For graphite monochromatized X-rays, $I_h(\theta)$ corresponding to $I_0^B(\varepsilon)$ is not constant and the integral in (31) cannot be evaluated. In spite of this it is common practice to consider $I_0 v/\alpha'$ as constant and to use (33) for the determination of observed structure factors on a relative scale. The error arising by neglect of the first part in (30) is about 1% as was estimated from three reflection profiles with different Bragg angles. However, this error scarcely varies with the Bragg angle so that for relative measurements the effective error reduces to about 0.2%.

The error caused by considering α' as constant in (33) may rise to about 2% depending upon which scan intervals are chosen and which Bragg-angle range is covered during data collection.

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On the Equivalence of Point Configurations due to Euclidean Normalizers (Cheshire Groups) of Space Groups

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Dedicated to Professor M. J. Buerger on the occasion of his 80th birthday

Abstract

The Euclidean normalizers of space groups form the appropriate mathematical tool for several problems treated independently by crystallographers in the past, *e.g.* the comparison, the classification and the standardized description of crystal structures. Explicit tables are presented that enable the user to handle Euclidean normalizers in an easy way and, especially, to calculate all descriptions of a crystal structure compatible with a chosen space-group setting. The use of the tables is illustrated by different examples, and the role of Euclidean normalizers for crystal-structure determination is discussed.

1. Introduction

Depending on the position of a representative point, point configurations (*i.e.* sets of symmetrically equivalent points) of a given space group in general differ with respect to their geometrical properties. For a study of these properties all different cases are covered if the coordinates of such a reference point are varied over the whole range of an asymmetric unit. In most space groups, however, it is possible to confine the parameter variation to a smaller region by taking into account the symmetry of the pattern of symmetry elements. In plane group *pgg*, for instance, Laves (1931) derived all possible plane partitions into Dirichlet domains by considering only the range $0 \leq x,y \leq \frac{1}{4}$ instead of the asymmetric unit $0 \leq x,y < \frac{1}{2}$ 'for reasons of symmetry'. Under the term 'reduced asymmetric units' this principle has been revived by Fischer (1968) in a paper on the packing of circles in a plane. Later it was applied in connection with sphere packings (Fischer, 1970, 1971, 1973, 1974) and Dirichlet partitions (Koch, 1972, 1973). For a classification of point configurations by means of symmetry, shortest dis-

tances and types of Dirichlet partitions the results are also given only for such reduced asymmetric units (Koch, 1983), *i.e.* in a most economic way.

Closely related to this is the problem of the different possibilities to describe a crystal structure or to place the first atom(s) in a trial structure, even if the size and the shape of the unit cell have been fixed. For all space groups, Hirshfeld (1968) has derived and tabulated the groups of all transformations that map such different possibilities onto each other and has called them *Cheshire groups*. He demonstrates by the example of $I4_122$ how all transformed coordinate triplets can be derived by means of Cheshire groups from the coordinate triplets listed in *International Tables for X-ray Crystallography* (1952).

As Hirshfeld's example shows, such a derivation is not always trivial, because the standard descriptions of a space group and its Cheshire group may differ with respect to the orientation of their unit cells and to the choice of origin. Therefore, it is helpful to have available explicit tables which enable the user to transform a given description of a crystal structure into all analogous ones. Such more detailed information has proved to be very useful for the classification of crystal structures (*cf.* Koch & Hellner, 1981; Hellner, Koch & Reinhardt, 1981), and is necessary if a standardized description of crystal structures is aimed at (Parthé & Gelato, 1983).

Similar relations between point configurations (or crystallographic orbits, *cf.* Wondratschek, 1976) play an important role in the assignment of Wyckoff positions to lattice complexes (Fischer & Koch, 1974, 1983; Koch & Fischer, 1978) and led to the derivation of the automorphism groups of the space groups (Koch & Fischer, 1975). Parallel to this, the related problems of interchangeable Wyckoff positions (Boyle & Lawrenson, 1973, 1978), of permissible origin shifts in direct methods (Giacovazzo, 1974), of interchangeable subgroups of space groups (Zarrouk & Billiet, 1975; Sayari & Billiet, 1975; Billiet, Sayari & Zarrouk, 1978), of automorphism groups of point groups (Billiet, 1975) and of standard settings of triclinic and monoclinic space groups (Sayari & Billiet, 1977) have been treated.

The mathematical concept underlying and connecting all these studies – though not mentioned in any of the corresponding papers – is that of the normalizer of a group with respect to one of its supergroups. Though this concept is well established in mathematics, its significance for such crystallographic problems was pointed out only a few years ago by Wondratschek (1980). Ascher (1974) did apply normalizers to determine the relativistic symmetry of a crystal structure. He introduced the term *symmetry of the symmetry* in this connection, but his paper seems to have escaped most crystallographers' notice. Subsequently, Burzlaff & Zimmermann (1980) have explicitly used normalizers when establishing 'privileged

origins'. Their table of the affine normalizers of space groups has been supplemented with respect to those of the monoclinic and triclinic groups by Billiet, Burzlaff & Zimmermann (1982). Another study on normalizers and automorphism groups of symmetry groups has recently been published by Gubler (1982), who tried to elaborate a strictly mathematical algorithm for the derivation of these groups. He himself admits, however, that two steps in his procedure 'still require some intuition'.

2. Normalizers of space groups

The *normalizer* $N_H(G)$ of a group G with respect to one of its supergroups H is the set of all elements $h \in H$ that map G onto itself by conjugation:

$$N_H(G): = \{h \in H | hGh^{-1} = G\}.$$

The normalizer $N_H(G)$ is always a group intermediate between G and H: $G \subseteq N_H(G) \subseteq H$. It is the largest such intermediate group that contains G as a normal subgroup. Therefore, it describes to a certain extent, fixed by the choice of H, the symmetry of the group G.

If G is a crystallographic group, the group elements, *i.e.* the symmetry operations, are isometries. So a natural choice for H is the Euclidean group E, the group of all isometries. The corresponding normalizer $N_E(G)$ is called the *Euclidean normalizer* of G.

If G especially is a space group its Euclidean normalizer is identical to the Cheshire group introduced by Hirshfeld (1968), *i.e.* the symmetry group of the pattern of symmetry elements (*cf.* Koch & Fischer, 1975; Gubler, 1982): Let g_1, $g_2 \in G$ be any pair of symmetry operations conjugate with respect to an element $h \in N_E(G)$, *i.e.* $hg_1h^{-1} = g_2$, and let x_1, x_1' be any pair of points mapped onto each other by g_1, *i.e.* $x_1' = g_1(x_1)$. As h also is an isometry, it operates on the points x_1 and x_1' and maps them onto $x_2 = h(x_1)$ and $x_2' = h(x_1')$. Then it follows that $x_2' = h(x_1') = hg_1(x_1) = hg_1h^{-1}(x_2) = g_2(x_2)$, *i.e.* h maps each pair of symmetry-related points onto another such pair, the symmetry element of g_1 onto the symmetry element of g_2 and the entire pattern of symmetry elements of G onto itself. Conversely, each symmetry operation of the pattern of symmetry elements of G is contained in the Euclidean normalizer $N_E(G)$ if symmetry elements are understood as geometric objects with certain qualities attached to them.

Euclidean normalizers may be used if, in a crystallographic problem, the lattice parameters have fixed values, *i.e.* if a specified space group from a given space-group type (Neubüser & Wondratschek, 1966; Wondratschek, 1983) is considered. This is the case for most of the problems connected with the determination, the description and the comparative discussion of crystal structures. As has also been stated by Gubler (1982),

space groups of the same type may differ with respect to the type of their Euclidean normalizers. This situation occurs if the same symmetry exists in symmetrically inequivalent directions (*e.g.* in *a*, *b* and *c* directions in *Pmmm*): special values or relationships for the lattice parameters ($a = b \neq c$ or $a = b = c$) may give rise to more comprehensive Euclidean normalizers (tetragonal or cubic, respectively, instead of orthorhombic for the general case).

For certain theoretical problems, like the derivation of subgroups and the definition of lattice complexes, the following choice of *H* is more advantageous: if *H* is the affine group *A*, the group of all affine mappings, the normalizer $N_A(G)$ is called the *affine normalizer* of *G*. The relation between a space group and its affine normalizer is the same for all space groups of the same type. $N_E(G)$ is a true subgroup of $N_A(G)$ for all triclinic and monoclinic space groups, but is equal to $N_A(G)$ for all tetragonal, trigonal, hexagonal and cubic ones. Within the orthorhombic crystal system, $N_E(G) = N_A(G)$ normally holds for all space groups of the same type; both normalizers differ, however, for space groups of type *P*222$_1$, *P*2$_1$2$_1$2, *C*222$_1$, *C*222, *Pmm*2, *Pcc*2, *Pba*2, *Pnn*2, *Cmm*2, *Ccc*2, *Fmm*2, *Fdd*2, *Imm*2, *Iba*2, *Pccm*, *Pban*, *Pbam*, *Pccn*, *Pnnm*, *Pmmn*, *Cmmm*, *Cccm*, *Cmma*, *Ccca*, *Ibam*, and *Imma* unless $a = b$, and for space groups of type *P*222, *P*2$_1$2$_1$2$_1$, *F*222, *I*222, *I*2$_1$2$_1$2$_1$, *Pmmm*, *Pnnn*, *Pbca*, *Fmmm*, *Fddd*, *Immm*, and *Ibca* unless $a = b = c$.

3. Equivalent point configurations and possible descriptions of crystal structures

As has been shown above, each element *h* of the Euclidean normalizer $N_E(G)$ of a space group *G* maps any pair of points symmetrically equivalent with respect to *G* onto another such pair. An element of $N_E(G)$, therefore, maps each point configuration of *G* onto a point configuration of the same space group. This property of the Euclidean normalizer gives rise to the following definition: Two point configurations of the same space group *G* are called *equivalent*, if they are mapped onto each other by an element $h \in N_E(G)$. As the elements of the Euclidean normalizer are isometries, such equivalent point configurations are always directly or inversely congruent. They form equivalence classes, each of which is generated by applying all elements of $N_E(G)$ to any point configuration out of the class. If *i* is the index of *G* with respect to its supergroup $N_E(G)$, the number of point configurations in such a class is *i* in the general case. This number may become less than *i*, however, for point configurations belonging to limiting complexes (*cf.* Fischer & Koch, 1983) and for point configurations of special positions.

Equivalent point configurations may belong to the same Wyckoff position. Then the part of the Wyckoff position within one asymmetric unit of the normalizer is smaller than that within one asymmetric unit of the space group. If, on the contrary, equivalent point configurations belong to different Wyckoff positions, all these positions together form a *Wyckoff set* (called *Konfigurationslage* by Koch & Fischer, 1975, *cf.* Wondratschek, 1983; Fischer & Koch, 1983). Such a Wyckoff set corresponds to one Wyckoff position of $N_E(G)$, if $N_E(G)$ itself is a space group (*cf.* below).

In the same way, sets made up from several point configurations may be duplicated. From one such set the Euclidean normalizer generates at most *i* equivalent sets, which may coincide in some of their point configurations. Different coordinate descriptions of one and the same crystal structure correspond to such equivalent sets of point configurations: if a crystal structure is described in the highest possible space group, then there exist exactly *i* different descriptions referring to the same space-group setting. All these possible descriptions are obtained by applying the Euclidean normalizer to a given description. In this procedure, the symmetry operations of the space group itself reproduce the original description and each of the $i - 1$ additional cosets of the space group within its Euclidean normalizer generates one of the additional possible descriptions. Different isometries from the same coset only result in interchanged points (or atoms) within the same description.

The ambiguity of crystal-structure description exists for all space groups except for *Im*3*m* and *Ia*3*d*. Each space group of one of these types coincides with its Euclidean normalizer and, therefore, shows unique point configurations and, in consequence, unique descriptions of crystal structures.

If less than *i* different descriptions of a crystal structure are produced by the Euclidean normalizer, at least one coset other than the space group itself reproduces the original description. In this case, the original space group is not properly chosen, because it does not contain the entire symmetry of the crystal structure, its *inherent symmetry*. For example, the structure of β-Hg$_4$Pt has been described in *Structure Reports* (1953), in space group *I*432 with Pt at 2(*a*) 0,0,0, and Hg at 8(*c*) $\frac{1}{4},\frac{1}{4},\frac{1}{4}$. As the subgroup index *i* of *I*432 in its Euclidean normalizer *Im*3*m* is 2, there should exist two different descriptions of this crystal structure. All additional symmetry operations of *Im*3*m*, however, leave the given description unchanged. The symmetry of β-Hg$_4$Pt, therefore, must at least be *Im*3*m*. This reasoning cannot be reversed, however: the number of different descriptions of a crystal structure in a given space group may be *i*, though this space group is not its inherent symmetry. The structure of β-tungsten, for instance, may be described in *Ia*3*d* by O at 16(*a*) 0,0,0 and W at 48(*g*) $\frac{1}{8}, x, \frac{1}{4} - x$ with $x = \frac{1}{4}$.

Table 1. *Characterization of the Euclidean normalizers of space groups: number and symbol of space group in columns 1 and 2, references to Tables 2 and 3 in columns 3 and 4, respectively*

No.	Symbol	T2	T3	No.	Symbol	T2	T3	No.	Symbol	T2	T3	No.	Symbol	T2	T3
1	$P1$	2	2A	33	$Pna2_1$	13	8B	102	$P4_2nm$	23	4G	163	$P\bar{3}1c$	37	4O
2	$P\bar{1}$	1	8D	34	$Pnn2$	13	8B	103	$P4cc$	23	4G	164	$P\bar{3}m1$	37	4O
3	$P112$	5	8B	35	$Cmm2$	13	4E	104	$P4nc$	23	4G	165	$P\bar{3}c1$	37	4O
3	$P121$	6	8A	36	$Cmc2_1$	13	4E	105	$P4_2mc$	23	4G	166	$R\bar{3}m$ (h)	25	2H
4	$P112_1$	5	8B	37	$Ccc2$	13	4E	106	$P4_2bc$	23	4G	166	$R\bar{3}m$ (r)	26	2G
4	$P12_11$	6	8A	38	$Amm2$	13	4E	107	$I4mm$	23	2E	167	$R\bar{3}c$ (h)	25	2H
5	$A112$	5	4E	39	$Abm2$	13	4E	108	$I4cm$	23	2E	167	$R\bar{3}c$ (r)	26	2G
5	$B112$	5	4F	40	$Ama2$	13	4E	109	$I4_1md$	24	2E	168	$P6$	39	4I
5	$I112$	5	4E	41	$Aba2$	13	4E	110	$I4_1cd$	24	2E	169	$P6_1$	35	2E
5	$C121$	6	4D	42	$Fmm2$	13	2D	111	$P\bar{4}2m$	18	8G	170	$P6_5$	35	2E
5	$A121$	6	4C	43	$Fdd2$	14	2D	112	$P\bar{4}2c$	18	8G	171	$P6_2$	35	2E
5	$I121$	6	4C	44	$Imm2$	13	4E	113	$P\bar{4}2_1m$	18	8G	172	$P6_4$	35	2E
6	$P11m$	7	4A	45	$Iba2$	13	4E	114	$P\bar{4}2_1c$	18	8G	173	$P6_3$	39	4I
6	$P1m1$	8	4B	46	$Ima2$	13	4E	115	$P\bar{4}m2$	18	8H	174	$P\bar{6}$	38	24B
7	$P11a$	7	4A	47	$Pmmm$	9	8D	116	$P\bar{4}c2$	18	8H	175	$P6/m$	37	4P
7	$P11n$	7	4A	48	$Pnnn$ (222)	9	8D	117	$P\bar{4}b2$	18	8H	176	$P6_3/m$	37	4P
7	$P11b$	7	4A	48	$Pnnn$ ($\bar{1}$)	9	8D	118	$P\bar{4}n2$	18	8H	177	$P622$	37	4P
7	$P1c1$	8	4B	49	$Pccm$	9	8D	119	$I\bar{4}m2$	22	8I	178	$P6_122$	29	2H
7	$P1n1$	8	4B	50	$Pban$ (222)	9	8D	120	$I\bar{4}c2$	22	8I	179	$P6_522$	32	2H
7	$P1a1$	8	4B	50	$Pban$ ($\bar{1}$)	9	8D	121	$I\bar{4}2m$	18	4M	180	$P6_222$	32	2H
8	$A11m$	7	2B	51	$Pmma$	9	8D	122	$I\bar{4}2d$	20	4M	181	$P6_422$	29	2H
8	$B11m$	7	2B	52	$Pnna$	9	8D	123	$P4/mmm$	18	4L	182	$P6_322$	37	4P
8	$I11m$	7	2B	53	$Pmna$	9	8D	124	$P4/mcc$	18	4L	183	$P6mm$	39	2E
8	$C1m1$	8	2C	54	$Pcca$	9	8D	125	$P4/nbm$ (422)	18	4L	184	$P6cc$	39	2E
8	$A1m1$	8	2C	55	$Pbam$	9	8D	125	$P4/nbm$ (2/m)	19	4L	185	$P6_3cm$	39	2E
8	$I1m1$	8	2C	56	$Pccn$	9	8D	126	$P4/nnc$ (422)	18	4L	186	$P6_3mc$	39	2E
9	$A11a$	7	2B	57	$Pbcm$	9	8D	126	$P4/nnc$ ($\bar{1}$)	19	4L	187	$P\bar{6}m2$	38	12B
9	$B11n$	7	2B	58	$Pnnm$	9	8D	127	$P4/mbm$	18	4L	188	$P\bar{6}c2$	38	12B
9	$I11b$	7	2B	59	$Pmmn$ (mm2)	9	8D	128	$P4/mnc$	18	4L	189	$P\bar{6}2m$	37	4O
9	$C1c1$	8	2C	59	$Pmmn$ ($\bar{1}$)	9	8D	129	$P4/nmm$ ($\bar{4}m2$)	18	4L	190	$P\bar{6}2c$	37	4O
9	$A1n1$	8	2C	60	$Pbcn$	9	8D	129	$P4/nmm$ (2/m)	19	4L	191	$P6/mmm$	37	2H
9	$I1a1$	8	2C	61	$Pbca$	9	8D	130	$P4/ncc$ ($\bar{4}$)	18	4L	192	$P6/mcc$	37	2H
10	$P112/m$	3	8D	62	$Pnma$	9	8D	130	$P4/ncc$ ($\bar{1}$)	19	4L	193	$P6_3/mcm$	37	2H
10	$P12/m1$	4	8D	63	$Cmcm$	9	4K	131	$P4_2/mmc$	18	4L	194	$P6_3/mmc$	37	2H
11	$P112_1/m$	3	8D	64	$Cmca$	9	4K	132	$P4_2/mcm$	18	4L	195	$P23$	46	8K
11	$P12_1/m1$	4	8D	65	$Cmmm$	9	4K	133	$P4_2/nbc$ ($\bar{4}$)	18	4L	196	$F23$	48	16D
12	$A112/m$	3	4L	66	$Cccm$	9	4K	133	$P4_2/nbc$ ($\bar{1}$)	19	4L	197	$I23$	46	4S
12	$B112/m$	3	4L	67	$Cmma$	9	4K	134	$P4_2/nnm$ ($\bar{4}2m$)	18	4L	198	$P2_13$	49	8L
12	$I112/m$	3	4K	68	$Ccca$ (222)	9	4K	134	$P4_2/nnm$ (2/m)	19	4L	199	$I2_13$	49	4T
12	$C12/m1$	4	4K	68	$Ccca$ ($\bar{1}$)	9	4K	135	$P4_2/mbc$	18	4L	200	$Pm3$	46	4Q
12	$A12/m1$	4	4L	69	$Fmmm$	9	2G	136	$P4_2/mnm$	18	4L	201	$Pn3$ (23)	46	4Q
12	$I12/m1$	4	4K	70	$Fddd$ (222)	10	2G	137	$P4_2/nmc$ ($\bar{4}m2$)	18	4L	201	$Pn3$ ($\bar{3}$)	47	4Q
13	$P112/a$	3	8D	70	$Fddd$ ($\bar{1}$)	11	2G	137	$P4_2/nmc$ ($\bar{1}$)	19	4L	202	$Fm3$	43	4Q
13	$P112/n$	3	8D	71	$Immm$	9	4K	138	$P4_2/ncm$ ($\bar{4}$)	18	4L	203	$Fd3$ (23)	44	4Q
13	$P112/b$	3	8D	72	$Ibam$	9	4K	138	$P4_2/ncm$ (2/m)	19	4L	203	$Fd3$ ($\bar{3}$)	45	4Q
13	$P12/c1$	4	8D	73	$Ibca$	9	4K	139	$I4/mmm$	18	2H	204	$Im3$	46	2J
13	$P12/n1$	4	8D	74	$Imma$	9	4K	140	$I4/mcm$	18	2H	205	$Pa3$	41	2G
13	$P12/a1$	4	8D	75	$P4$	23	8C	141	$I4_1/amd$ ($\bar{4}m2$)	20	2H	206	$Ia3$	49	2K
14	$P112_1/a$	3	8D	76	$P4_1$	17	4G	141	$I4_1/amd$ (2/m)	21	2H	207	$P432$	46	4R
14	$P112_1/n$	3	8D	77	$P4_2$	23	8C	142	$I4_1/acd$ ($\bar{4}$)	20	2H	208	$P4_232$	46	4R
14	$P112_1/b$	3	8D	78	$P4_3$	17	4G	142	$I4_1/acd$ ($\bar{1}$)	21	2H	209	$F432$	43	4Q
14	$P12_1/c1$	4	8D	79	$I4$	23	4H	143	$P3$	40	24A	210	$F4_132$	44	4Q
14	$P12_1/n1$	4	8D	80	$I4_1$	24	4H	144	$P3_1$	36	12A	211	$I432$	46	2I
14	$P12_1/a1$	4	8D	81	$P\bar{4}$	18	16B	145	$P3_2$	36	12A	212	$P4_332$	42	2G
15	$A112/a$	3	4L	82	$I\bar{4}$	22	16C	146	$R3$ (h)	27	4I	213	$P4_132$	42	2G
15	$B112/b$	3	4L	83	$P4/m$	18	8H	146	$R3$ (r)	28	4J	214	$I4_132$	49	2I
15	$I112/b$	3	4K	84	$P4_2/m$	18	8H	147	$P\bar{3}$	37	8J	215	$P\bar{4}3m$	46	4R
15	$C12/c1$	4	4K	85	$P4/n$ ($\bar{4}$)	18	8H	148	$R\bar{3}$ (h)	25	4N	216	$F\bar{4}3m$	48	8F
15	$A12/n1$	4	4L	85	$P4/n$ ($\bar{1}$)	19	8H	148	$R\bar{3}$ (r)	26	4Q	217	$I\bar{4}3m$	46	2I
15	$I12/a1$	4	4K	86	$P4_2/n$ ($\bar{4}$)	18	8H	149	$P312$	38	24B	218	$P\bar{4}3n$	46	4R
16	$P222$	9	16A	86	$P4_2/n$ ($\bar{1}$)	19	8H	150	$P321$	37	8J	219	$F\bar{4}3c$	48	8F
17	$P222_1$	9	16A	87	$I4/m$	18	4P	151	$P3_112$	31	12B	220	$I\bar{4}3d$	49	2I
18	$P2_12_12$	9	16A	88	$I4_1/a$ ($\bar{4}$)	20	4M	152	$P3_121$	30	4O	221	$Pm3m$	46	2G
19	$P2_12_12_1$	9	16A	88	$I4_1/a$ ($\bar{1}$)	21	4M	153	$P3_212$	34	12B	222	$Pn3n$ (432)	46	2G
20	$C222_1$	9	8E	89	$P422$	18	8H	154	$P3_221$	33	4O	222	$Pn3n$ ($\bar{3}$)	47	2G
21	$C222$	9	8E	90	$P42_12$	18	8H	155	$R32$ (h)	25	4N	223	$Pm3n$	46	2G
22	$F222$	12	8F	91	$P4_122$	16	4L	155	$R32$ (r)	26	4Q	224	$Pn3m$ ($\bar{4}3m$)	46	2G
23	$I222$	9	8E	92	$P4_12_12$	15	4L	156	$P3m1$	40	12A	224	$Pn3m$ ($\bar{3}m$)	47	2G
24	$I2_12_12_1$	9	8E	93	$P4_222$	18	8H	157	$P31m$	39	4I	225	$Fm3m$	43	2G
25	$Pmm2$	13	8B	94	$P4_22_12$	18	8H	158	$P3c1$	40	12A	226	$Fm3c$	43	2G
26	$Pmc2_1$	13	8B	95	$P4_322$	16	4L	159	$P31c$	39	4I	227	$Fd3m$ ($\bar{4}3m$)	44	2G
27	$Pcc2$	13	8B	96	$P4_32_12$	15	4L	160	$R3m$ (h)	27	2E	227	$Fd3m$ ($\bar{3}m$)	45	2G
28	$Pma2$	13	8B	97	$I422$	18	4P	160	$R3m$ (r)	28	2F	228	$Fd3c$ (23)	44	2G
29	$Pca2_1$	13	8B	98	$I4_122$	20	4M	161	$R3c$ (h)	27	2E	228	$Fd3c$ ($\bar{3}$)	45	2G
30	$Pnc2$	13	8B	99	$P4mm$	23	4G	161	$R3c$ (r)	28	2F	229	$Im3m$	46	1A
31	$Pmn2_1$	13	8B	100	$P4bm$	23	4G	162	$P\bar{3}1m$	37	4O	230	$Ia3d$	49	1A
32	$Pba2$	13	8B	101	$P4_2cm$	23	4G								

Here, the description is unique and $i = 1$, though the inherent symmetry is higher, namely the supergroup $Pm3n$ of $Ia3d$.

For most space groups, the Euclidean normalizer is a space group again and then the corresponding subgroup index i is finite. This is not the case, however, for all space groups from crystal classes 1, 2, 3, 4, 6, m, $mm2$, $3m$, $4mm$, and $6mm$: the pattern of symmetry elements for such a space group is mapped onto itself by continuous translations in at least one direction and each symmetry operation is transformed into itself by conjugation with each such translation. The Euclidean normalizer then may be imagined as a limiting case of a space group due to infinitesimal shrinking of lattice translations in one, two, or three direction(s) of degeneration, but is not a space group itself. Accord-

Table 2. *Euclidean normalizers of space groups: reference number according to Table 1 in column 1, symbol of the Euclidean normalizer in column 2, basis vectors of the Euclidean normalizer referred to the basis vectors of the space group and, eventually, site of origin in column 3*

1	$P\bar{1}$	$a/2, b/2, c/2$
2	$Z^3\bar{1}$	$\mu a, \mu b, \mu c$
3	$P112/m$	$a/2, b/2, c/2$
4	$P12/m1$	$a/2, b/2, c/2$
5	Z^1112/m	$a/2, b/2, \mu c$
6	$Z^112/m1$	$a/2, \mu b, c/2$
7	Z^2112/m	$\mu a, \mu b, c/2$
8	$Z^212/m1$	$\mu a, b/2, \mu c$
9	$Pmmm$	$a/2, b/2, c/2$
10	$Pnnn\ (222)$	$a/2, b/2, c/2$
11	$Pnnn\ (\bar{1})$	$a/2, b/2, c/2$
12	$Immm$	$a/2, b/2, c/2$
13	Z^1mmm	$a/2, b/2, \mu c$
14	$Z^1ban\ (222)$	$a/2, b/2, \mu c$
15	$P4_222$	$a/2 - b/2, a/2 + b/2, c/2$
16	$P4_222$	$a/2 - b/2, a/2 + b/2, c/2; 0,0,\frac{1}{8}$
17	Z^1422	$a/2 - b/2, a/2 + b/2, \mu c$
18	$P4/mmm$	$a/2 - b/2, a/2 + b/2, c/2$
19	$P4/mmm$	$a/2 - b/2, a/2 + b/2, c/2; \frac{1}{4},\frac{1}{4},0$
20	$P4_2/nnm\ (\bar{4}2m)$	$a/2 - b/2, a/2 + b/2, c/2$
21	$P4_2/nnm\ (\bar{4}2m)$	$a/2 - b/2, a/2 + b/2, c/2; 0,\frac{1}{4},\frac{1}{8}$
22	$I4/mmm$	$a/2 - b/2, a/2 + b/2, c/2$
23	Z^14/mmm	$a/2 - b/2, a/2 + b/2, \mu c$
24	$Z^14/nbm\ (422)$	$a/2 - b/2, a/2 + b/2, \mu c; \frac{1}{4},\frac{1}{4},0$
25	$R\bar{3}m\ (h)$	$-a, -b, c/2$
26	$R\bar{3}m\ (r)$	$-a/2 + b/2 + c/2, a/2 - b/2 + c/2, a/2 + b/2 - c/2$
27	$Z^1\bar{3}1m$	$2a/3 + b/3, -a/3 + b/3, \mu c$
28	$Z^1\bar{3}1m$	$2a/3 - b/3 - c/3, -a/3 + 2b/3 - c/3, \mu a + \mu b + \mu c$
29	$P6_222$	$a, b, c/2$
30	$P6_222$	$a + b, -a, c/2$
31	$P6_222$	$2a/3 + b/3, -a/3 + b/3, c/2$
32	$P6_422$	$a, b, c/2$
33	$P6_422$	$a + b, -a, c/2$
34	$P6_422$	$2a/3 + b/3, -a/3 + b/3, c/2$
35	Z^1622	$a, b, \mu c$
36	Z^1622	$2a/3 + b/3, -a/3 + b/3, \mu c$
37	$P6/mmm$	$a, b, c/2$
38	$P6/mmm$	$2a/3 + b/3, -a/3 + b/3, c/2$
39	Z^16/mmm	$a, b, \mu c$
40	Z^16/mmm	$2a/3 + b/3, -a/3 + b/3, \mu c$
41	$Ia3$	a, b, c
42	$I4_132$	a, b, c
43	$Pm3m$	$a/2, b/2, c/2$
44	$Pn3m\ (\bar{4}3m)$	$a/2, b/2, c/2$
45	$Pn3m\ (3m)$	$a/2, b/2, c/2$
46	$Im3m$	$a, b, c; \frac{1}{4},\frac{1}{4},\frac{1}{4}$
47	$Im3m$	$a, b, c; \frac{1}{4},\frac{1}{4},\frac{1}{4}$
48	$Im3m$	$a/2, b/2, c/2$
49	$Ia3d$	a, b, c

Table 3. *Transformations generating all equivalent point configurations from a given one (column 1: reference symbol according to Table 1)*

$1A$ (x,y,z)

$2A$ $(r,s,t) \pm (x,y,z)$
$2B$ $(r,s,0) \pm (x,y,z)$
$2C$ $(r,0,t) \pm (x,y,z)$
$2D$ $(0,0,t) + (x,y,z; x,-y,-z)$
$2E$ $(0,0,t) + (x,y,z; y,x,-z)$
$2F$ $(r,r,r) \pm (x,y,z)$
$2G$ $(0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) + (x,y,z)$
$2H$ $(0,0,0; 0,0,\frac{1}{2}) + (x,y,z)$
$2I$ $\pm(x,y,z)$
$2J$ $(x,y,z; y,x,z)$
$2K$ $(x,y,z; \frac{1}{4} + y, \frac{1}{4} + x, \frac{1}{4} + z)$

$4A$ $(r,s,0; r,s,\frac{1}{2}) \pm (x,y,z)$
$4B$ $(r,0,t; r,\frac{1}{2},t) \pm (x,y,z)$
$4C$ $(0,s,0; \frac{1}{2},s,0) \pm (x,y,z)$
$4D$ $(0,s,0; 0,s,\frac{1}{2}) \pm (x,y,z)$
$4E$ $(0,0,t; \frac{1}{2},0,t) \pm (x,y,z)$
$4F$ $(0,0,t; 0,\frac{1}{2},t) \pm (x,y,z)$
$4G$ $(0,0,t;\frac{1}{2},\frac{1}{2},t) + (x,y,z;y,x,-z)$
$4H$ $(0,0,t) + (x,y,z; -y,x,-z; y,x,-z; -x,y,z)$
$4I$ $(0,0,t) \pm (x,y,z; y,x,-z)$
$4J$ $(r,r,r) \pm (x,y,z; y,x,z)$
$4K$ $(0,0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}; 0,\frac{1}{2},\frac{1}{2}) + (x,y,z)$
$4L$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{2},\frac{1}{2},0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) + (x,y,z)$
$4M$ $(0,0,0; 0,0,\frac{1}{2}) + (x,y,z; -x,y,z)$
$4N$ $(0,0,0; 0,0,\frac{1}{2}) + (x,y,z; -y,-x,z)$
$4O$ $(0,0,0; 0,0,\frac{1}{2}) + (x,y,z; -x,-y,z)$
$4P$ $(0,0,0; 0,0,\frac{1}{2}) + (x,y,z; y,x,z)$
$4Q$ $(0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) + (x,y,z; y,x,z)$
$4R$ $(0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm (x,y,z)$
$4S$ $\pm(x,y,z; y,x,z)$
$4T$ $\pm(x,y,z; \frac{1}{4} + y, \frac{1}{4} + x, \frac{1}{4} + z)$

$8A$ $(0,s,0; \frac{1}{2},s,0; 0,s,\frac{1}{2}; \frac{1}{2},s,\frac{1}{2}) \pm (x,y,z)$
$8B$ $(0,0,t; \frac{1}{2},0,t; 0,\frac{1}{2},t; \frac{1}{2},\frac{1}{2},t) \pm (x,y,z)$
$8C$ $(0,0,t; \frac{1}{2},\frac{1}{2},t) \pm (x,y,z; y,x,z)$
$8D$ $(0,0,0;\frac{1}{2},0,0;0,\frac{1}{2},0;0,0,\frac{1}{2};0,\frac{1}{2},\frac{1}{2};\frac{1}{2},0,\frac{1}{2};\frac{1}{2},\frac{1}{2},0;\frac{1}{2},\frac{1}{2},\frac{1}{2}) + (x,y,z)$
$8E$ $(0,0,0; 0,0,\frac{1}{2}; 0,\frac{1}{2},0; 0,\frac{1}{2},\frac{1}{2}) + (x,y,z)$
$8F$ $(0,0,0; \frac{1}{4},\frac{1}{4},\frac{1}{4}; \frac{1}{2},\frac{1}{2},\frac{1}{2}; \frac{3}{4},\frac{3}{4},\frac{3}{4}) \pm (x,y,z)$
$8G$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{2},\frac{1}{2},0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) + (x,y,z; -x,y,z)$
$8H$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{2},\frac{1}{2},0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) + (x,y,z; y,x,z)$
$8I$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{2},0,\frac{1}{2}; 0,\frac{1}{2},\frac{1}{2}) + (x,y,z)$
$8J$ $(0,0,0; 0,0,\frac{1}{2}) + (x,y,z; -y,-x,z; y,x,z; -x,-y,z)$
$8K$ $(0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm (x,y,z; y,x,z)$
$8L$ $(0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm (x,y,z; \frac{1}{4} + y, \frac{1}{4} + x, \frac{1}{4} + z)$

$12A$ $(0,0,t; \frac{1}{3},\frac{2}{3},t; \frac{2}{3},\frac{1}{3},t) + (x,y,z; y,x,-z; -x,-y,z; -y,-x,-z)$
$12B$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{3},\frac{2}{3},0; \frac{1}{3},\frac{2}{3},\frac{1}{2}; \frac{2}{3},\frac{1}{3},0; \frac{2}{3},\frac{1}{3},\frac{1}{2}) + (x,y,z; -x,-y,z)$

$16A$ $(0,0,0; \frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}; 0,\frac{1}{2},\frac{1}{2}; \frac{1}{2},0,\frac{1}{2}; \frac{1}{2},\frac{1}{2},0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm (x,y,z)$
$16B$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{2},\frac{1}{2},0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm (x,y,z; y,x,z)$
$16C$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{2},0,\frac{1}{2}; 0,\frac{1}{2},\frac{1}{2}) \pm (x,y,z; y,x,z)$
$16D$ $(0,0,0; \frac{1}{4},\frac{1}{4},\frac{1}{4}; \frac{1}{2},\frac{1}{2},\frac{1}{2}; \frac{3}{4},\frac{3}{4},\frac{3}{4}) \pm (x,y,z; y,x,z)$

$24A$ $(0,0,t; \frac{1}{3},\frac{2}{3},t; \frac{2}{3},\frac{1}{3},t) \pm (x,y,z; y,x,-z; -x,-y,z; -y,-x,-z)$
$24B$ $(0,0,0; 0,0,\frac{1}{2}; \frac{1}{3},\frac{2}{3},0; \frac{1}{3},\frac{2}{3},\frac{1}{2}; \frac{2}{3},\frac{1}{3},0; \frac{2}{3},\frac{1}{3},\frac{1}{2}) \pm (x,y,z; -x,-y,z)$

ingly, here the index of the space group in its Euclidean normalizer is infinite, *i.e.* to any point configuration there exists an infinite number of equivalent ones. These may, however, be distributed among a finite number *j* of sets in such a way that two point configurations from the same set are shifted against each other parallel to a direction of degeneration, *i.e.* all corresponding isometries only differ by a translation component in such a direction.

4. Tables of Euclidean normalizers and of isometries generating equivalent point configurations

The information necessary for the direct generation of all equivalent point configurations or all possible descriptions of a crystal structure from a given one has been condensed into three tables.

Table 1 gives for each space group two references leading to its Euclidean normalizer (Cheshire group) in Table 2 and to a set of isometries generating complete sets of equivalent point configurations in Table 3. Each space group is characterized by its number and by its Hermann–Mauguin symbol (columns 1 and 2). If a space group is explicitly described in different settings within *International Tables for Crystallography* (1983, abbreviated IT 1983 in the following) all these settings are treated. They are distinguished either by different Hermann–Mauguin symbols (monoclinic space groups); or by (*r*) or (*h*) for rhombohedral or hexagonal coordinate description, respectively (rhombohedral space groups); or by the site symmetry of the origin.

The reference to Table 2 is given by a number in column 3. Table 3 is referred to by a symbol in column 4, each such symbol containing a number and a capital letter: the number is the index *i* of the space group as subgroup of its Euclidean normalizer (or *j* in case of degeneration), the letter gives an arbitrary labelling for the different sets of isometries with the same value of *i* (or *j*).

Table 2 is similar to Table 2 in Hirshfeld's paper and contains all Euclidean normalizers in settings corresponding to the space-group descriptions of Table 1. The number of entries is larger than in Hirshfeld's table because of the additional settings of space groups and because an eventual shift of origin between a space group and its Euclidean normalizer is indicated. For each entry, the reference number is followed by the symbol of the Euclidean normalizer. In case of degeneration, Z^n is used instead of the Bravais letter, *n* giving the number of independent directions with degeneration (*cf.* Hirshfeld, 1968). If the Euclidean normalizer is a space group described in different settings in IT 1983, these settings are identified as in Table 1. The last column contains the basis vectors of the Euclidean normalizer expressed in terms of the basis vectors of the corresponding space group. In a

few cases there does not exist a setting in IT 1983 such that the origins of space group and Euclidean normalizer coincide. Then the location of the origin of the Euclidean normalizer is added, referred to the coordinate system of the space group. Degenerate directions are indicated by the factor μ for the corresponding basis vectors.

Table 3 gives sets of isometries that generate all equivalent point configurations from a given one. The symbols from column 4 of Table 1 serve as an entry to this table. Following each such symbol, a set of representatives for all cosets of the space group in its Euclidean normalizer is specified. As each coset is infinite, these representative isometries can be chosen in infinitely many different ways. Even if a reduction modulo the translations is used, there remain several ambiguities. The selection made for Table 3, therefore, has been arbitrary to some extent, but the following rules have been taken into account: (1) Each coset containing translations is represented by a translation. (2) If possible, isometries with the origin as fixed point are chosen. (3) Translations selected by the first rule are also used in combination with the other isometries. (4) An attempt has been made to minimize the number of entries.

Each set of isometries is described in a condensed way by means of two subsets in separate parentheses: the subset of translations and a minimal subset of other isometries. The complete set of isometries is produced by combining each triplet from the first parentheses with each triplet from the second ones. In case of degeneration the continuous translations are indicated by letters *r,s,t* which may take any values.

The material in Tables 1–3 is limited with respect to space groups with specialized metric. As discussed above, the Euclidean normalizer of such a group may be higher than for the ordinary space groups of the same type. No additional information on the Euclidean normalizer is given here for such an exceptional case.

For the comparison of two crystal structures, it may be necessary to apply a basis transformation to one of the space groups in addition to the isometries of the Euclidean normalizer. Normally this situation is easily recognized, because the two descriptions refer to obviously different settings of the same space group. Care has to be taken, however, in the case of a space group for which the Euclidean normalizer differs from the affine normalizer. If then the metric is near to one of the specialized cases, it may be necessary to transform the basis vectors in order to arrive at comparable descriptions. Another exceptional situation occurs in connection with enantiomorphic pairs of space groups. Here, without physical reasons, the second crystal structure may be described by means of the enantiomorphic counterpart of the space group of the first structure. The required transformation then may be performed by changing the signs of all coordinates. In

all these cases, Tables 1–3 can be used as shown in the following examples after the appropriate basis transformation has been carried out.

5. Examples for the use of the tables

Geometrical studies on point configurations

As mentioned above, studies on geometrical properties of point configurations frequently have been confined to an asymmetric unit of the Euclidean normalizer, but in most cases it is necessary to extend the results to an asymmetric unit of the space group. This extension can be done by means of Tables 1–3, even if both asymmetric units are complicated, as in the following examples. The procedure indeed is not based on the knowledge of any asymmetric units at all.

According to Fischer (1974), a point configuration with reference point $0,\frac{1}{4},\frac{7}{8}$ in the general position of $P2_13$ fulfils the condition for a sphere packing of type $8/3/c1$. The complete set of point configurations equivalent to this one, and therefore with the same sphere-packing property, may be calculated as follows. The appropriate item in Table 1 reads

$$198 \quad P2_13 \quad 49 \quad 8L.$$

Here, 49 is the reference number to the table of Euclidean normalizers (Table 2) and leads to

$$49 \quad Ia3d \quad a,b,c.$$

Therefore, $Ia3d$ with the same basis vectors and the same origin as $P2_13$ is the Euclidean normalizer of $P2_13$. The subgroup index of $P2_13$ with respect to $Ia3d$ is 8, as can be learned from the symbol $8L$. This symbol in addition defines the entry to Table 3 where the isometries representing the eight cosets of $P2_13$ in its Euclidean normalizer $Ia3d$ are found in the abbreviated form

$$8L \quad (0,0,0;\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) \pm (x,y,z;\tfrac{1}{4}+y,\tfrac{1}{4}+x,\tfrac{1}{4}+z).$$

Combining the contents of the two pairs of parentheses results in the eight isometries listed explicitly in the entry column of Table 4. Then the reference point $0,\frac{1}{4},\frac{7}{8}$ of the original point configuration has to be transformed by each of these isometries (next column). Normally, the resulting points represent different but equivalent configurations and may directly be used as reference points for these. It has to be checked, however, whether all cosets really give rise to different point configurations. For this, it is sufficient to show that none of the transformed reference points is contained in the original configuration. As can be seen from Table 4, this condition is violated in the example: only two different point configurations are generated, each by four out of the eight representative isometries. As has been shown above, the inherent symmetry of these point configurations must be higher than $P2_13$, and indeed it is $I\bar{4}3d$ 12 (a,b) with site symmetry $\bar{4}$.

Different descriptions of the same crystal structure

Na_3AsS_3 (Sommer & Hoppe, 1977) may be used as an example for the evaluation of all possible descriptions of a given crystal structure. As the space-group symmetry is $P2_13$ again, the isometries necessary to generate all these descriptions are the same as in the previous example. The resulting eight descriptions are given in Table 5. All of them are different, as can easily be seen, for example, by choosing appropriate reference points for the sites of the sulphur atoms (last column). If these coordinates are idealized to multiples of $\frac{1}{8}$, they correspond to those of the sphere packing of the previous example. The deviations of the sulphur atoms from the idealized positions, however, as well as the positions of the metal atoms uniquely characterize each single description.

Comparison of crystal structures

The comparison of different crystal structures requires analogous descriptions for all these structures.

Table 4. *Generation of all point configurations equivalent to that with reference point* $0,\frac{1}{4},\frac{7}{8}$ *in space group* $P2_13$
(Euclidean normalizer $Ia3d$)

Cyclic permutations of all coordinate triplets have to be added.

Isometries from $Ia3d$	x,y,z	$\tfrac{1}{2}-x,-y,\tfrac{1}{2}+z$	$-x,\tfrac{1}{2}+y,\tfrac{1}{2}-z$	$\tfrac{1}{2}+x,\tfrac{1}{2}-y,-z$
		Isometries from $P2_13$		
x,y,z	$0,\tfrac{1}{4},\tfrac{7}{8}$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{3}{8}$	$0,\tfrac{3}{4},\tfrac{5}{8}$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{1}{8}$
$\tfrac{1}{4}+y,\tfrac{1}{4}+x,\tfrac{1}{4}+z$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{7}{8}$	$0,\tfrac{3}{4},\tfrac{5}{8}$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{3}{8}$	$0,\tfrac{1}{4},\tfrac{1}{8}$
$\tfrac{1}{2}+x,\tfrac{1}{2}+y,\tfrac{1}{2}+z$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{3}{8}$	$0,\tfrac{1}{4},\tfrac{7}{8}$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{1}{8}$	$0,\tfrac{3}{4},\tfrac{5}{8}$
$\tfrac{3}{4}+y,\tfrac{3}{4}+x,\tfrac{3}{4}+z$	$0,\tfrac{3}{4},\tfrac{5}{8}$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{1}{8}$	$0,\tfrac{1}{4},\tfrac{7}{8}$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{3}{8}$
$-x,-y,-z$	$0,\tfrac{3}{4},\tfrac{1}{8}$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{5}{8}$	$0,\tfrac{1}{4},\tfrac{3}{8}$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{7}{8}$
$\tfrac{1}{4}-y,\tfrac{3}{4}-x,\tfrac{3}{4}-z$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{7}{8}$	$0,\tfrac{1}{4},\tfrac{1}{8}$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{5}{8}$	$0,\tfrac{3}{4},\tfrac{3}{8}$
$\tfrac{1}{2}-x,\tfrac{1}{2}-y,\tfrac{1}{2}-z$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{5}{8}$	$0,\tfrac{3}{4},\tfrac{1}{8}$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{7}{8}$	$0,\tfrac{1}{4},\tfrac{3}{8}$
$\tfrac{3}{4}-y,\tfrac{1}{4}-x,\tfrac{1}{4}-z$	$0,\tfrac{1}{4},\tfrac{3}{8}$	$\tfrac{1}{2},\tfrac{3}{4},\tfrac{7}{8}$	$0,\tfrac{3}{4},\tfrac{1}{8}$	$\tfrac{1}{2},\tfrac{1}{4},\tfrac{5}{8}$

Frequently, this condition is not fulfilled by the original data. A simple procedure that may be used in such a case is illustrated by the example of sodalite $Na_4Cl(AlSiO_4)_3$ (Löns & Schulz, 1967), its aluminate analog $Ca_4O(AlO_2)_6$ (Ponomarev, Kheiker & Belov, 1971), and $Zn_4O(BO_2)_6$ (Smith-Verdier & Garcia-Blanco, 1980).

Arbitrarily, sodalite has been picked out and all of its possible descriptions have been calculated (Table 6). The space group of sodalite is $P\bar{4}3n$ with the Euclidean normalizer $Im3m$ which generates four different descriptions. These can directly be compared with the original descriptions of the other two structures, though these show the higher symmetry $I\bar{4}3m$. Due to this, the Wyckoff positions $P\bar{4}3n$ $6(c)$ and $6(d)$ occupied by Si and Al in an ordered way in sodalite combine to one Wyckoff position of $I\bar{4}3m$ and the oxygen position in $I\bar{4}3m$ is restricted to $x = y$. As can be seen from Table 6, the structures of sodalite and of $Zn_4O(BO_2)_6$ are closely related to each other. The structure of $Ca_4O(AlO_2)_6$, however, differs from these, because the orientation of the Ca tetrahedron around the origin is opposite to that of the Na or Zn tetrahedra if referred to the same description of the anion framework (cf. Koch & Hellner, 1981).

In such a comparison care has to be taken that appropriate reference points are used for all descriptions. The selection of such reference points for all kinds of atoms normally poses no problem if done by hand. In an automatic procedure either additional rules for the choice of all reference points have to be established (Parthé & Gelato, 1983) or all atoms inside a unit cell have to be included in the comparison.

6. The role of Euclidean normalizers in crystal-structure determination

A crystal-structure determination may result in any of the descriptions compatible with the chosen space-group setting. It depends on arbitrary choices during the course of the structure determination which of these equivalent descriptions is obtained. The nature of these choices is subject to the method of structure determination used.

Each description of a crystal structure corresponds to a list of structure factors and each change of the description causes alterations in this list. In this respect two kinds of changes of the description may be differentiated: those which only influence phases of

Table 5. *The eight different descriptions of the* Na_3AsS_3 *structure in space group* $P2_13$

	As x,x,x	Na(2) x,x,x	Na(1) x,x,x	Na(3) x,x,x	S x,y,z Generated point	x,y,z Preferred reference point
x,y,z	0·0281	0·3181	0·5785	0·8104	0·2220, 0·6040, 0·4981	−0·0019, 0·2780, 0·3960
$\frac{1}{4}+y,\frac{1}{4}+x,\frac{1}{4}+z$	0·2781	0·5681	0·8285	0·0604	0·8540, 0·4720, 0·7481	0·0280, 0·2519, 0·3540
$\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}+z$	0·5281	0·8181	0·0785	0·3104	0·7220, 0·1040, 0·9981	0·0019, 0·2220, 0·3960
$\frac{3}{4}+y,\frac{3}{4}+x,\frac{3}{4}+z$	0·7781	0·0681	0·3285	0·5604	0·3540, 0·9720, 0·2481	−0·0280, 0·2481, 0·3540
$-x,-y,-z$	0·9719	0·6819	0·4215	0·1896	0·7780, 0·3960, 0·5019	−0·0019, 0·2220, 0·8960
$\frac{3}{4}-y,\frac{3}{4}-x,\frac{3}{4}-z$	0·7219	0·4319	0·1715	0·9396	0·1460, 0·5280, 0·2519	0·0280, 0·2481, 0·8540
$\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$	0·4719	0·1819	0·9215	0·6896	0·2780, 0·8960, 0·0019	0·0019, 0·2780, 0·8960
$\frac{1}{4}-y,\frac{1}{4}-x,\frac{1}{4}-z$	0·2219	0·9319	0·6715	0·4396	0·6460, 0·0280, 0·7519	−0·0280, 0·2519, 0·8540

Table 6. *Comparison of the structures of sodalite (four descriptions),* $Zn_4O(BO_2)_6$ *and* $Ca_4O(AlO_2)_6$

$P\bar{4}3n$	$2(a)$ $0,0,0$	$6(c)$ $\frac{1}{4},\frac{1}{2},0$	$6(d)$ $\frac{1}{4},0,\frac{1}{2}$	$8(e)$ x,x,x	$24(i)$ x,y,z	Transformation
Sodalite	Cl	Al	Si	Na 0·1777	O 0·1487, 0·1401, 0·4385	x,y,z
Sodalite	Cl	Si	Al	Na 0·1777	O 0·1401, 0·1487, 0·4385	$\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}+z$
Sodalite	Cl	Al	Si	Na −0·1777	O 0·1487, 0·1401, −0·4385	$-x,-y,-z$
Sodalite	Cl	Si	Al	Na −0·1777	O 0·1401, 0·1487, −0·4385	$\frac{1}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$
$I\bar{4}3m$	$2(a)$ $0,0,0$	$12(d)$ $\frac{1}{4},\frac{1}{2},0$	$8(c)$ x,x,x	$24(g)$ x,x,z		
$Zn_4O(BO_2)_6$	O	B	Zn 0·1533	O 0·1398, 0·4147		x,y,z
$Ca_4O(AlO_2)_6$	O	Al	Ca −0·160	O 0·135, 0·413		x,y,z

structure factors but leave the structure amplitudes unchanged, and those which in addition lead to different structure amplitudes for the same triplet of indices. In the latter case, each alteration of the description is associated with a permutation of the set of indices. Changes of the first type can always be represented by a translation or an inversion; changes of the second type only exist in a space group, the Laue class of which differs from that of its Euclidean normalizer (*e.g.* $P2_13$ with normalizer $Ia3d$). The Laue class of G then is a subgroup of index $n \neq 1$ of the Laue class of $N_E(G)$.

Independent of the method used, a structure determination normally starts from a set of structure amplitudes with attached indices. In the case of different Laue classes, some of the possible descriptions have already been singled out by indexing the diffraction pattern. The selection among the remaining $1/n$ of all equivalent descriptions is done by arbitrary restrictions on certain phases in direct methods, or by fixing the position of the first atom(s) in Patterson and trial-and-error procedures (*cf.* Hirshfeld, 1968).

In Table 3, representative isometries that may cause a change of the indexing are always listed at the end. In the example of $P2_13$ the subgroup index of the Laue classes is 2, and the four isometries $(0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}) \pm (\frac{1}{4} + y, \frac{1}{4} + x, \frac{1}{4} + z)$ give rise to a change of hkl into khl. Therefore, only the first, third, fifth and seventh descriptions of Na_3AsS_3 in Table 5 are compatible with the indexing of the original data.

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