation for further research.

In an important paper [3], the phase transitions of the diperiodic structures have been analysed within Landau theory. For that purpose the real representations related to the special points are used to find the Molien functions generating the invariants and the order parameters. They are constructed by the subduction from the space supergroup, and they essentially correspond to a part of our results. In fact, the choice of the generators is not always the same (ours is based on the internal factorization of the diperiodic group, while in [3] it was determined by the correspondence of the invariants of the diperiodic and space groups), while, due to the different methods of construction the many-dimensional representations do not have the same matrices, although they are equivalent. In this context, now it is possible to investigate the incommensurate transitions (related to the special lines and general points) from the same point of view.

While the first investigations on the diperiodic groups, [1], reflected the interest for the semiconductors, this paper has been inspired by the theoretical investigations on the high-

Table 26. The irrs of the hexagonal diperiodic groups **Dg**67 = $\mathbf{D}_3\mathbf{T}$ = gr$\{C_3, U, (I|1\,0), (I|0\,1)\}$, **Dg**69 = $\mathbf{C}_{3v}\mathbf{T}$ = gr$\{C_3, \sigma, (I|1\,0), (I|0\,1)\}$ and **Dg**78 = $\mathbf{D}_{3h}\mathbf{T}$ = gr$\{C_3, U, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the elements U and σ from the irrs of the groups **Dg**65 and **Dg**74 (table 24). The quasi angular momentum m takes on the values -1, 0 and 1. The irreducible domain of the Brillouin zone is presented in figure 4(*e*). Here, $D_3 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}(k_1+k_2)}, \mathrm{e}^{-\mathrm{i}k_2}, \mathrm{e}^{-\mathrm{i}k_1})$ and $N_3 = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}k_2}, \mathrm{e}^{\mathrm{i}k_1}, \mathrm{e}^{-\mathrm{i}(k_1+k_2)})$.

Irr	D	C_3	σ or U	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
${}^{v}\Gamma_0^{\pm}$	1	1	$(-1)^v$	± 1	1	1
$\Gamma_1^{\pm}$	2	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} \end{pmatrix}$	A_2	$\pm I_2$	I_2	I_2
$Q_m^{\pm}$	2	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}m} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}m} \end{pmatrix}$	A_2	$\pm I_2$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} \end{pmatrix}$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} \end{pmatrix}$
${}^{v}_{k}\Delta^{\pm}$	3	B_3	$(-1)^v \begin{pmatrix} 1 & 0 \\ 0 & A_2 \end{pmatrix}$	$\pm I_3$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}k} & 0 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}k} & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}k} \end{pmatrix}$
${}^{v}_{k}\Phi^{\pm}$	3	B_3	$(-1)^v A_3$	$\pm I_3$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k} & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}k} \end{pmatrix}$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}k} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}k} \end{pmatrix}$
${}_{\boldsymbol{k}}G^{\pm}$	6	$\begin{pmatrix} B_3 & 0 \\ 0 & B_3^{-1} \end{pmatrix}$	$\begin{pmatrix} 0 & I_3 \\ I_3 & 0 \end{pmatrix}$	$\pm I_6$	$\begin{pmatrix} E_3 & 0 \\ 0 & D_3 \end{pmatrix}$	$\begin{pmatrix} N_3 & 0 \\ 0 & N_3^* \end{pmatrix}$

Table 27. The irrs of the hexagonal diperiodic groups **Dg**66 = $\mathbf{S}_6\mathbf{T}$ = gr$\{C_6\sigma_h, (I|1\,0), (I|0\,1)\}$, **Dg**73 = $\mathbf{C}_6\mathbf{T}$ = gr$\{C_6, (I|1\,0), (I|0\,1)\}$ and **Dg**75 = $\mathbf{C}_{6h}\mathbf{T}$ = gr$\{C_6, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the elements of the axial point groups $\mathbf{C}_6$ or $\mathbf{S}_6$ from the irrs of the groups **Dg**1 and **Dg**4 (table 2). For the points Γ, X and Q the quasi angular momentum m takes on the integer values from the intervals $[-2, 3]$, $[0, 1]$ and $[-1, 1]$, respectively. The irreducible domain of the Brillouin zone is presented in figure 4(*d*).

Irr	D	C_6 or $C_6\sigma_h$	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
$\Gamma_m^{\pm}$	1	$\mathrm{e}^{\mathrm{i}\frac{\pi}{3}m}$	± 1	1	1
$Q_m^{\pm}$	2	$\begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}m\frac{2\pi}{3}} \\ \mathrm{e}^{-\mathrm{i}m\frac{2\pi}{3}} & 0 \end{pmatrix}$	$\pm I_2$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} \end{pmatrix}$	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} \end{pmatrix}$
$X_m^{\pm}$	3	$(-1)^m B_3^{-1}$	$\pm I_3$	$\begin{pmatrix} -I_2 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -I_2 \end{pmatrix}$
${}_{\boldsymbol{k}}G^{\pm}$	6	$\begin{pmatrix} 0 & 1 \\ I_5 & 0 \end{pmatrix}$	$\pm I_6$	$\begin{pmatrix} S_3 & 0 \\ 0 & S_3^* \end{pmatrix}$	$\begin{pmatrix} O_3 & 0 \\ 0 & O_3^* \end{pmatrix}$

temperature superconducting materials. Most of those 3D structures are periodical in two dimensions only, since such compounds contain the different and even aperiodically (along the z-axis) arranged layers, with several CuO_2 conducting layers always present. The most frequently discussed compounds are with the symmetry of **Dg**61 = $\mathbf{D}_{4h}\mathbf{T}$, table 21. The possible topology of the band shapes can be calculated by the compatibility relations: when the general point $\boldsymbol{k}$ tends to the boundary of the irreducible domain, i.e. to some of the special lines or points, the representations $G^{\pm}$ become reducible, and their irreducible components reveal the bands stickings at the boundary. This analysis for the CuO_2 layers give the band shapes for the relevant electronic states (figure 5). Analogously, the symmetry classification of the ionic vibrations as well as of the other electronic states of these superconducting materials, can be performed with the help of the irrs of the diperiodic groups. Although the detailed symmetry analysis of such systems will be presented elsewhere, it should be stressed

Table 28. The irrs of the hexagonal diperiodic groups $\mathbf{Dg}71 = \mathbf{D}_{3d}\mathbf{T} = \mathrm{gr}\{C_6\sigma_h, \sigma_x, (I|1\,0), (I|0\,1)\}$, $\mathbf{Dg}72 = \mathbf{D}_{3d}\mathbf{T} = \mathrm{gr}\{C_6\sigma_h, U_x, (I|1\,0), (I|0\,1)\}$, $\mathbf{Dg}76 = \mathbf{D}_6\mathbf{T} = \mathrm{gr}\{C_6, U_x, (I|1\,0), (I|0\,1)\}$, $\mathbf{Dg}77 = \mathbf{C}_{6v}\mathbf{T} = \mathrm{gr}\{C_6, \sigma_x, (I|1\,0), (I|0\,1)\}$ and $\mathbf{Dg}80 = \mathbf{D}_{6h}\mathbf{T} = \mathrm{gr}\{C_6, \sigma_x, \sigma_h, (I|1\,0), (I|0\,1)\}$ induced by the elements σ_x or U_x from the irrs of the groups **Dg**66, **Dg**73 and **Dg**75 (table 27). For ${}^v\Gamma_m^\pm$, $\Gamma_m^\pm$ and ${}^vX_m^\pm$ the quasi angular momentum m takes on the values from the sets $\{0, 3\}$, $\{1, 2\}$ and $\{0, 1\}$, respectively. The irreducible domain of the Brillouin zone is presented in figure 4(c). Here, $V_3 = \mathrm{diag}\,(\mathrm{e}^{-\mathrm{i}(k_1+k_2)}, \mathrm{e}^{-\mathrm{i}k_1}, \mathrm{e}^{\mathrm{i}k_2})$.

Irr	D	C_6 or $C_6\sigma_h$	U_x or σ_x	σ_h	$(I\|1\,0)$	$(I\|0\,1)$
${}^v\Gamma_m^\pm$	1	$(-1)^m$	$(-1)^v$	± 1	1	1
$\Gamma_m^\pm$	2	$\begin{pmatrix} \mathrm{e}^{\mathrm{i}m\frac{\pi}{3}} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}m\frac{\pi}{3}} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\pm I_2$	I_2	I_2
${}^vQ_0^\pm$	2	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(-1)^v I_2$	$\pm I_2$	K_2	K_2
${}^vX_m^\pm$	3	$(-1)^m B_3^{-1}$	$(-1)^v \begin{pmatrix} A_2 & 0 \\ 0 & 1 \end{pmatrix}$	$\pm I_3$	$\begin{pmatrix} -I_2 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -I_2 \end{pmatrix}$
$Q_1^\pm$	4	$\begin{pmatrix} R_2^* & 0 \\ 0 & R_2 \end{pmatrix}$	$\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$	$\pm I_4$	$\begin{pmatrix} K_2 & 0 \\ 0 & K_2 \end{pmatrix}$	$\begin{pmatrix} K_2 & 0 \\ 0 & K_2 \end{pmatrix}$
${}_k^v\Sigma^\pm$	6	$\begin{pmatrix} 0 & 1 \\ I_5 & 0 \end{pmatrix}$	$(-1)^v \begin{pmatrix} A_5 & 0 \\ 0 & 1 \end{pmatrix}$	$\pm I_6$	$\begin{pmatrix} K_3 & 0 \\ 0 & K_3^* \end{pmatrix}$	$\begin{pmatrix} J_3 & 0 \\ 0 & J_3^* \end{pmatrix}$
${}_k^v\Delta^\pm$	6	$\begin{pmatrix} 0 & 1 \\ I_5 & 0 \end{pmatrix}$	$(-1)^v A_6$	$\pm I_6$	$\begin{pmatrix} P_3 & 0 \\ 0 & P_3^* \end{pmatrix}$	$\begin{pmatrix} R_3 & 0 \\ 0 & R_3^* \end{pmatrix}$
${}_k^v\Lambda^\pm$	6	$\begin{pmatrix} 0 & 1 \\ I_5 & 0 \end{pmatrix}$	$(-1)^v \begin{pmatrix} A_3 & 0 \\ 0 & A_3 \end{pmatrix}$	$\pm I_6$	$\begin{pmatrix} J_3 & 0 \\ 0 & J_3^* \end{pmatrix}$	$\begin{pmatrix} L_3 & 0 \\ 0 & L_3^* \end{pmatrix}$
${}_kG^\pm$	12	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ I_5 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_5 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & I_6 \\ I_6 & 0 \end{pmatrix}$	$\pm I_{12}$	$\begin{pmatrix} S_3 & 0 & 0 & 0 \\ 0 & S_3^* & 0 & 0 \\ 0 & 0 & S_3 & 0 \\ 0 & 0 & 0 & S_3^* \end{pmatrix}$	$\begin{pmatrix} O_3 & 0 & 0 & 0 \\ 0 & O_3^* & 0 & 0 \\ 0 & 0 & V_3 & 0 \\ 0 & 0 & 0 & V_3^* \end{pmatrix}$

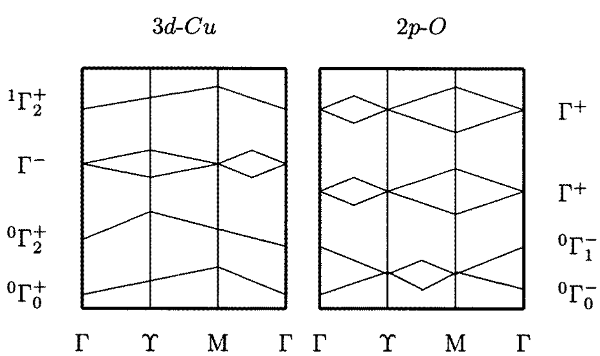

Figure 5. The scheme of the bands induced by 3d–Cu and 2p–O electronic orbitals of CuO_2 layer. The energies are not calculated, and only the trends along the bands are roughly estimated, [9], in order to represent the bands sticking together predicted by the compatibility relations of the irrs $G^\pm$ at the boundary of the irreducible domain of the Brillouin zone. The special positions at the boundary, specified below the figures, are separated by the general positions of the interior.

that the simultaneous classifications of the vibrational and electronic states has revealed some kind of the anomalous vibronic coupling, [14]: surprisingly enough, it appears that there are degenerate electronic states which are not coupled vibronically to the phonons. This is the first known breakdown of the Jahn–Teller theorem, which had been previously verified for the molecules [15], polymers [16], and a number of the 3D crystals. There are some experimental results supporting this prediction [17].

Finally, let it be emphasized that the determination of generators of the diperiodic groups (being simplified by the factorization of the groups) enables the direct computer implementation. Indeed, the modified group projector method, involving the only the generators, can be employed straightforwardly. The program, analogous to the one designed for the systems with the translational periodicity in one direction, using this method, [18], is in progress; particularly, it has already been applied to check the results of this paper independently.

Appendix. Construction of irrs

The structural properties of the diperiodic groups allow us to avoid the general induction procedure, and to reduce the task to the three especially simple cases, being elaborated in the literature [7].

Method 1. The group **G** is the product of its subgroups **H** and **K**. The irrs of **H** and **K** ($\{D^{(\mu)}(\mathbf{H})\}$, and $\{D^{(\nu)}(\mathbf{K})\}$) suffice to find the irrs of **G**: these are $D^{(\mu,\nu)}(\mathbf{G})$, defined by $D^{(\mu,\nu)}(g) = D^{(\mu)}(h) \otimes D^{(\nu)}(k)$, for each element $g = hk$ of **G**, and each pair of irrs of **H** and **K**.

Method 2. The group **G** is semidirect product of its subgroups **H** and **K**, **H** being Abelian (with 1D irrs $\{\Delta^{(\mu)}(\mathbf{H})\}$). Then the subgroup $\mathbf{K}_\mu$ of **K** for each μ, consists of the elements $l \in \mathbf{K}$ satisfying $\Delta^{(\mu)}(l^{-1}hl) = Z^{-1}\Delta^{(\mu)}(h)Z$ (for all h in **H** and fixed nonsingular matrix Z). For each irr $\delta^{(\nu)}(\mathbf{K}_\mu)$ of $\mathbf{K}_\mu$, the irr $\Gamma^{(\mu,\nu)}(hk_\mu) = \Delta^{(\mu)}(h) \otimes \delta^{(\nu)}(k_\mu)$ of the little group $\mathbf{HK}_\mu$ yields one induced irr of **G**: $D^{(\mu,\nu)}(\mathbf{G}) = \Gamma^{(\mu,\nu)}(\mathbf{HK}_\mu) \uparrow \mathbf{G}$.

In both cases the set of the generators of **G** is the union of the sets of the generators of **H** and **K**.

Method 3. The group is of the form $\mathbf{G} = \mathbf{H} + s\mathbf{H}$, where **H** is halving subgroup (with the set of all nonequivalent irrs $\{\Delta^{(\mu)}(\mathbf{H})\}$), and s is an element of the coset of **H**. If there is nonsingular matrix Z satisfying $Z^2 = \Delta^{(\mu)}(s^2)$ and $\Delta^{(\mu)}(s^{-1}hs) = Z^{-1}\Delta^{(\mu)}(h)Z$, for each $h \in \mathbf{H}$, two irrs of **G** are obtained:

$$\{D^{(\mu\pm)}(h) \stackrel{\text{def}}{=} \Delta^{(\mu)}(h),\, D^{(\mu\pm)}(sh) \stackrel{\text{def}}{=} \pm Z\Delta^{(\mu)}(h) \mid h \in \mathbf{H}\}$$

if there is no such Z, then the induced representation $D^{(\mu)}(\mathbf{G}) = \Delta^{(\mu)}(\mathbf{H}) \uparrow \mathbf{G}$, defined by the matrices

$$\left\{D^{(\mu)}(h) = \begin{pmatrix} \Delta^{(\mu)}(h) & 0 \\ 0 & Z^{-1}\Delta^{(\mu)}(h)Z \end{pmatrix},\right.$$
$$\left. D^{(\mu)}(sh) = \begin{pmatrix} 0 & \Delta^{(\mu)}(s^2)Z^{-1}\Delta^{(\mu)}(h)Z \\ \Delta^{(\mu)}(h) & 0 \end{pmatrix} \right\}$$

is irreducible. If $\{h_1, \ldots, h_k\}$ are the generators of **H**, then the set $\{h_1, \ldots, h_k, s\}$ generates **G**. In some cases, this set is not minimal, since some of the elements h_i are monomials over s and the remaining generators.

To make the calculations completely clear, the paths of the induction will be given explicitly, for each type of the Brillouin zone separately. As for the oblique groups,

Dg1, **Dg**4 and **Dg**5 are direct products and their irrs are obtained by method 1. For the remaining groups the induction by method 3 is indicated by $\xrightarrow{g}$, where g stands for the coset representative:

$$\mathbf{Dg}1\begin{cases}\xrightarrow{C_2\sigma_h}\mathbf{Dg}2\\ \xrightarrow{C_2}\mathbf{Dg}3\xrightarrow{(\sigma_h|0\,\frac{1}{2})}\mathbf{Dg}7\end{cases}\qquad \mathbf{Dg}4\xrightarrow{C_2}\mathbf{Dg}6.$$

The irrs of the rectangular groups are obtained by method 3 in the following seven chains, each one starting from the one of the oblique group.

$$\mathbf{Dg}1\begin{cases}\xrightarrow{U_x}\mathbf{Dg}8\begin{cases}\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}10\\ \xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}31\end{cases}\\ \xrightarrow{(U_y|0\,\frac{1}{2})}\mathbf{Dg}9\begin{cases}\xrightarrow{C_2\sigma_h}\mathbf{Dg}15\\ \xrightarrow{C_2}\mathbf{Dg}20\\ \xrightarrow{\sigma_y}\mathbf{Dg}26\end{cases}\\ \xrightarrow{\sigma_x}\mathbf{Dg}11\begin{cases}\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}13\\ \xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}32\end{cases}\\ \xrightarrow{(\sigma_y|0\,\frac{1}{2})}\mathbf{Dg}12\begin{cases}\xrightarrow{C_2\sigma_h}\mathbf{Dg}17\\ \xrightarrow{U_x}\mathbf{Dg}27\\ \xrightarrow{C_2}\mathbf{Dg}28\end{cases}\end{cases}\qquad \mathbf{Dg}2\begin{cases}\xrightarrow{U_x}\mathbf{Dg}14\begin{cases}\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}16\\ \xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}42\end{cases}\\ \xrightarrow{(\sigma|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}18\end{cases}$$

$$\mathbf{Dg}3\begin{cases}\xrightarrow{U_x}\mathbf{Dg}19\begin{cases}\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}22\\ \xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}39\end{cases}\\ \xrightarrow{(U|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}21\\ \xrightarrow{\sigma_x}\mathbf{Dg}23\begin{cases}\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}34\\ \xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}46\end{cases}\\ \xrightarrow{(\sigma|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}33\end{cases}\qquad \mathbf{Dg}4\begin{cases}\xrightarrow{U_x}\mathbf{Dg}24\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}36\\ \xrightarrow{(U_y|0\,\frac{1}{2})}\mathbf{Dg}25\xrightarrow{C_2}\mathbf{Dg}40\end{cases}$$

$$\mathbf{Dg}5\begin{cases}\xrightarrow{U_x}\mathbf{Dg}29\\ \xrightarrow{(U_x|\frac{1}{2}\,0)}\mathbf{Dg}30\begin{cases}\xrightarrow{U_y}\mathbf{Dg}43\\ \xrightarrow{C_2}\mathbf{Dg}45\end{cases}\\ \xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}36\end{cases}\qquad \mathbf{Dg}6\begin{cases}\xrightarrow{U_x}\mathbf{Dg}37\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}47\\ \xrightarrow{(\sigma|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}44\end{cases}$$

$$\mathbf{Dg}7\begin{cases}\xrightarrow{U_y}\mathbf{Dg}38\\ \xrightarrow{\sigma_y}\mathbf{Dg}41\xrightarrow{(I|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}48.\end{cases}$$

The irrs of the square groups are derived in two chains, starting from the square oblique groups **Dg**1 and **Dg**4; besides the induction from the halving subgroup, method 2 has been used (the subgroup **K** is in these cases indicated by $\xRightarrow{\mathbf{K}}$):

$$\mathbf{Dg}1\left\{\begin{array}{l} \xRightarrow{\mathbf{C}_4}\mathbf{Dg}49\left\{\begin{array}{l}\xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}52\\ \xrightarrow{U_x}\mathbf{Dg}53\\ \xrightarrow{(U|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}54\\ \xrightarrow{\sigma_x}\mathbf{Dg}55\\ \xrightarrow{(\sigma|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}56\end{array}\right.\\ \xRightarrow{\mathbf{S}_4}\mathbf{Dg}50\left\{\begin{array}{l}\xrightarrow{U_x}\mathbf{Dg}57\xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}64\\ \xrightarrow{(U|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}58\\ \xrightarrow{U}\mathbf{Dg}59\xrightarrow{(\sigma_h|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}62\\ \xrightarrow{(\sigma|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}60\end{array}\right.\end{array}\right.\qquad \mathbf{Dg}4\xRightarrow{\mathbf{C}_4}\mathbf{Dg}51\left\{\begin{array}{l}\xrightarrow{U_x}\mathbf{Dg}61\\ \xrightarrow{(\sigma|\frac{1}{2}\,\frac{1}{2})}\mathbf{Dg}63.\end{array}\right.$$

For the hexagonal groups there are two chains again, starting from the hexagonal oblique groups **Dg**1 and **Dg**4, respectively. Also, the second and third induction procedures were necessary

$$\mathbf{Dg}1\left\{\begin{array}{l} \xRightarrow{\mathbf{C}_3}\mathbf{Dg}65\left\{\begin{array}{l}\xrightarrow{U}\mathbf{Dg}67\\ \xrightarrow{U_x}\mathbf{Dg}68\\ \xrightarrow{\sigma}\mathbf{Dg}69\\ \xrightarrow{\sigma_x}\mathbf{Dg}70\end{array}\right.\\ \xRightarrow{\mathbf{S}_6}\mathbf{Dg}66\left\{\begin{array}{l}\xrightarrow{U}\mathbf{Dg}71\\ \xrightarrow{U_x}\mathbf{Dg}72\end{array}\right.\\ \xRightarrow{\mathbf{C}_6}\mathbf{Dg}73\xrightarrow{\sigma_x}\mathbf{Dg}77\end{array}\right.\qquad \mathbf{Dg}4\left\{\begin{array}{l}\xRightarrow{\mathbf{C}_3}\mathbf{Dg}74\left\{\begin{array}{l}\xrightarrow{U}\mathbf{Dg}78\\ \xrightarrow{U_x}\mathbf{Dg}79\end{array}\right.\\ \xRightarrow{\mathbf{C}_6}\mathbf{Dg}75\xrightarrow{U_x}\mathbf{Dg}80\end{array}\right. .$$

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