

Subgroups of Black-White Point Groups

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The necessity of distinguishing the orientations of a subgroup in a group is pointed out. The numbers of different subgroups and normal subgroups of the black-white point groups are given first by taking into account this distinction, secondly by not distinguishing the orientations, and thirdly by not distinguishing isomorphic subgroups. Groups that can be constructed by successive formation of direct products are assembled into seven families, each of which contains precisely one black-white point group that is not isomorphic to an ordinary point group.

There are 25 non-isomorphic (abstract) black-white point groups that give rise to a total of 122 non-equivalent (crystallographic) black-white point groups (Table 1, column I).

Table 2. *Subgroups that are normal or not, depending on their orientation*

Table 1. *Numbers of isomorphs and subgroups of the abstract black-white point groups*

Ab- stract group	I		II		III	
	Non- equivalent realiza- tions	Ab- stract sub- groups	Abstract normal sub- groups	Total number of sub- groups	Total number of normal subgroups	
C_1	1	1	1	1	1	
C_2	7	2	2	2	2	
D_2	12	3	3	5	5	
D_{2h}	7	4	4	16	16	
$D_{2h} \times \theta$	1	5	5	67	67	
C_4	4	3	3	3	3	
C_{4h}	6	5	5	8	8	
$C_{4h} \times \theta$	1	7	7	27	27	
D_4	10	5	5	10	6	
D_{4h}	9	8	8	35	19	
$D_{4h} \times \theta$	1	11	11	146	78	
C_3	1	2	2	2	2	
C_6	7	4	4	4	4	
C_{6h}	7	6	6	10	10	
$C_{6h} \times \theta$	1	7	7	32	32	
D_3	4	4	3	6	3	
D_6	16	7	6	16	7	
D_{6h}	10	10	9	54	21	
$D_{6h} \times \theta$	1	13	12	236	83	
T	1	5	3	10	3	
T_h	3	8	6	26	6	
$T_h \times \theta$	1	10	8	88	15	
O	4	9	4	30	4	
O_h	6	16	8	98	9	
$O_h \times \theta$	1	23	11	420	26	

The 7 black-white point groups that are not isomorphic to an ordinary point group are:

$$D_{2h} \times \theta, C_{4h} \times \theta, D_{4h} \times \theta, C_{6h} \times \theta, D_{6h} \times \theta, T_h \times \theta, O_h \times \theta.$$

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Group	Subgroup	Number of orientations	Number of normal orientations
D_4	C_2	5	1
D_{2d}	C_2	3	1
$D_4(D_2)$	C_2	3	1
$D_{2d}(D_2)$	C_2	3	1
D_{4h}	C_2	5	1
	S_1	5	1
	C_{2v}	6	2
	C_{2h}	5	1
$D_4 \times \theta$	C_2	5	1
	$C_2(C_1)$	5	1
	$D_2(C_2)$	6	2
	$C_2 \times \theta$	5	1
$D_{4h}(D_4)$	C_2	5	1
	$S_1(C_1)$	5	1
	$C_{2v}(C_2)$	6	2
	$C_{2h}(C_2)$	5	1
$D_{4h}(D_{2h})$	C_2	3	1
	S_1	3	1
	C_{2v}	3	1
	C_{2h}	3	1
$D_{2d} \times \theta$	C_2	3	1
	$C_2(C_1)$	3	1
	$D_2(C_2)$	3	1
	$C_2 \times \theta$	3	1
$D_{4h}(D_{2d})$	C_2	3	1
	$S_1(C_1)$	3	1
	$C_{2v}(C_2)$	3	1
	$C_{2h}(C_2)$	3	1
$D_{4h} \times \theta$	C_2	5	1
	S_1	5	1
	$C_2(C_1)$	5	1
	$S_1(C_1)$	5	1
	C_{2v}	6	2
	$D_2(C_2)$	6	2
	$C_{2v}(C_2)$	6	2
	C_{2h}	5	1
	$C_2 \times \theta$	5	1
	$C_{2h}(C_2)$	5	1
	$C_{2h}(S_2)$	5	1
	$S_1 \times \theta$	5	1
	$C_{2h}(S_1)$	5	1
	$C_{2h} \times \theta$	5	1

Table 3(c). Subgroups of the black-white point groups

POINT GROUP		60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122
3	C_3	60	1																																																													
3	C_3	60	1																																																													
60	C_2	60	1																																																													
61	C_2	61	1	1																																																												
107	T	107	4																																																													

θ is the group consisting of the identity and of the colour reversal operators.

The usual notation $G(H)$ for black-white point group means that it has a subgroup H of index two, containing all elements that are not multiplied by the colour reversal operator (see *e.g.* Hamermesh, 1962).

When considering the subgroups of the black-white point groups, it is advisable to distinguish not only the different crystallographic black-white point groups but also the different orientations that may occur with respect to a given group. There are several reasons for doing so.

Isomorphic groups must have the same number of subgroups. Thus the abstract group D_{2h} has 4 non-isomorphic subgroups: C_1 , C_2 , D_2 , and D_{2h} all of which are normal. If we distinguish all non-equivalent

black-white point groups but not the various orientations, there are 7 groups isomorphic to D_{2h} : D_{2h} , $D_2 \times \theta$ and $D_{2h}(D_2)$ each have 8 subgroups, whereas $D_{2h}(C_{2h})$, $C_{2v} \times \theta$, and $D_{2h}(C_{2v})$ have each 12 subgroups; $C_{2h} \times \theta$ even has 16 of them. If now we distinguish between the different orientations, each of the 7 groups again has the same number of subgroups, *viz.* 16 that are all normal. In Table 1 we indicate the number of non-isomorphic subgroups and non-isomorphic normal subgroups (in column II), and the total number of different subgroups and different normal subgroups (in column III) for each of the 25 abstract black-white point groups. The number of subgroups without distinction of orientation within the group may be found in Tables 3(a) and 3(b).

A more stringent reason appears when we wish to single out the normal subgroups; this can generally

Table 4(a). Normal subgroups within the heavy frame of Table 3(a)

POINT GROUP		SUBGROUP																												
4 2 2	D_4	40	1	1												2														
$\bar{4} 2 m$	D_{2d}	41	1	1											1	1														
$4' 2 2'$	$D_4 (D_2)$	42	1	1											1		1													
$\bar{4}' 2' m'$	$D_{2d} (D_2)$	43	1	1											1			1												
4 mm	C_{4v}	44	1	1												2														
$4' 2 2'$	$D_4 (C_4)$	45	1	1													2													
$4 m' m'$	$C_{4v} (C_4)$	46	1	1														2												
$\bar{4}' 2' m'$	$D_{2d} (S_4)$	47	1	1															1	1										
$4' m m'$	$C_{4v} (C_{2v})$	48	1	1												1		1												
$\bar{4}' 2' m$	$D_{2d} (C_{2v})$	49	1	1												1	1													
4/mmm	D_{4h}	50	1	1	1			1						2	2			1							2					
$4 2 2 1'$	$D_4 \times \theta$	51	1	1	1			1						2	2			1							2					
$4/m' m' m'$	$D_{4h} (D_4)$	52	1	1			1						1	2			2		1							2				
$4'/m m m'$	$D_{4h} (D_{2h})$	53	1	1	1			1					1	1	1	1	1	1					1			1				
$\bar{4} 2 m 1'$	$D_{2d} \times \theta$	54	1	1	1			1					1	1	1	1	1	1						1		1				
$4/m' m' m'$	$D_{4h} (D_{2d})$	55	1	1			1					1	1	1	1	1	1	1							1		1			
$4/m m' m'$	$D_{4h} (C_{4h})$	56	1	1	1			1						2	2	1											2			
4 mm 1'	$C_{4v} \times \theta$	57	1	1	1			1						2	2	1											2			
$4/m' m m$	$D_{4h} (C_{4v})$	58	1	1			1						2	2			1										2			
$4/m m m 1'$	$D_{4h} \times \theta$	59	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2	1	1	1	1	1	1	1	2	2	2	2	2	1

not be done if the orientation of the subgroup is not specified. In D_{4h} for instance the subgroup C_{2v} occurs in 6 different orientations; two of them give rise to a normal subgroup, four of them do not. Table 2 gives a complete list of groups with subgroups that are normal or not according to their orientation.

In Tables 3(a), 3(b), 3(c) we indicate the number of times each subgroup occurs in one of the 122 black-white point groups. All subgroups outside the heavy frame are normal. The normal subgroups occurring within the heavy frame are indicated in Tables 4(a) and 4(b). So far as Table 3(c) is concerned, none of the subgroups within the heavy frame is normal.

One word about the order we have adopted for the enumeration of groups. First of all, isomorphic groups are placed together. Furthermore, groups that can be constructed by successive formation of direct

products with the abstract group of order two are assembled together. Besides C_1 we thus have the 7 families:

$$\begin{aligned}
 &C_2, D_2 = C_2^z \times C_2^y, D_{2h}, D_{2h} \times \theta \\
 &C_4, C_{4h}, C_{4h} \times \theta \\
 &D_4, D_{4h}, D_{4h} \times \theta \\
 &C_3, C_6^z = C_3^z \times C_2^z, C_{6h}, C_{6h} \times \theta \\
 &D_3, D_6^z = D_3^z \times C_2^z, D_{6h}, D_{6h} \times \theta \\
 &T, T_h, T_h \times \theta \\
 &O, O_h, O_h \times \theta.
 \end{aligned}$$

Each family contains precisely one black-white point group that is not isomorphic to an ordinary point group.

We wish to thank the Cobalt Information Centre, Brussels (*cf.* Janner & Ascher, 1963) and the Battelle Institute, Geneva, for their support of this research.

Table 4(b). Normal subgroups within the heavy frame of Table 3(b)

POINT GROUP																																																														
32	D ₄	76	1																																																											
3 m	C _{3v}	77	1																																																											
32'	D _{2d} (C ₂)	78	1																																																											
3 m'	C _{3v} (C ₂)	79	1																																																											
622	D ₆	80	1																																																											
3 m	D _{3d}	81	1																																																											
321'	D _{3d} θ	82	1																																																											
3 m'	D _{3d} (D ₂)	83	1																																																											
3 m'	D _{3d} (C ₂)	84	1																																																											
3 m1'	C _{3v} θ	85	1																																																											
3 m	D _{3d} (C _{2v})	86	1																																																											
6 m2	D _{3h}	87	1																																																											
622'	D _{3d} (D ₂)	88	1																																																											
6 m2	D _{3d} (D ₂)	89	1																																																											
6 mm	C _{6v}	90	1																																																											
62 2'	D ₆ (C ₂)	91	1																																																											
6 m m'	C _{6v} (C ₂)	92	1																																																											
6 m 2'	D _{3h} (C _{2v})	93	1																																																											
6 m m'	C _{6v} (C _{2v})	94	1																																																											
6 m 2'	D _{3h} (C _{2v})	95	1																																																											
6/mmm	D _{6h}	96	1																																																											
6221'	D _{3h} θ	97	1																																																											
6/m m m'	D _{6h} (D ₂)	98	1																																																											
6/m m m'	D _{6h} (D _{3d})	99	1																																																											
6 m 21'	D _{3h} θ	100	1																																																											
6/m m m'	D _{3h} (D _{2h})	101	1																																																											
6/m m m'	D _{3h} (C _{2v})	102	1																																																											
6 mm1'	C _{6v} θ	103	1																																																											
6/m m m'	D _{3h} (C _{2v})	104	1																																																											
3 m1'	D _{3d} θ	105	1																																																											
6/m m m1'	D _{6h} θ	106	1																																																											
23	T	107	1																																																											
m3	T _h	108	1																																																											
231'	Tθ	109	1																																																											
m3	T _h (T)	110	1																																																											
m31'	T _h θ	111	1																																																											
432	O	112	1																																																											
43m	T _h	113	1																																																											
432'	O(T)	114	1																																																											
43m'	T _h (T)	115	1																																																											
m3m	O _h	116	1																																																											
4321'	Oθ	117	1																																																											
m3m'	O _h (O)	118	1																																																											
m3m'	O _h (T _h)	119	1																																																											
43 m1'	T _h θ	120	1																																																											
m3m	O _h (T _d)	121	1																																																											
m3m1'	O _h θ	122	1																																																											
1	C ₁	1	1																																																											
2	C ₂	2	1																																																											
m	S ₆	3	1																																																											
2'	C ₂ (C ₂)	4	1																																																											
m'	S ₆ (C ₂)	5	1																																																											
1'	S ₂	6	1																																																											
1'	C ₂ θ	7	1																																																											
1'	S ₆ (C ₂)	8	1																																																											
222	D ₂	9	1																																																											
mm2	C _{2v}	10	1																																																											
222'	D ₂ (C ₂)	11	1																																																											
m'm'2	C _{2v} (C ₂)	12	1																																																											
2/m	C _{2h}	13	1																																																											
21'	C _{2v} θ	14	1																																																											
2/m'	C _{2h} (C ₂)	15	1																																																											
2/m'	C _{2h} (D ₂)	16	1																																																											
m'	S ₂ θ	17	1																																																											
2/m	C _{2h} (S ₂)	18	1																																																											
m'm'2'	C _{2v} (S ₂)	19	1																																																											
1'	S ₂ θ	20	1																																																											
mmm	D _{2h}	21	1																																																											
2221'	D ₂ θ	22	1																																																											
m'm'm'	D _{2h} (D ₂)	23	1																																																											
m'm'm'	D _{2h} (C _{2v})	24	1																																																											
m m 21'	C _{2v} θ	25	1																																																											
mmm'	D _{2h} (C _{2v})	26	1																																																											
2/m1'	C _{2h} θ	27	1																																																											
mmmm1'	D _{2h} θ	28	1																																																											
4	C ₄	29	1																																																											
4	S ₈	30	1																																																											
4'	C ₄ (C ₂)	31	1																																																											
2'	S ₈ (C ₂)	32	1																																																											
4/m	C _{4h}	33	1																																																											
41'	C ₄ θ	34	1																																																											
4/m'	C _{4h} (C ₂)	35	1																																																											
4/m	C _{4h} (C _{2v})	36	1																																																											
41'	S ₈ θ	37	1																																																											
4/m'	C _{4h} (S ₂)	38	1																																																											
4/m1'	C _{4h} θ	39	1																																																											
422	D ₄	40	1																																																											
42m	D _{2d}	41	1																																																											
422'	D _{2d} (D ₂)	42	1																																																											
4'2m'	D _{2d} (D ₂)	43	1																																																											
4 mm	C _{4v}	44	1																																																											
422'	D _{2d} (C _{2v})	45	1																																																											
4 m m'	C _{4v} (C ₂)	46	1																																																											
4'2m'	D _{2d} (S ₂)	47	1																																																											
4' m m'	C _{4v} (C _{2v})	48	1																																																											
4'2m'	D _{2d} (C _{2v})	49	1																																																											
4/mmm	D _{4h}	50	1																																																											
4221'	D _{2d} θ	51	1																																																											
4/m m m'	D _{4h} (D ₂)	52	1																																																											
4/m m m'	D _{4h} (D _{2d})	53	1																																																											
4'2m1'	D _{2d} θ	54	1																																																											
4/m m m m'	D _{4h} (D _{2d})	55	1																																																											
4/m m m m'	D _{4h} (C _{2v})	56	1																																																											
4 mm1'	C _{4v} θ	57	1																																																											
4/m m m m'	D _{4h} (C _{2v})	58	1																																																											
4/m m m m'	D _{4h} θ	59	1																																																											

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