We are grateful to the United Kingdom Science Research Council for the award of a Research Studentship (to JEL).

References

ASCHER, E. (1966). *Phys. Letters*, **20**, 352.

ASCHER, E. (1967). *Chem. Phys. Letters*, **1**, 69.

ASCHER, E. (1968). *Lattices of equi-translation subgroups of the space groups*. Internal report of the Battelle Institute Advanced Studies Centre, Geneva, 2nd ed.

ASCHER, E., GRAMLICH, V. & WONDRATSCHEK, H. (1969). *Acta Cryst*. B**25**, 2154.

FELSCH, V. & NEUBÜSER, J. (1963). *Mitteilung des Rheinische-Westfälische Instituts für Instrumentelle Mathematik (Bonn)*, **2**, 39.

HERMANN, C. (1929). *Z. Kristallogr*. **69**, 533.

HILTON, H. (1903). *Mathematical Crystallography and the Theory of Groups of Movements*. Oxford Univ. Press.

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). Vol. I. Berlin: Borntraeger.

KOPTSIK, V. A. (1966). *Shubnikov Groups*, Table 10. Moscow Univ. Press.

LANDAU, L. D. (1937). *Phys. Z. Sowjet*. **11**, 26.

LIFSHITZ, E. M. (1942). *J. Phys. Moscow*, **6**, 61.

NEUBÜSER, J. & WONDRATSCHEK, H. (1966). *Krist. Tech*. **1**, 529.

NEUBÜSER, J. & WONDRATSCHEK, H (1969). *Maximal subgroups of the space-groups*. Internal report, 2nd typing. (This differs only in a very few minor misprints and improvements from the original 1965 edition. The whole work was prepared for publication in the next edition of Vol. I of *International Tables for X-ray Crystallography*).

NEUBÜSER, J. & WONDRATSCHEK, H (1970). *Minimal supergroups of the space-groups*. Internal report.

NIGGLI, P. (1919). *Geometrische Kristallographie des Diskontinuums*, Table 1. Leipzig: Borntraeger.

Acta Cryst. (1972). A**28**, 489

Klassengleichen Supergroup–Subgroup Relationships between the Space Groups

BY L. L. BOYLE AND J. E. LAWRENSON

University Chemical Laboratory, Canterbury, Kent, England

(*Received* 18 *February* 1972)

A list of physically significant klassengleichen subgroups and supergroups of the 230 space groups is presented with a discussion of the criteria governing the limitations on the allowed changes in volume of the unit cell.

In a previous paper (Boyle & Lawrenson, 1972) we have enumerated the zellengleichen supergroups of the 230 Fedorov space groups. By definition, no change in the volume of the unit cell was involved and although such relationships are extremely useful for many physical applications, klassengleichen changes are often necessary if radical simplifications of a crystal structure are to be effected. In a klassengleiche ascent in symmetry, the volume of the unit cell is reduced so that not only does the number of molecules per unit cell, Z, change, but also the sites occupied by the various molecules and ions comprising the crystal attain a higher point symmetry. By definition, a klassengleiche relationship can only hold between two space groups having the same crystal class (unit cell group) and therefore in Schönflies notation only the superscript in the space group symbol may change. The principles underlying these relationships were laid down by Hermann (1929) and again in a useful paper by Neubüser & Wondratschek (1966). The enumeration of the black-and-white space groups (Belov, Neronova &

Table 1. *Klassengleichen relationships between the triclinic space groups*

S_2	1
1	z

Code: $z=2$.

Table 2. *Klassengleichen relationships between the monoclinic space groups*

C_2	1	2	3
1	z	.	e
2	z	z	e
3	v	.	z

C_{1h}	1	2	3	4
1	z	.	e	.
2	z	z	e	e
3	v	.	z	.
4	.	v	z	v

C_{2h}	1	2	3	4	5	6
1	z	.	e	.	.	.
2	z	z	e	.	.	.
3	v	.	z	.	.	.
4	z	.	e	z	.	e
5	v	z	e	z	z	e
6	a	.	z	v	.	v

Code: $e=1, 2, 4, 8$; $z=2, 4, 8$; $v=4, 8$; $a=8$ with the restriction that $Z_{\max}=4$ for C_2 and C_{1h} groups and 8 for C_{2h} groups.

Smirnova, 1955) involved the determination of all the halving subgroups of the space groups. Of the 1191 different possibilities, 674 represent zellengleichen and 517 klassengleichen descents. In Koptsik's (1966) monograph, the klassengleichen relationships are distinguished from the zellengleichen (on pp. 625–723) by a rectangular black frame around the catalogue number. These also correspond to the occurrence of P_s, P_c, P_I, C_c, C_a, C_A, F_s, I_c and R_I black-and-white lattices while the zellengleichen correspond to the *P*, *C*, *F*, *I* and *R* lattices. Of the 36 different lattices used for constructing Shubnikov space groups the 14 Bravais lattices are used in the zellengleichen descents and the 22 black-and-white lattices in the klassengleichen descents. A list (with some misprints) of the halving klassengleichen subgroups of the space groups appears in Table 10 of Koptsik's (1966) monograph, and reference to the more accurate list on pp. 625–723 must be made

Table 3. *Klassengleichen relationships between the orthorhombic space groups*

D_2	1	2	3	4	5	6	7	8	9
1	z	.	.	.	.	e	e	e	.
2	z	z	.	.	e	e	e	z	e
3	v	z	z	.	e	e	e	e	z
4	a	v	z	.	e	z	e	z	b
5	a	v	.	.	v	z	e	a	v
6	v	.	.	.	.	z	e	v	.
7	a	.	.	.	.	a	a	a	.
8	a	.	.	.	.	z	z	a	.
9	a	.	.	.	.	z	z	a	.

C_{2v}	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	z	.	.	.	.	.	.	.	.	.	z	.	.	e	.	.	.	e	.	e	.	.
2	z	z	.	.	.	.	.	.	.	.	z	e	.	e	e	.	.	e	.	z	.	e
3	z	.	z	.	.	.	.	.	.	.	z	.	e	z	e	.	.	e	.	z	e	.
4	z	.	.	z	.	.	.	.	.	.	e	.	.	z	e	e	.	e	.	z	.	e
5	v	z	.	z	z	.	.	.	.	.	z	e	.	z	e	z	e	e	.	v	e	z
6	v	.	z	z	.	z	.	.	.	.	z	.	e	e	z	z	e	e	.	v	z	e
7	z	z	.	z	.	.	z	.	.	.	z	e	.	e	e	e	.	e	.	e	.	e
8	v	.	.	z	.	.	.	z	.	.	e	.	.	v	z	z	e	e	.	v	e	z
9	z	z	.	v	z	.	z	z	.	.	z	e	.	z	z	e	e	e	.	z	z	e
10	a	.	v	v	.	z	.	z	.	.	z	.	e	z	v	b	z	e	.	b	z	z
11	v	.	.	.	.	.	.	.	.	.	z	.	.	v	.	.	.	e	.	v	.	.
12	a	v	.	.	.	.	.	.	.	.	z	v	.	v	v	.	.	e	.	a	.	v
13	a	.	v	.	.	.	.	.	.	.	z	.	v	a	v	.	.	e	.	a	v	.
14	v	.	.	.	.	.	.	.	.	.	a	.	.	z	.	.	.	e	.	v	.	.
15	v	.	.	.	.	.	.	.	.	.	a	.	.	v	z	.	.	e	.	v	.	.
16	a	.	.	v	.	.	.	.	.	.	v	.	.	z	v	v	.	e	.	a	.	v
17	a	.	.	v	.	.	.	.	.	.	v	.	.	z	z	v	.	e	.	a	.	v
18	a	.	.	.	.	.	.	.	.	.	s	.	.	a	.	.	.	a	.	a	.	.
19	.	.	.	.	.	s	.	s	.	A	s	.	a	s	.	A	s	a	.	A	s	s
20	a	.	.	.	.	.	.	.	.	.	z	.	.	z	.	.	.	z	.	a	.	.
21	a	.	.	.	.	.	.	.	.	.	z	.	.	a	z	.	.	z	.	a	.	.
22	a	.	.	.	.	.	.	.	.	.	z	.	.	z	z	.	.	z	.	a	.	.

D_{2h}	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
1	z	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	e	.	.	.	e	.	e	.	.	.
2	a	.	v	z	.	.	.	.	.	.	.	.	.	.	.	.	.	.	z	b	v	z	e	.	c	z	.	.
3	z	.	z	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	z	e	e	.	e	.	z	e	.	.
4	v	.	z	z	.	.	.	.	.	.	.	.	.	.	.	.	.	.	e	z	z	e	e	.	v	e	.	.
5	z	.	.	.	z	.	.	.	.	.	.	.	.	.	.	.	z	.	e	.	e	.	e	.	z	v	.	e
6	a	.	v	z	.	.	z	z	.	.	.	.	.	.	.	.	b	z	z	e	z	e	e	.	a	z	z	e
7	v	.	z	.	z	.	z	.	.	.	.	.	.	.	.	.	z	e	e	e	z	.	e	.	v	z	.	e
8	v	.	z	.	z	.	.	z	.	.	.	.	.	.	.	.	z	e	z	z	e	e	e	.	v	z	e	z
9	v	.	.	.	z	.	.	.	z	.	.	.	.	.	.	.	z	e	e	.	z	.	e	.	v	e	.	z
10	a	.	v	.	v	.	.	z	.	.	.	.	z	.	.	.	z	z	z	b	z	z	e	.	z	b	z	v
11	v	.	.	.	z	.	.	.	.	.	z	.	.	.	.	.	e	e	z	.	e	.	e	.	v	e	.	z
12	a	.	v	.	v	.	z	.	z	.	.	.	.	.	.	.	e	z	z	e	v	.	e	.	c	z	.	z
13	v	.	.	.	z	.	.	.	.	.	.	.	z	.	.	.	e	.	e	.	z	.	e	.	e	a	.	z
14	a	.	v	.	.	.	z	z	.	.	z	.	.	.	.	.	e	e	z	z	z	e	e	.	a	e	z	z
15	a	.	.	.	v	.	.	.	.	.	z	.	.	.	.	.	z	e	v	.	z	.	e	.	a	z	E	v
16	a	.	.	.	.	.	.	.	z	.	z	.	z	.	.	.	e	e	z	.	z	.	e	.	z	z	.	e
17	a	.	.	.	v	.	.	.	.	.	.	.	.	.	.	.	v	.	z	.	v	.	e	.	a	s	.	v
18	a	.	.	.	v	.	.	.	.	.	.	.	.	.	.	.	v	.	v	.	z	.	e	.	a	a	.	v
19	v	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	z	.	.	.	e	.	v	.	.	.
20	a	.	v	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	z	v	v	.	e	.	a	v	.	.
21	v	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	v	.	z	.	e	.	v	v	.	.
22	a	.	v	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	a	v	z	.	e	.	a	v	.	.
23	a	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	a	.	.	.	a	.	a	.	.	.
24	s	A	d	s	.	.	.	.	.	.	.	.	.	.	.	.	.	.	s	d	d	s	z	.	a	s	.	.
25	s	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	z	.	.	.	z	.	a	.	.	.
26	s	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	z	.	z	.	z	.	a	a	.	.
27	s	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	a	.	z	.	z	.	s	a	.	.
28	s	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	z	.	.	.	z	.	a	.	.	.

Code: $e=1, 2, 4, 8, 16, 32$; $E=1$; $b=1, 4, 8, 16, 32$; $c=1, 8, 16, 32$; $z=2, 4, 8, 16, 32$; $v=4, 8, 16, 32$; $a=8, 16, 32$; $A=8$; $s=16, 32$; $d=32$; with the restrictions that $Z_{\max}=8$ for D_2 groups, 16 for C_{2v} groups and 32 for D_{2h} groups.

Table 4. *Klassengleichen relationships between the trigonal space groups*

C_3	1	2	3	4
1	*d*	.	.	*e*
2	*d*	*d*	.	*e*
3	*d*	.	*d*	*e*
4	*n*	.	.	*d*

S_6	1	2
1	*b*	*e*
2	*n*	*b*

D_{3d}	1	2	3	4	5	6
1	*b*	.	*d*	.	*d*	.
2	*z*	.	*s*	*D*	*s*	*D*
3	*d*	.	*b*	.	*e*	.
4	*s*	*D*	*z*	.	*s*	*E*
5	*n*	.	.	.	*b*	.
6	*a*	*n*	.	.	*z*	.

C_{3v}	1	2	3	4	5	6
1	*b*	*d*	.	.	*e*	.
2	*d*	*b*	.	.	*d*	.
3	*z*	*s*	*D*	*D*	*s*	*E*
4	*s*	*z*	*D*	*D*	*s*	*D*
5	.	*n*	.	.	*b*	.
6	.	*a*	.	*n*	*z*	.

D_3	1	2	3	4	5	6	7
1	*b*	*d*	.	.	.	.	*d*
2	*d*	*b*	.	.	.	.	*e*
3	*d*	*n*	*b*	*d*	*z*	*s*	*d*
4	*n*	*d*	*d*	*b*	*s*	*z*	*e*
5	*d*	*n*	*z*	*s*	*b*	*d*	*d*
6	*n*	*d*	*s*	*z*	*d*	*b*	*e*
7	*n*	.	.	.	.	.	*b*

Code: $e=1, 2, 3, 4, 6, 9, 12, 18, 36$; $E=3$; $z=2, 4, 6, 8, 12, 18, 36$; $d=3, 6, 9, 12, 18, 36$; $D=3$; $b=2, 3, 4, 6, 9, 12, 18, 36$; $s=6, 12, 18, 36$; $n=9, 18, 36$; $a=18, 36$ with the restriction that $Z_{\max}=9$ for C_3, 18 for S_6, D_3, C_{3v} and 36 for D_{3d}. For the space groups based on a rhombohedral unit cell, ascent or descent to a hexagonal cell is assumed.

Table 5. *Klassengleichen relationships between the tetragonal space groups*

C_4	1	2	3	4	5	6
1	*z*	.	.	.	*e*	.
2	*v*	*z*	*z*	.	*z*	*e*
3	*z*	.	*z*	.	*e*	*z*
4	*v*	.	*z*	*z*	*z*	*e*
5	*v*	.	.	.	*v*	.
6	*a*	.	*v*	.	*v*	*v*

S_4	1	2
1	*z*	*e*
2	*v*	*v*

C_{4h}	1	2	3	4	5	6
1	*z*	.	.	.	*e*	.
2	*z*	*z*	.	.	*e*	.
3	*z*	.	*z*	.	*e*	.
4	*v*	*z*	*z*	.	*e*	.
5	*v*	.	.	.	*v*	.
6	*s*	*a*	*a*	*V*	*v*	.

D_4	1	2	3	4	5	6	7	8	9	10
1	*z*	.	.	.	.	.	.	.	*e*	.
2	*z*	*z*	*z*	.	*v*	.	*s*	.	*e*	*z*
3	*v*	.	*z*	.	*z*	.	.	.	*z*	*e*
4	*a*	*v*	*z*	.	*v*	*Z*	.	.	*z*	*e*
5	*z*	.	.	.	*z*	.	.	.	*e*	.
6	*v*	*z*	*v*	.	*z*	.	.	.	*e*	*v*
7	*v*	.	*z*	.	*z*	.	*z*	.	*z*	*e*
8	*a*	*v*	*v*	.	*v*	*Z*	*z*	.	*z*	*e*
9	*v*	.	.	.	.	.	.	.	*v*	.
10	*a*	.	.	.	*v*	.	.	.	*v*	.

C_{4v}	1	2	3	4	5	6	7	8	9	10	11	12
1	*z*	.	.	.	.	.	.	.	*e*	.	.	.
2	*z*	*z*	.	.	.	.	.	.	*z*	*e*	.	.
3	*z*	.	*h*	.	.	.	*g*	.	*z*	*f*	.	.
4	*v*	*z*	*h*	.	.	.	*g*	.	*e*	*z*	.	.
5	*z*	.	.	.	*z*	.	.	.	*z*	*e*	.	.
6	*v*	*z*	.	.	*z*	.	.	.	*b*	*z*	.	.
7	*z*	.	*g*	.	.	.	*h*	.	*e*	.	.	.
8	*v*	*z*	*g*	.	.	.	*h*	.	*v*	*e*	.	.
9	*v*	.	.	.	.	.	.	.	*v*	.	.	.
10	*v*	.	.	.	.	.	.	.	*v*	.	.	.
11	*s*	*a*	*S*	*V*	.	.	*k*	.	*v*	*a*	.	.
12	*s*	*a*	*S*	*V*	.	.	*k*	.	*v*	*a*	.	.

D_{2d}	1	2	3	4	5	6	7	8	9	10	11	12
1	*z*	.	.	.	*z*	.	.	.	*z*	.	*e*	.
2	*z*	*h*	.	.	*v*	*g*	.	.	*v*	*g*	*e*	.
3	*v*	.	*z*	.	*z*	.	.	.	*z*	.	*e*	.
4	*a*	*h*	*z*	.	*v*	*g*	.	.	*v*	*g*	*e*	.
5	*z*	.	.	.	*z*	.	.	.	*e*	.	*z*	.
6	*v*	*g*	.	.	*z*	*h*	.	.	*z*	*f*	*z*	.
7	*z*	.	.	.	*v*	.	*z*	.	*v*	*e*	*z*	.
8	*v*	*g*	.	.	*a*	*h*	*z*	.	*c*	*z*	*z*	.
9	*v*	.	.	.	*a*	.	.	.	*a*	.	*v*	.
10	*v*	.	.	.	*a*	.	.	.	*a*	.	*v*	.
11	*a*	.	.	.	*v*	.	.	.	*v*	.	*a*	.
12	*s*	*k*	.	.	.	*S*	*a*	*V*	*j*	*a*	*a*	.

D_{4h}	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	*z*	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	*e*	.	.	.
2	*z*	*z*	.	.	.	.	.	.	.	.	.	.	.	.	.	.	*z*	*e*	.	.
3	*z*	.	*z*	.	.	.	.	.	.	.	.	.	.	.	.	.	*z*	*e*	.	.
4	*v*	*z*	*z*	.	.	.	.	.	.	.	.	.	.	.	.	.	*b*	*z*	.	.
5	*a*	.	.	.	*z*	.	.	.	.	.	.	.	.	.	.	.	*z*	*e*	.	.
6	*v*	*z*	.	.	*z*	.	.	.	.	.	.	.	.	.	.	.	*e*	*z*	.	.
7	*a*	.	.	.	.	.	*z*	.	.	.	.	.	.	.	.	.	*e*	.	.	.
8	*v*	*z*	.	.	.	.	*z*	.	.	.	.	.	.	.	.	.	*z*	*e*	.	.
9	*a*	.	.	.	.	.	.	.	*h*	*g*	.	.	.	.	.	.	*e*	*z*	.	.
10	*a*	.	.	.	.	.	.	.	*g*	*h*	.	.	.	.	.	.	*z*	*b*	.	.
11	*v*	.	*z*	.	.	.	.	.	*h*	*g*	.	.	.	.	.	.	*v*	*e*	.	.
12	*v*	.	*z*	.	.	.	.	.	*g*	*h*	.	.	.	.	.	.	*e*	*z*	.	.
13	*v*	.	.	.	*z*	.	.	.	*h*	*g*	.	.	.	.	.	.	*v*	*e*	.	.
14	*v*	.	.	.	*z*	.	.	.	*g*	*h*	.	.	.	.	.	.	*e*	*z*	.	.
15	*v*	.	.	.	.	.	*z*	.	*h*	*g*	.	.	.	.	.	.	*b*	*z*	.	.
16	*v*	.	.	.	.	.	*z*	.	*g*	*h*	.	.	.	.	.	.	*z*	*b*	.	.
17	*v*	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
18	*v*	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	*v*	.	.	.
19	*s*	.	*a*	.	.	.	.	.	*k*	*S*	.	*V*	.	.	.	.	*v*	*a*	.	.
20	*s*	.	*a*	.	.	.	.	.	*k*	*S*	.	*V*	.	.	.	.	*v*	*a*	.	.

Code: $e=1, 2, 4, 8, 16, 32$; $f=1, 4, 16$; $b=1, 4, 8, 16, 32$; $c=1, 8, 16, 32$; $E=1$; $z=2, 4, 8, 16, 32$; $g=2, 8, 32$; $Z=2$; $v=4, 8, 16, 32$; $h=4, 16$; $j=4, 32$; $V=4$; $a=8, 16, 32$; $k=8, 32$; $A=8$; $s=16, 32$; $S=16$; $d=32$ with the restrictions that $Z_{\max}=8$ for C_4 and S_4 groups; 16 for C_{4h}, D_4, C_{4v} and D_{2d} groups; and 32 for D_{4h} groups.

Table 6. *Klassengleichen relationships between the hexagonal space groups*

C_6	1	2	3	4	5	6
1	*b*	.	.	.	.	.
2	*s*	.	.	*z*	.	*D*
3	*s*	.	.	.	*z*	*D*
4	*d*	.	.	*b*	*z*	.
5	*d*	.	.	*z*	*b*	.
6	*z*	.	.	.	.	*D*

D_6	1	2	3	4	5	6
1	*b*	.	.	.	.	.
2	*s*	.	.	*z*	*v*	*D*
3	*s*	.	.	*v*	*z*	*D*
4	*d*	.	.	*b*	*z*	.
5	*d*	.	.	*z*	*b*	.
6	*z*	.	.	.	.	*D*

C_{3h}	1
1	*b*

C_{6h}	1	2
1	*b*	.
2	*z*	*D*

C_{6v}	1	2	3	4
1	*b*	.	.	.
2	*z*	*D*	.	.
3	*z*	.	.	*D*
4	*z*	.	*D*	.

D_{3h}	1	2	3	4
1	*b*	.	*d*	.
2	*z*	.	*s*	*D*
3	*d*	.	*b*	.
4	*s*	*D*	*z*	.

D_{6h}	1	2	3	4
1	*b*	.	.	.
2	*z*	*D*	.	.
3	*z*	.	.	*D*
4	*z*	.	*D*	.

Code: b=2, 3, 4, 6, 8, 12, 24; z=2, 4, 6, 8, 12, 24; d=3, 6, 12, 24; D=3; v=4, 8, 12, 24; s=6, 12, 24; with the restrictions that $Z_{\max}=6$ for C_6 groups and C_{3h} groups; 12 for D_6, C_{6h}, C_{6v} and D_{3h} groups; and 24 for D_{6h} groups.

with great care since although the convention of writing G/H for the black-and-white space group arising from a space group G and its halving subgroup H holds, the ordering principle is on G if the descent is zellengleich, but on H if it is klassengleich.

A complete list of maximal klassengleichen subgroups has been given in an internal report by Neubüser & Wondratschek (1969) in Hermann–Mauguin notation and the inverse list of minimal klassengleichen supergroups has been produced more recently (Neubüser & Wondratschek, 1970). These lists do not include the possibilities of enlargement of cell size without change of space group since these can be effected by increasing an axis by any desired number of times subject to the restriction that any equivalent axes are also similarly increased (Hermann, 1929; Neubüser & Wondratschek, 1966), provided that such an increase is allowable for the symmetry elements in question. A list of derivative symmetries and their translational multiplicities, for one and two-dimensional symmetry operations only, has been given by Buerger (1949). In general it can be said that improper operations (screws and glides) have derivatives which are seldom allowed on physical grounds but we have considered all cases in detail on the lines of Buerger's analysis.

There is an important difference between the number in double parentheses of Neubüser & Wondratschek (1969) and that in parentheses in Table 10 of Koptsik (1966). In both works it is properly defined but the Russian text of Koptsik (1966) may hinder appreciation of the difference. Neubüser & Wondratschek have used this number to denote the index of the subgroup, *i.e.* the ratio of the orders of supergroup and subgroup. Koptsik has used it to denote the actual ratio of the volumes of the unit cell of the subgroup to that of the supergroup. This is the quantity which is relevant to physical applications and in order to obtain it from the index one must multiply the index by the ratio of the volumes of the unit cell of the subgroup to that of the supergroup. This ratio of the volumes can conveniently be determined from the diagrams defining the black-and-white lattices of Belov, Neronova & Smirnova (1955) for the halving subgroup cases and can take the value $\frac{1}{2}$ as well as certain integral values.

The problem of determining the klassengleichen relationships between two space groups may now be divided into the problems of first enumerating all (*i.e.* not necessarily maximal) klassengleichen subgroups of a given group and then the possible volume changes accompanying each relationship. The latter problem is infinite, and virtually intractable if an attempt is made to specify the different orientations through which a given volume ratio may be obtained. There are, however, physical restrictions on the number of useful volume changes. It would not be desirable to reduce the number of molecules per unit cell to less than one: further the number of molecules per unit cell is limited (if crystallographic equivalence of chemically and spectroscopically equivalent molecules or ions is to be maintained). The maximum value of Z is the product of the order of the crystal class and the number of lattice points per unit cell (1 for primitive, 2 for end-centred and body-centred cells, 3 for an hexagonal cell and 4 for face-centred cells). The maximum value may appear to have been exceeded if the 'formula' of the compound has been over-simplified to the extent that it represents only a fraction of the entity that should be associated with a general position (site of C_1 symmetry). Such formulae cannot distinguish chemical or crystallographic inequivalence of the constituent groups and only represent a statement of the composition determinable by chemical analysis. It will henceforth be assumed that the formula meets the basic requirements. A further physical restriction is that Z shall be integral and thus any cell volume change must be a factor of Z; since all possible Z values are factors of the maximum Z discussed above, the only cell volume changes that need be considered are those which are factors of the maximum Z.

The Tables

Tables 1–7 give the possible volume changes within the physically significant range as a ratio of the volume of the unit cell in the subgroup symmetry to that in the supergroup. To simplify printing, various code letters have been used and have been explained in the rubric to the Table in which they appear. Where no entry appears at the intersection of a row and column either no klassengleiche relationship occurs or the relationship is of no physical significance. The supergroups have been written along the top of each table so that the subgroups can be read off from the column below the group being studied. The subgroups have

Table 7. *Klassengleichen relationships between the cubic space groups*

T	1	2	3	4	5
1	*a*	*e*	*e*	.	.
2	*a*	*a*	*a*	.	.
3	*a*	*a*	*a*	.	.
4	*a*	*e*	*a*	.	*E*
5	*a*	*a*	*a*	.	.

T_h	1	2	3	4	5	6	7
1	*a*	.	*e*	.	*e*	.	.
2	*a*	.	*e*	.	*e*	.	.
3	*a*	.	*a*	.	*a*	.	.
4	.	*A*	*a*	.	*a*	.	.
5	*a*	.	*a*	.	*a*	.	.
6	*a*	.	*e*	.	*a*	.	*E*
7	*a*	.	*a*	.	*a*	.	.

T_d	1	2	3	4	5	6
1	*a*	*e*	*e*	.	.	.
2	*a*	*a*	*a*	.	.	.
3	*a*	*a*	*a*	.	.	.
4	.	.	*e*	.	*E*	.
5	*a*	*a*	*a*	.	.	.
6	.	.	*a*	*A*	*A*	.

O	1	2	3	4	5	6	7	8
1	*a*	.	*e*	.	*e*	.	.	.
2	*a*	*a*	*e*	.	*e*	.	.	.
3	*a*	.	*a*	.	*a*	.	.	.
4	.	*a*	*a*	.	*a*	.	.	.
5	*a*	.	*a*	.	*a*	.	.	.
6	.	*a*	*a*	*E*	*a*	.	.	*E*
7	.	*a*	*a*	*E*	*a*	.	.	*E*
8	.	*a*	*a*	.	*a*	.	.	.

O_h	1	2	3	4	5	6	7	8	9	10
1	*a*	.	.	.	*e*	.	.	.	*e*	.
2	*a*	.	.	.	*a*	*e*	.	.	*e*	.
3	*a*	.	.	.	*a*	*e*	.	.	*e*	.
4	*a*	.	.	.	*e*	.	.	.	*e*	.
5	*a*	.	.	.	*a*	.	.	.	*a*	.
6	*a*	.	.	.	*a*	*a*	.	.	*a*	.
7	*s*	.	.	*A*	*a*	.	.	.	*a*	.
8	*s*	.	.	*A*	*a*	.	.	.	*a*	.
9	*a*	.	.	.	*a*	.	.	.	*a*	.
10	*s*	.	*A*	.	*a*	*a*	.	.	*a*	.

Code: $e=1, 8, 64$; $E=1$; $a=8, 64$; $A=8$; $s=64$; with there strictions that $Z_{\max}=48$ for T groups; 96 for T_h, T_d and O groups and 192 for O_h.

been written in the vertical column so that their supergroups can be read off from the relevant row. Where enantiomorphic pairs of groups appear, klassengleichen relationships are possible but the cell volume ratios are not in the physically significant range. This is not unreasonable since it should not be possible to radically affect predictions of the optical acivity of a crytal by effecting a klassengleiche change of space group. Increase of the unit-cell volume by descent in symmetry to a subgroup is allowed for many more cell volume ratios, but is seldom a useful process.

We would like to thank Professor Dr H. Wondratschek for a most helpful discussion with LLB during a recent visit to Karlsruhe which elucidated some of the finer points of the problem. We would also like to thank the United Kingdom Science Research Council for the award of a Research Studentship to JEL.

References

BELOV, N. V., NERONOVA, N. N. & SMIRNOVA, T. S. (1955). *Trudy Akad. Nauk SSSR. Inst. Kristallogr.* **11**, 33; a translation into imperfect English has appeared in *Colored Symmetry* (1964). Edited by W. T. HOLSER, pp. 175–210. Oxford: Pergamon.

BOYLE, L. L. & LAWRENSON, J. E. (1972). *Acta Cryst.* **A28**, 485.

BUERGER, M. J. (1949). *J. Chem. Phys.* **15**, 1.

HERMANN, C. (1929). *Z. Kristallogr.* **69**, 533.

KOPTSIK, V. A. (1966). *Shubnikov Groups.* Moscow Univ. Press.

NEUBÜSER, J. & WONDRATSCHEK, H. (1966). *Krist. Tech.* **1**, 529.

NEUBÜSER, J. & WONDRATSCHEK, H. (1969). *Maximal subgroups of the space-groups.* Internal report, 2nd typing.

NEUBÜSER, J. & WONDRATSCHEK, H. (1970). *Minimal supergroups of the space-groups.* Internal report.