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Q-reducible two-dimensional space groups and layer groups

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Abstract. The theory of Q-reducible space groups is applied to determine those line groups in two dimensions which are isomorphic to factor groups of Q-reducible two-dimensional space groups. The concept of Q reducibility is extended to subperiodic groups, and the strip groups isomorphic to factor groups of the subperiodic layer groups are determined.

The action of the point group of a space group on the underlying vector space is Q-reducible if the vector space splits into invariant subspaces such that the point group operators can be expressed by rational matrices on each subspace. It has been shown by Kopsky (1986) that if the point group is Q-reducible then (i) the point group is a subdirect product of point groups of lower dimension, (ii) the space group is a subdirect product of space groups of lower dimension and (iii) the space group has complementary normal translational subgroups of lower dimension and corresponding factor groups which are isomorphic to subperiodic groups. Q reducibility gives insight into the structure of space groups with Q-reducible point groups and can be used for the derivation of higher-dimensional space or subperiodic groups as well as for the introduction of a hierarchy of these groups (Jarrat 1980). The occurrence of subperiodic groups as factor groups is also of importance in the consideration of lattices of subgroups of space groups and can be used to develop representation theory of space groups by ascent from lower to higher dimensions (Fuksa and Kopsky 1987).

We determine the subperiodic groups isomorphic to factor groups of Q-reducible two-dimensional space groups taken with respect to the normal subgroups which span each of the invariant subspaces of the underlying vector space: nine of the seventeen two-dimensional space groups are Q-reducible. These are the oblique and rectangular two-dimensional space groups numbered from one to nine in the *International Tables for Crystallography* (Hahn 1983). The rotational part of the symbols for these groups is given in a ZXY coordinate system where XY are the coordinates of the two-dimensional space. We shall also use the notation G_2 (Bohm and Dornberger-Schiff 1967) as a notation for an arbitrary two-dimensional space group.

Factor groups G_2/T_{G_i}, where T_{G_i} is a one-dimensional subgroup spanning an invariant subspace, are isomorphic to line groups G_{21} in two dimensions. The seven groups G_{21} are listed along with their generators in table 1. The rotational part of the symbols of these groups are given in a ZXY coordinate system where the unique plane is the XY plane and the unique axis the X axis.

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Table 1. Generators of the seven line groups in two dimensions G_{21}.

(1) $\not{p}111$	$\left\langle \left(\begin{array}{cc\|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\rangle$
(2) $\not{p}11m$	$\left\langle \left(\begin{array}{cc\|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\rangle$
(3) $\not{p}1m1$	$\left\langle \left(\begin{array}{cc\|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\rangle$
(4) $\not{p}211$	$\left\langle \left(\begin{array}{cc\|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\rangle$
(5) $\not{p}2mm$	$\left\langle \left(\begin{array}{cc\|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\rangle$
(6) $\not{p}11g$	$\left\langle \left(\begin{array}{cc\|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\rangle$
(7) $\not{p}2mg$	$\left\langle \left(\begin{array}{cc\|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc\|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\rangle$

Table 2. Groups G_{21} isomorphic to factor groups G_2/T_{Gi}.

	G_{21}	
G_2	G_2/T_{GX}	G_2/T_{GY}
(1) *p*1	$\not{p}111$	$\not{p}111$
(2) *p*2	$\not{p}211$	$\not{p}211$
(3) *p*1*m*1	$\not{p}1m1$ ($\not{p}11m$)	$\not{p}1m1$
(4) *p*1*g*1	$\not{p}1g1$ ($\not{p}11g$)	$\not{p}1m1$
(5) *c*1*m*1	$\not{p}_{1/2}1m1$ ($\not{p}_{1/2}11m$)	$\not{p}_{1/2}1m1$
(6) *p*2*mm*	$\not{p}2mm$	$\not{p}2mm$
(7) *p*2*mg*	$\not{p}2mm$	$\not{p}2mg$
(8) *p*2*gg*	$\not{p}2gm$ ($\not{p}2mg$)	$\not{p}2mg$
(9) *c*2*mm*	$\not{p}_{1/2}2mm$	$\not{p}_{1/2}2mm$

In table 2 we list to the right of each Q-reducible two-dimensional space group G_2 those line groups G_{21} which are isomorphic to factor groups G_2/T_{GX} and G_2/T_{GY}. The symbols for these isomorphic groups G_{21} are given in the same coordinate system as that of the corresponding group G_2. For factor groups G_2/T_{GY}, the symbol for the isomorphic group G_{21} is thus in the same coordinate system as used in table 1. For factor groups G_2/T_{GX}, one must interchange the X and Y coordinates to obtain the coordinate system used in table 1. If on interchange of coordinates one obtains a new

Table 3. Groups G_{321} isomorphic to factor groups G_{32}/T_{Gi}.

G_{32}	G_{321}	
	G_{32}/T_{GX}	G_{32}/T_{GY}
(1) $p1$	$\not{p}1$	$\not{p}1$
(2) $p\bar{1}$	$\not{p}\bar{1}$	$\not{p}\bar{1}$
(3) $p211$	$\not{p}211$	$\not{p}211$
(4) $pm11$	$\not{p}m11$	$\not{p}m11$
(5) $pb11$	$\not{p}b11$ ($\not{p}a11$)	$\not{p}m11$
(6) $p\frac{2}{m}11$	$\not{p}\frac{2}{m}11$	$\not{p}\frac{2}{m}11$
(7) $p\frac{2}{b}11$	$\not{p}\frac{2}{b}11\left(\not{p}\frac{2}{a}11\right)$	$\not{p}\frac{2}{m}11$
(8) $p112$	$\not{p}112$ ($\not{p}121$)	$\not{p}112$
(9) $p112_1$	$\not{p}112_1$ ($\not{p}12_11$)	$\not{p}112$
(10) $c112$	$\not{p}_{1/2}112$ ($\not{p}_{1/2}121$)	$\not{p}_{1/2}112$
(11) $p11m$	$\not{p}11m$ ($\not{p}1m1$)	$\not{p}11m$
(12) $p11a$	$\not{p}11m$ ($\not{p}1m1$)	$\not{p}11a$
(13) $c11m$	$\not{p}_{1/2}11m$ ($\not{p}_{1/2}1m1$)	$\not{p}11m$
(14) $p11\frac{2}{m}$	$\not{p}11\frac{2}{m}\left(\not{p}1\frac{2}{m}1\right)$	$\not{p}11\frac{2}{m}$
(15) $p11\frac{2_1}{m}$	$\not{p}11\frac{2_1}{m}\left(\not{p}1\frac{2_1}{m}1\right)$	$\not{p}11\frac{2}{m}$
(16) $c11\frac{2}{m}$	$\not{p}_{1/2}11\frac{2}{m}\left(\not{p}_{1/2}1\frac{2}{m}1\right)$	$\not{p}_{1/2}11\frac{2}{m}$
(17) $p11\frac{2}{a}$	$\not{p}11\frac{2}{m}\left(\not{p}1\frac{2}{m}1\right)$	$\not{p}11\frac{2}{a}$
(18) $p11\frac{2_1}{a}$	$\not{p}11\frac{2_1}{m}\left(\not{p}1\frac{2_1}{m}1\right)$	$\not{p}11\frac{2}{a}$
(19) $p222$	$\not{p}222$	$\not{p}222$
(20) $p222_1$	$\not{p}222_1$ ($\not{p}22_12$)	$\not{p}222$
(21) $p22_12_1$	$\not{p}222_1$ ($\not{p}22_12$)	$\not{p}22_12$
(22) $c222$	$\not{p}_{1/2}222$	$\not{p}_{1/2}222$
(23) $p2mm$	$\not{p}2mm$	$\not{p}2mm$
(24) $pmm2$	$\not{p}mm2$ ($\not{p}m2m$)	$\not{p}mm2$
(25) $pm2_1a$	$\not{p}m2m$ ($\not{p}mm2$)	$\not{p}m2_1a$
(26) $pbm2_1$	$\not{p}bm2_1$ ($\not{p}a2_1m$)	$\not{p}mm2$
(27) $pbb2$	$\not{p}bb2$ ($\not{p}a2a$)	$\not{p}mm2$
(28) $p2ma$	$\not{p}2mm$	$\not{p}2ma$
(29) $pam2$	$\not{p}mm2$ ($\not{p}m2m$)	$\not{p}am2$
(30) $pab2_1$	$\not{p}mb2_1$ ($\not{p}m2_1a$)	$\not{p}am2$
(31) $pnb2$	$\not{p}bb2$ ($\not{p}a2a$)	$\not{p}am2$
(32) $pnm2_1$	$\not{p}bm2_1$ ($\not{p}a2_1m$)	$\not{p}am2$
(33) $p2ba$	$\not{p}2bm$ ($\not{p}2ma$)	$\not{p}2ma$
(34) $c2mm$	$\not{p}_{1/2}2mm$	$\not{p}_{1/2}2mm$
(35) $cmm2$	$\not{p}_{1/2}mm2$ ($\not{p}_{1/2}m2m$)	$\not{p}_{1/2}mm2$
(36) $cam2$	$\not{p}_{1/2}mm2$ ($\not{p}_{1/2}m2m$)	$\not{p}_{1/2}mm2$
(37) $p\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}\frac{2}{m}\frac{2}{m}\frac{2}{m}$
(38) $\not{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}$	$\not{p}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}$
(39) $p\frac{2}{n}\frac{2}{b}\frac{2}{a}$	$\not{p}\frac{2}{b}\frac{2}{b}\frac{2}{m}\left(\not{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}\right)$	$\not{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}$

Table 3. (continued)

	G_{321}	
G_{32}	G_{32}/T_{GX}	G_{32}/T_{GY}
(40) $p\frac{2}{m}\frac{2_1}{m}\frac{2}{a}$	$\not{p}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}\frac{2}{m}\frac{2_1}{m}\frac{2}{a}$
(41) $p\frac{2}{a}\frac{2_1}{m}\frac{2}{m}$	$\not{p}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}\frac{2}{a}\frac{2_1}{m}\frac{2}{m}$
(42) $p\frac{2}{n}\frac{2}{m}\frac{2_1}{a}$	$\not{p}\frac{2}{b}\frac{2}{m}\frac{2_1}{m}\left(\not{p}\frac{2}{a}\frac{2_1}{m}\frac{2}{m}\right)$	$\not{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}$
(43) $p\frac{2}{a}\frac{2}{b}\frac{2_1}{a}$	$\not{p}\frac{2}{m}\frac{2}{b}\frac{2_1}{m}\left(\not{p}\frac{2}{m}\frac{2_1}{m}\frac{2}{a}\right)$	$\not{p}\frac{2}{a}\frac{2}{m}\frac{2}{a}$
(44) $p\frac{2}{m}\frac{2_1}{b}\frac{2_1}{a}$	$\not{p}\frac{2}{m}\frac{2}{b}\frac{2_1}{m}\left(\not{p}\frac{2}{m}\frac{2_1}{m}\frac{2}{a}\right)$	$\not{p}\frac{2}{m}\frac{2_1}{m}\frac{2}{a}$
(45) $p\frac{2}{a}\frac{2_1}{b}\frac{2_1}{m}$	$\not{p}\frac{2}{m}\frac{2}{b}\frac{2_1}{m}\left(\not{p}\frac{2}{m}\frac{2_1}{m}1\frac{2}{a}\right)$	$\not{p}\frac{2}{a}\frac{2_1}{m}\frac{2}{m}$
(46) $p\frac{2}{n}\frac{2_1}{m}\frac{2_1}{m}$	$\not{p}\frac{2}{b}\frac{2}{m}\frac{2_1}{m}\left(\not{p}\frac{2}{a}\frac{2_1}{m}\frac{2}{m}\right)$	$\not{p}\frac{2}{a}\frac{2_1}{m}\frac{2}{m}$
(47) $c\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}_{1/2}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}_{1/2}\frac{2}{m}\frac{2}{m}\frac{2}{m}$
(48) $c\frac{2}{a}\frac{2}{m}\frac{2}{m}$	$\not{p}_{1/2}\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\not{p}_{1/2}\frac{2}{m}\frac{2}{m}\frac{2}{m}$

distinct symbol, it is given in parentheses. For example, for $G_2 = p1g1$:

$$G_2 = ((E|00) + (M_X|0\tfrac{1}{2}))(T_{GX} + (E|01)T_{GX} + \ldots)$$

$$G_2/T_{GX} \approx ((E|00) + (M_X|0\tfrac{1}{2}))((E|00) + (E|01) + \ldots).$$

The isomorphic group G_{21} is $\not{p}1g1$ which on interchanging the X and Y coordinates becomes $\not{p}11g$. The notation $\not{p}_{1/2}$ in table 2 denotes that the translational subgroup of the line group is isomorphic to a translational group generated by one-half a translation along the conventional unit cell of the corresponding centred two-dimensional space group. For example, for $G_2 = c1m1$:

$$G_2 = ((E|00) + (M_X|00))(T_{GY} + (E|\tfrac{1}{2}\tfrac{1}{2})T_{GY} + \ldots)$$

$$G_2/T_{GY} \approx ((E|00) + (M_X|00))((E|00) + (E|\tfrac{1}{2}0) + (E|10) + \ldots).$$

The isomorphic line group is denoted by $\not{p}_{1/2}1m1$.

The concept of Q reducibility can also be extended to subperiodic groups. The action of the point group of a subperiodic group on the underlying vector space will be defined as Q-reducible if the vector space spanned by the translational subgroup splits into invariant subspaces such that the action of point group operators on these subspaces can be expressed by rational matrices on each subspace. A subperiodic group with a Q-reducible point group has complementary normal subgroups of lower dimension and corresponding factor groups isomorphic to lower-dimensional subperiodic groups.

We consider the subperiodic layer groups G_{32} (Wood 1964a, b). In the left-hand column of table 3 we list the 48 Q-reducible layer groups in the numbering and notation of Wood (1964a,b). The rotational part of the group symbol is given in a ZXY coordinate system where the invariant plane is the XY plane. The factor groups G_{32}/T_{Gi} are isomorphic to strip groups G_{321} (Bohm and Dornberger-Schiff 1967). The rotational part of the group symbol of groups G_{321} is given in a ZXY coordinate system where the unique plane is the XY plane and unique axis the X axis. In table 3, to the right of each layer group G_{32} we list those strip groups G_{321} isomorphic to the factor groups G_{32}/T_{GX} and G_{32}/T_{GY}.

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References

Bohm J and Dornberger-Schiff K 1967 *Acta Crystallogr.* **23** 913
Fuksa J and Kopsky V 1987 in preparation
Hahn T (ed) 1983 *International Tables for Crystallography* (Dordrecht: Reidel)
Jarrat J D 1980 *Proc. Camb. Phil. Soc.* **88** 245
Kopsky V 1986 *J. Phys. A: Math. Gen.* **19** L181
Wood E A 1964a *Bell Telephone Tech. Publ.* Monograph 4680
—— 1964b *Bell Telephone Tech. J.* **43** 541