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On symmetry classes of crystal structures

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An open-ended classification scheme for crystal structures based on Wyckoff sets and affine normalizer groups is proposed. It is free of metrical and geometrical considerations. All structures of one structure type belong to the same symmetry class. An application is given for the Inorganic Crystal Structure Database (version 2, 2007).

1. Introduction

A recent report on the use of structure types in the description and handling of inorganic crystal structures (Allmann & Hinek, 2007) was the point of origin of the following considerations. Since the methods applied by Allmann & Hinek utilize metrical and geometrical properties that include the selection of the setting and the origin of a structure, the question arose as to whether it is possible to develop a notation system for a structural classification independent of metrical and geometrical properties. Moreover, the system should be open ended, *i.e.* suitable for new crystal structures and crystal structures of arbitrary size. The proposal given below is based on the application of Wyckoff positions and Wyckoff sets under the influence of the affine normalizer of a space group.

2. Wyckoff positions, Wyckoff sets and affine normalizers

In crystal structure descriptions Wyckoff-position labels are used. As was shown by Boyle & Lawrenson (1973), the atoms of a structure may be described by different sets of Wyckoff labels. A careful inspection shows that the Wyckoff positions related to these labels are equivalent under the operations of the affine normalizer of the space group. A set of Wyckoff positions which are equivalent under those operations forms a Wyckoff set (Wondratschek, 1983; Fischer & Koch, 1983–2002). Wyckoff sets were originally introduced by Fischer & Koch (1974) and tabulated by Koch & Fischer (1975), using the German term *Konfigurationslage*; for a more recent survey, see Koch & Fischer (2006).

As a consequence, Wyckoff sets are independent of metrical and geometrical properties. Thus, Wyckoff sets can be used as the basic principle for crystal structure classification as considered above.

Tables 1 to 5 contain notations for the normalizers and Wyckoff positions and their distribution among the related Wyckoff sets for all 230 space-group types; Table 1 for the anorthic and monoclinic crystal families, Tables 2 to 5 for the orthorhombic, tetragonal, hexagonal and cubic crystal families. In the headings of each table a codification for the normalizers is given as presented by Burzlaff & Zimmermann (1980). In this notation the normalizer and space group make use of the same basis in their presentation to show their subgroup relation as simply as possible. Thus, the mutual relation is invariant under base transformation. Some improvements of the notation were introduced by Burzlaff & Zimmermann (1993). The changes concern the following:

(i) Instead of zero the letters *r*, *s*, *t* are adopted to indicate arbitrary translations.

(ii) By origin shifts, the symbols c_c, b_v and b_b used in the 1980 paper can be replaced by *d*, the indicator symbol '4' is replaced by '4_1'. The symbols for the normalizers $P_{222}4_1/mmc_c$, $C_{110}4/amb_v$, $P_{220}4/db_bm$ are thus changed to $P_{222}4_1/amd$, $C_{11t}4_1/amd$, $P_{22t}4_1/ddm$.

Since these symbols are modified Hermann–Mauguin symbols, the generating operations of the normalizers can be derived in the same way as described for the Hermann–Mauguin symbols of space groups (Burzlaff & Zimmermann, 1983). Necessary origin shifts can easily be derived using the origins of the symbols. It is noteworthy that the first part of the symbol does not only indicate a transformation but should be read as centrings of the unit cell.

The affine normalizers of anorthic and monoclinic space groups cannot be characterized by modified Hermann–Mauguin symbols (see Koch *et al.*, 1983–2002); however, it is sufficient to apply only the translation groups of the normalizers with the exception of space group 15: *C*2/*c*. For this space group the normalizer operation (M_{12}, v_9): [(1 0 1 / 0 1 0 / 0 0 1),($\frac{1}{4}$ $\frac{1}{4}$ 0)] has to be applied in addition to show that the Wyckoff positions *a*, *b*, *c*, *d* belong to the same Wyckoff set (Koch *et al.*, 1983–2002).

The Wyckoff sets are completely described by Fischer & Koch (1983–2002); however, no codification of the Wyckoff sets is given.

In Tables 1 to 5 the line for each space group contains first the space-group number of *International Tables* followed by

Table 1
Translation groups of normalizers and Wyckoff sets of anorthic and monoclinic space groups.

Code: A: = P_{222}; B: = P_{2s2}; C: = P_{r2t}; D: = P_{rst}.

Space group		Code	Wyckoff sets				
1	$P1$	D	C_1 I *a*				
2	$P\bar{1}$	A	C_i I *a–h*	C_1 I *i*			
3	$P2$	B	C_2 I *a–d*	C_1 I *e*			
4	$P2_1$	B	C_1 I *a*				
5	$C2$	B	C_2 I *a–b*	C_1 I *c*			
6	Pm	C	C_s I *a–b*	C_1 I *c*			
7	Pc	C	C_1 I *a*				
8	Cm	C	C_s I *a*	C_1 I *b*			
9	Cc	C	C_1 I *a*				
10	$P2/m$	A	C_{2h} I *a–h*	C_2 I *i–l*	C_s I *m–n*	C_1 I *o*	
11	$P2_1/m$	A	C_i I *a–d*	C_s I *e*	C_1 I *f*		
12	$C2/m$	A	C_{2h} I *a–d*	C_i I *e–f*	C_2 I *g–h*	C_s I *i*	C_1 I *j*
13	$P2/c$	A	C_i I *a–d*	C_2 I *e–f*	C_1 I *g*		
14	$P2_1/c$	A	C_i I *a–d*	C_1 I *e*			
15	$C2/c$	A	C_i I *a–d*	C_2 I *e*	C_1 I *f*		

an international space-group symbol (for elucidation only). The next column contains the code for the normalizer as presented in the table caption; in the following columns information for the Wyckoff sets of the space group is given. The label of a Wyckoff set consists of a symbol for the site symmetry of the related Wyckoff position in Schoenflies notation (emphasizing the independence of metrics and settings) followed by Roman numerals. Different Roman numerals indicate that these site symmetries are not conjugated under the normalizer operations, thus leading to different Wyckoff sets. This is followed by a list of labels for Wyckoff positions belonging to the same set.

3. Symmetry classes of crystal structures; Pearson symbols and Wyckoff sequences

Pearson symbols (PS) are well established in crystal structure descriptions as the number of atoms in the unit cell indicates the size of the structure. Pearson symbols consist of the combination of a lower-case letter for the crystal family and an upper case letter for the centrings followed by the number N of atoms in the unit cell: aP–, mP–, mS–, oP–, oS–, oF–, oI–, tP–, tI–, hP–, hR–, cP–, cF–, cI–, replace '–' by N.

The content of the unit cell can be evaluated in two ways:

(i) The number of atoms in the sum formula is multiplied by Z (number of formula units per cell) resulting in $N1$. This procedure is adopted in the Inorganic Crystal Structure Database (ICSD).[1]

(ii) The multiplicities of all Wyckoff positions used in the structure description that differ from each other in their coordinates are added up and lead to $N2$. Note that this number represents possible sites rather than atoms themselves. This procedure is adopted in this report [see example (5) below].

[1] Note the inconsistency in the database notation for rhombohedral structures: they use a hexagonal cell and do not count the *R*-centring.

Another application of Wyckoff positions for crystal structure descriptions was introduced by Parthé (1990). He classified crystal structures by the space-group number and the sequence of used Wyckoff positions connected with a trailing number which indicates how often a Wyckoff position is used [Wyckoff sequences (WS)]; however, standardized structure data must be used.

To avoid structure data standardization with all its ambiguities, the classification terms are changed:

(i) Following Parthé (1990), the space-group number is used as a reference. As the space-group number represents the class of all equivalent space groups, the group of affine mappings has to be considered.

(ii) Instead of the multiplicity of Wyckoff positions in the conventional unit cell, the number of sites refers to primitive cells to be independent from the choice of the basis.

(iii) These reduced multiplicities for all occupied Wyckoff positions belonging to one Wyckoff set are added up resulting in an occupation number of the Wyckoff set.

(iv) The sequence of these numbers, separated by slashes, results in a pattern that characterizes the symmetry properties and the size of a crystal structure without use of metrical and geometrical properties. It represents a fingerprint for the structure with respect to size and symmetry. This sequence of numbers defines a symmetry class of crystal structures and is suitable for an open-ended classification system.

Examples are taken from the ICSD.

(1) The structures of $AuCu_3$ [Collection (Coll.) code 40351] and ReO_3 (Coll. code 77679), space group 221: $Pm\bar{3}m$, occupy the following Wyckoff positions:

Au 1 *a* 000
Cu 3 *c* $0\frac{1}{2}\frac{1}{2}$
PS = cP4, WS = *ca*,

Re 1 *a* 000
O 3 *d* $\frac{1}{2}00$
PS = cP4, WS = *da*.

According to Table 5, the fingerprint for both structures is 221: 4 1/3.

According to Lima-de-Faria *et al.* (1990), the structures are not isotypic but belong to the same symmetry class because the *I*-centring of the normalizer maps the position *c* on position *d*.

(2) The structures of CaB_6 (Coll. codes 26753 and 26893), space group 221: $Pm\bar{3}m$, occupy the following Wyckoff positions:

Ca 1 *b* $\frac{1}{2}\frac{1}{2}\frac{1}{2}$
B 6 *e* 0 0 .293
PS = cP7, WS = *be*,

Ca 1 *a* 000
B 6 *f* $\frac{1}{2}\frac{1}{2}$ .2
PS = cP7, WS = *af*.

Following Table 5, the fingerprint for both structures is 221: 7 1/0/6.

Table 2
Normalizers and Wyckoff sets of orthorhombic space groups.

Code: A: $P_{222}m3m$; B: $P_{222}m3d$; C: $P_{222}d3m$; D: $I_{222}m3m$; E: $P_{222}m3$; F: $P_{22t}mmm$; G: $P_{22t}4/mmm$; H: $P_{22t}4_1/ddm$; I: $P_{222}4/mmm$; J: $P_{222}4_1/amd$; K: $P_{222}mmm$.

Space group		Code	Wyckoff sets						
16	$P222$	A	D_2 I *a–h*	C_2 I *i–t*	C_1 I *u*				
17	$P222_1$	J	C_2 I *a–d*	C_1 I *e*					
18	$P2_12_12$	I	C_2 I *a–b*	C_1 I *c*					
19	$P2_12_12_1$	B	C_1 I *a*						
20	$C222_1$	J	C_2 I *a–b*	C_1 I *e*					
21	$C222$	I	D_2 I *a–d*	C_2 I *e–h* II *i–j* III *k*	C_1 I *l*				
22	$F222$	D	D_2 I *a–d*	C_2 I *e–h*	C_1 I *i*				
23	$I222$	A	D_2 I *a–d*	C_2 I *e–j*	C_1 I *k*				
24	$I2_12_12_1$	B	C_2 I *a–c*	C_1 I *d*					
25	$Pmm2$	G	C_{2v} I *a–d*	C_s I *e–h*	C_1 I *i*				
26	$Pmc2_1$	F	C_s I *a–b*	C_1 I *c*					
27	$Pcc2$	G	C_2 I *a–d*	C_1 I *e*					
28	$Pma2$	F	C_2 I *a–b*	C_s I *c*	C_1 I *d*				
29	$Pca2_1$	F	C_1 I *a*						
30	$Pnc2$	F	C_2 I *a–b*	C_1 I *c*					
31	$Pmn2_1$	F	C_s I *a*	C_1 I *b*					
32	$Pba2$	G	C_2 I *a–b*	C_1 I *c*					
33	$Pna2_1$	F	C_1 I *a*						
34	$Pnn2$	G	C_2 I *a–b*	C_1 I *c*					
35	$Cmm2$	G	C_{2v} I *a–b*	C_2 I *c*	C_s I *d–e*	C_1 I *f*			
36	$Cmc2_1$	F	C_s I *a*	C_1 I *b*					
37	$Ccc2$	G	C_2 I *a–b* II *c*	C_1 I *d*					
38	$Amm2$	F	C_{2v} I *a–b*	C_s I *c* II *d–e*	C_1 I *f*				
39	$Abm2$	F	C_2 I *a–b*	C_s I *c*	C_1 I *d*				
40	$Ama2$	F	C_2 I *a*	C_s I *b*	C_1 I *c*				
41	$Aba2$	F	C_2 I *a*	C_1 I *b*					
42	$Fmm2$	G	C_{2v} I *a*	C_2 I *b*	C_s I *c–d*	C_1 I *e*			
43	$Fdd2$	H	C_2 I *a*	C_1 I *b*					
44	$Imm2$	G	C_{2v} I *a–b*	C_s I *c–d*	C_1 I *e*				
45	$Iba2$	G	C_2 I *a–b*	C_1 I *c*					
46	$Ima2$	F	C_2 I *a*	C_s I *b*	C_1 I *c*				
47	$Pmmm$	A	D_{2h} I *a–h*	C_{2v} I *i–t*	C_s I *u–z*	C_1 I *a*			
48	$Pnnn$	A	D_2 I *a–d*	C_i I *e–f*	C_2 I *g–l*	C_1 I *m*			
49	$Pccm$	I	C_{2h} I *a–d*	D_2 I *e–h*	C_2 I *i–l* II *m–p*	C_s I *q*	C_1 I *r*		
50	$Pban$	I	D_2 I *a–d*	C_i I *e–f*	C_2 I *g–j* II *k–l*	C_1 I *m*			
51	$Pmma$	K	C_{2h} I *a–d*	C_{2v} I *e–f*	C_2 I *g–h*	C_s I *i–j* II *k*	C_1 I *l*		
52	$Pnna$	K	C_i I *a–b*	C_2 I *c* II *d*	C_1 I *e*				
53	$Pmna$	K	C_{2h} I *a–d*	C_2 I *e–f* II *g*	C_s I *h*	C_1 I *i*			
54	$Pcca$	K	C_i I *a–b*	C_2 I *c* II *d–e*	C_1 I *f*				
55	$Pbam$	I	C_{2h} I *a–d*	C_2 I *e–f*	C_s I *g–h*	C_1 I *i*			
56	$Pccn$	I	C_i I *a–b*	C_2 I *c–d*	C_1 I *e*				
57	$Pbcm$	K	C_i I *a–b*	C_2 I *c*	C_s I *d*	C_1 I *e*			
58	$Pnnm$	I	C_{2h} I *a–d*	C_2 I *e–f*	C_s I *g*	C_1 I *h*			
59	$Pmmn$	I	C_{2v} I *a–b*	C_i I *c–d*	C_s I *e–f*	C_1 I *g*			
60	$Pbcn$	K	C_i I *a–b*	C_2 I *c*	C_1 I *d*				
61	$Pbca$	E	C_i I *a–b*	C_1 I *c*					
62	$Pnma$	K	C_i I *a–b*	C_s I *c*	C_1 I *d*				
63	$Cmcm$	K	C_{2h} I *a–b*	C_{2v} I *c*	C_i I *d*	C_2 I *e*	C_s I *f* II *g*	C_1 I *h*	
64	$Cmce$	K	C_{2h} I *a–b*	C_i I *c*	C_2 I *d* II *e*	C_s I *f*	C_1 I *g*		
65	$Cmmm$	I	D_{2h} I *a–d*	C_{2h} I *e–f*	C_{2v} I *g–j* II *k–l*	C_2 I *m*	C_s I *n–o* II *p–q*	C_1 I *r*	
66	$Cccm$	I	D_2 I *a–b*	C_{2h} I *c–d* II *e–f*	C_2 I *g–h* II *i–j* III *k*	C_s I *l*	C_1 I *m*		
67	$Cmme$	I	D_2 I *a–b*	C_{2h} I *c–f*	C_{2v} I *g*	C_2 I *h–k* II *l*	C_s I *m–n*	C_1 I *o*	
68	$Ccce$	I	D_2 I *a–b*	C_i I *c–d*	C_2 I *e–f* II *g* III *h*	C_1 I *i*			
69	$Fmmm$	A	D_{2h} I *a–b*	C_{2h} I *c–e*	D_2 I *f*	C_{2v} I *g–i*	C_2 I *j–l*	C_s I *m–o*	C_1 I *p*
70	$Fddd$	C	D_2 I *a–b*	C_i I *c–d*	C_2 I *e–g*	C_1 I *h*			
71	$Immm$	A	D_{2h} I *a–d*	C_{2v} I *e–j*	C_i I *k*	C_s I *l–n*	C_1 I *o*		
72	$Ibam$	I	D_2 I *a–b*	C_{2h} I *c–d*	C_i I *e*	C_2 I *f–g* II *h–i*	C_s I *j*	C_1 I *k*	
73	$Ibca$	B	C_i I *a–b*	C_2 I *c–e*	C_1 I *f*				
74	$Imma$	J	C_{2h} I *a–d*	C_{2v} I *e*	C_2 I *f–g*	C_s I *h–i*	C_1 I *j*		

Table 3
Normalizers and Wyckoff sets of tetragonal space groups.

Code: A: $C_{11t}4/mmm$; B: $C_{11t}422$; C: $C_{11t}4_1/amd$; D: $C_{112}4/mmm$; E: $C_{112}4_122$; F: $F_{112}4/mmm$; G: $C_{112}4_1/amd$.

Space group		Code	Wyckoff sets							
75	$P4$	A	C_4 I *a–b*	C_2 I *c*	C_1 I *d*					
76	$P4_1$	B	C_1 I *a*							
77	$P4_2$	A	C_2 I *a–b* II *c*	C_1 I *d*						
78	$P4_3$	B	C_1 I *a*							
79	$I4$	A	C_4 I *a*	C_2 I *b*	C_1 I *c*					
80	$I4_1$	C	C_2 I *a*	C_1 I *b*						
81	$P\bar{4}$	D	S_4 I *a–d*	C_2 I *e–f* II *g*	C_1 I *h*					
82	$I\bar{4}$	F	S_4 I *a–d*	C_2 I *e–f*	C_1 I *g*					
83	$P4/m$	D	C_{4h} I *a–d*	C_{2h} I *e–f*	C_4 I *g–h*	C_2 I *i*	C_s I *j–k*	C_1 I *l*		
84	$P4_2/m$	D	C_{2h} I *a–b* II *c–d*	S_4 I *e–f*	C_2 I *g–h* II *i*	C_s I *j*	C_1 I *k*			
85	$P4/n$	D	S_4 I *a–b*	C_4 I *c*	C_i I *d–e*	C_2 I *f*	C_1 I *g*			
86	$P4_2/n$	D	S_4 I *a–b*	C_i I *c–d*	C_2 I *e* II *f*	C_1 I *g*				
87	$I4/m$	D	C_{4h} I *a–b*	C_{2h} I *c*	S_4 I *d*	C_4 I *e*	C_i I *f*	C_2 I *g*	C_s I *h*	C_1 I *i*
88	$I4_1/a$	G	S_4 I *a–b*	C_i I *c–d*	C_2 I *e*	C_1 I *f*				
89	$P422$	D	D_4 I *a–d*	D_2 I *e–f*	C_4 I *g–h*	C_2 I *i* II *j–k* III *l–o*	C_1 I *p*			
90	$P42_12$	D	D_2 I *a–b*	C_4 I *c*	C_2 I *d* II *e–f*	C_1 I *g*				
91	$P4_122$	E	C_2 I *a–b* II *c*	C_1 I *d*						
92	$P4_12_12$	E	C_2 I *a*	C_1 I *b*						
93	$P4_222$	D	D_2 I *a–b* II *c–d* III *e–f*	C_2 I *g–h* II *i* III *j–m* IV *n–o*	C_1 I *p*					
94	$P4_22_12$	D	D_2 I *a–b*	C_2 I *c* II *d* III *e–f*	C_1 I *g*					
95	$P4_322$	E	C_2 I *a–b* II *c*	C_1 I *d*						
96	$P4_32_12$	E	C_2 I *a*	C_1 I *b*						
97	$I422$	D	D_4 I *a–b*	D_2 I *c* II *d*	C_4 I *e*	C_2 I *f* II *g* III *h–i* IV *j*	C_1 I *k*			
98	$I4_122$	G	D_2 I *a–b*	C_2 I *c* II *d–e* III *f*	C_1 I *g*					
99	$P4mm$	A	C_{4v} I *a–b*	C_{2v} I *c*	C_s I *d* II *e–f*	C_1 I *g*				
100	$P4bm$	A	C_4 I *a*	C_{2v} I *b*	C_s I *c*	C_1 I *d*				
101	$P4_2cm$	A	C_{2v} I *a–b*	C_2 I *c*	C_s I *d*	C_1 I *e*				
102	$P4_2nm$	A	C_{2v} I *a*	C_2 I *b*	C_s I *c*	C_1 I *d*				
103	$P4cc$	A	C_4 I *a–b*	C_2 I *c*	C_1 I *d*					
104	$P4nc$	A	C_4 I *a*	C_2 I *b*	C_1 I *c*					
105	$P4_2mc$	A	C_{2v} I *a–b* II *c*	C_s I *d–e*	C_1 I *f*					
106	$P4_2bc$	A	C_2 I *a* II *b*	C_1 I *c*						
107	$I4mm$	A	C_{4v} I *a*	C_{2v} I *b*	C_s I *c* II *d*	C_1 I *e*				
108	$I4cm$	A	C_4 I *a*	C_{2v} I *b*	C_s I *c*	C_1 I *d*				
109	$I4_1md$	C	C_{2v} I *a*	C_s I *b*	C_1 I *c*					
110	$I4_1cd$	C	C_2 I *a*	C_1 I *b*						
111	$P\bar{4}2m$	D	D_{2d} I *a–d*	D_2 I *e–f*	C_{2v} I *g–h*	C_2 I *i–l* II *m*	C_s I *n*	C_1 I *o*		
112	$P\bar{4}2c$	D	D_2 I *a,c* II *b,d*	S_4 I *e–f*	C_2 I *g–j* II *k–l* III *m*	C_1 I *n*				
113	$P\bar{4}2_1m$	D	S_4 I *a–b*	C_{2v} I *c*	C_2 I *d*	C_s I *e*	C_1 I *f*			
114	$P\bar{4}2_1c$	D	S_4 I *a–b*	C_2 I *c* II *d*	C_1 I *e*					
115	$P\bar{4}m2$	D	D_{2d} I *a–d*	C_{2v} I *e–f* II *g*	C_2 I *h–i*	C_s I *j–k*	C_1 I *l*			
116	$P\bar{4}c2$	D	D_2 I *a–b*	S_4 I *c–d*	C_2 I *e–f* II *g–h* III *i*	C_1 I *j*				
117	$P\bar{4}b2$	D	S_4 I *a–b*	D_2 I *c–d*	C_2 I *e* II *f* III *g–h*	C_1 I *i*				

Table 3 (continued)

Space group		Code	Wyckoff sets									
118	*P*$\bar{4}$*n*2	D	S_4 I *a–b*	D_2 I *c–d*	C_2 I *e* II *f–g* III *h*	C_1 I *i*						
119	*I*$\bar{4}$*m*2	F	D_{2d} I *a–d*	C_{2v} I *e–f*	C_2 I *g–h*	C_s I *i*	C_1 I *j*					
120	*I*$\bar{4}$*c*2	F	D_2 I *a,d*	S_4 I *b–c*	C_2 I *e,h* II *f–g*	C_1 I *i*						
121	*I*$\bar{4}$2*m*	D	D_{2d} I *a–b*	D_2 I *c*	S_4 I *d*	C_{2v} I *e*	C_2 I *f–g* II *h*	C_s I *i*	C_1 I *j*			
122	*I*$\bar{4}$2*d*	G	S_4 I *a–b*	C_2 I *c* II *d*	C_1 I *e*							
123	*P*4/*mmm*	D	D_{4h} I *a–d*	D_{2h} I *e–f*	C_{4v} I *g–h*	C_{2v} I *i* II *j–k* III *l–o*	C_s I *p–q* II *r* III *s–t*	C_1 I *u*				
124	*P*4/*mcc*	D	D_4 I *a,c*	C_{4h} I *b,d*	C_{2h} I *e*	D_2 I *f*	C_4 I *g–h*	C_2 I *i* II *j* III *k–l*	C_s I *m*	C_1 I *n*		
125	*P*4/*nbm*	D	D_4 I *a–b*	D_{2d} I *c–d*	C_{2h} I *e–f*	C_4 I *g*	C_{2v} I *h*	C_2 I *i–j* II *k–l*	C_s I *m*	C_1 I *n*		
126	*P*4/*nnc*	D	D_4 I *a–b*	D_2 I *c*	S_4 I *d*	C_4 I *e*	C_i I *f*	C_2 I *g* II *h* III *i–j*	C_1 I *k*			
127	*P*4/*mbm*	D	C_{4h} I *a–b*	D_{2h} I *c–d*	C_4 I *e*	C_{2v} I *f* II *g–h*	C_s I *i–j* II *k*	C_1 I *l*				
128	*P*4/*mnc*	D	C_{4h} I *a–b*	C_{2h} I *c*	D_2 I *d*	C_4 I *e*	C_2 I *f* II *g*	C_s I *h*	C_1 I *i*			
129	*P*4/*nmm*	D	D_{2d} I *a–b*	C_{4v} I *c*	C_{2h} I *d–e*	C_{2v} I *f*	C_2 I *g–h*	C_s I *i* II *j*	C_1 I *k*			
130	*P*4/*ncc*	D	D_2 I *a*	S_4 I *b*	C_4 I *c*	C_i I *d*	C_2 I *e* II *f*	C_1 I *g*				
131	*P*4$_2$/*mmc*	D	D_{2h} I *a–b* II *c–d*	D_{2d} I *e–f*	C_{2v} I *g–h* II *i* III *j–m*	C_2 I *n*	C_s I *o–p* II *q*	C_1 I *r*				
132	*P*4$_2$/*mcm*	D	D_{2h} I *a,c*	D_{2d} I *b,d*	D_2 I *e*	C_{2h} I *f*	C_{2v} I *g–h* II *i–j*	C_2 I *k* II *l–m*	C_s I *n* II *o*	C_1 I *p*		
133	*P*4$_2$/*nbc*	D	D_2 I *a* II *b* III *c*	S_4 I *d*	C_i I *e*	C_2 I *f* II *g* III *h–i* IV *j*	C_1 I *k*					
134	*P*4$_2$/*nnm*	D	D_{2d} I *a–b*	D_2 I *c* II *d*	C_{2h} I *e–f*	C_{2v} I *g*	C_2 I *h* II *i–j* III *k–l*	C_s I *m*	C_1 I *n*			
135	*P*4$_2$/*mbc*	D	C_{2h} I *a*	S_4 I *b*	C_{2h} I *c*	D_2 I *d*	C_2 I *e* II *f* III *g*	C_s I *h*	C_1 I *i*			
136	*P*4$_2$/*mnm*	D	D_{2h} I *a–b*	C_{2h} I *c*	S_4 I *d*	C_{2v} I *e* II *f–g*	C_2 I *h*	C_s I *i* II *j*	C_1 I *k*			
137	*P*4$_2$/*nmc*	D	D_{2d} I *a–b*	C_{2v} I *c* II *d*	C_i I *e*	C_2 I *f*	C_s I *g*	C_1 I *h*				
138	*P*4$_2$/*ncm*	D	D_2 I *a*	S_4 I *b*	C_{2h} I *c–d*	C_{2v} I *e*	C_2 I *f* II *g–h*	C_s I *i*	C_1 I *j*			
139	*I*4/*mmm*	D	D_{4h} I *a–b*	D_{2h} I *c*	D_{2d} I *d*	C_{4v} I *e*	C_{2h} I *f*	C_{2v} I *g* II *h* III *i–j*	C_2 I *k*	C_s I *l* II *m* III *n*	C_1 I *o*	
140	*I*4/*mcm*	D	D_4 I *a*	D_{2d} I *b*	C_{4h} I *c*	D_{2h} I *d*	C_{2h} I *e*	C_4 I *f*	C_{2v} I *g* II *h*	C_2 I *i* II *j*	C_s I *k* II *l*	C_1 I *m*
141	*I*4$_1$/*amd*	G	D_{2d} I *a–b*	C_{2h} I *c*	C_{2v} I *e*	C_2 I *f* II *g*	C_s I *h*	C_1 I *i*				
142	*I*4$_1$/*acd*	G	S_4 I *a*	D_2 I *b*	C_i I *c*	C_2 I *d* II *e* III *f*	C_1 I *g*					

According to Lima-de-Faria *et al.* (1990), the structures are isotypic and belong to the same symmetry class.

(3) The structures of FeS_2 (Coll. code 316) and CO_2 (Coll. code 16428), space group 205: *Pa*$\bar{3}$, occupy the following Wyckoff positions:

Fe 4 *a* 000
S 8 *c* .385 .385 .385
PS = cP12, WS = *ca*,

C 4 *a* 000
O 8 *c* .1185 .1185 .1185
PS = cP12, WS = *ca*.

According to Table 5, the fingerprint for both structures is 205: 12 4/8.

According to Lima-de-Faria *et al.* (1990), the structures are not isotypic but belong to the same symmetry class; they differ in their coordinations.

(4) The structures of $Co_{0.93}Mn_{1.07}O_4Si$ (Coll. code 2) and $CdNaO_4P$ (Coll. code 6210), space group 62: *Pnma*, occupy the following Wyckoff positions:

Mn/Co 4 *a* 0 0 0
Mn/Co 4 *c* .22 .25 .51
Si 4 *c* .41 .25 .08
O1 4 *c* .41 .25 .74
O2 4 *c* .05 .25 .28
O3 8 *d* .34 .46 .22
PS = oP28, WS = *dc*4*a*.
Lattice parameters:
$a = 10.51$, $b = 6.13$, $c = 4.82$ Å,

Table 4
Normalizers and Wyckoff sets of hexagonal space groups.

Code: A: $H_{11t}6/mmm$; B: $P_{11t}622$; C: $H_{11t}622$; D: $H_{11t}\bar{3}m$; E: $P_{11t}6/mmm$; F: $P_{112}6/mmm$ G: $H_{112}6/mmm$; H: $P_{112}6_122$; I: $P_{112}6_522$; J: $H_{112}6_122$; K: $H_{112}6_522$; L: $'R_{112}\bar{3}m$.

Space group		Code	Wyckoff sets										
143	$P3$	A	C_3 I *a–c*	C_1 I *d*									
144	$P3_1$	C	C_1 I *a*										
145	$P3_2$	C	C_1 I *a*										
146	$R3$	D	C_3 I *a*	C_1 I *b*									
147	$P\bar{3}$	F	C_{3i} I *a–b*	C_3 I c II *d*	C_i I *e–f*	C_1 I *g*							
148	$R\bar{3}$	L	C_{3i} I *a–b*	C_3 I *c*	C_i I *d–e*	C_1 I *f*							
149	$P312$	G	D_3 I *a–f*	C_3 I *g–i*	C_2 I *j–k*	C_1 I *l*							
150	$P321$	F	D_3 I *a–b*	C_3 I c II *d*	C_2 I *e–f*	C_1 I *g*							
151	$P3_112$	J	C_2 I *a–b*	C_1 I *c*									
152	$P3_121$	H	C_2 I *a–b*	C_1 I *c*									
153	$P3_212$	K	C_2 I *a–b*	C_1 I *c*									
154	$P3_221$	I	C_2 I *a–b*	C_1 I *c*									
155	$R32$	L	D_3 I *a–b*	C_3 I *c*	C_2 I *d–e*	C_1 I *f*							
156	$P3m1$	A	C_{3v} I *a–c*	C_s I *d*	C_1 I *e*								
157	$P31m$	E	C_{3v} I *a*	C_3 I *b*	C_s I *c*	C_1 I *d*							
158	$P3c1$	A	C_3 I *a–c*	C_1 I *d*									
159	$P31c$	E	C_3 I *a* II *b*	C_1 I *c*									
160	$R3m$	D	C_{3v} I *a*	C_s I *b*	C_1 I *c*								
161	$R3c$	D	C_3 I *a*	C_1 I *b*									
162	$P\bar{3}1m$	F	D_{3d} I *a–b*	D_3 I *c–d*	C_{3v} I *e*	C_{2h} I *f–g*	C_3 I *h*	C_2 I *i–j*	C_s I *k*	C_1 I *l*			
163	$P\bar{3}1c$	F	D_3 I *a* II *c–d*	C_{3i} I *b*	C_3 I *e* II *f*	C_i I *g*	C_2 I *h*	C_1 I *i*					
164	$P\bar{3}m1$	F	D_{3d} I *a–b*	C_{3v} I c II *d*	C_{2h} I *e–f*	C_2 I *g–h*	C_s I I	C_1 I *j*					
165	$P\bar{3}c1$	F	D_3 I *a*	C_{3i} I *b*	C_3 I c II *d*	C_i I *e*	C_2 I *f*	C_1 I *g*					
166	$R\bar{3}m$	L	D_{3d} I *a–b*	C_{3v} I *c*	C_{2h} I *d–e*	C_2 I *f–g*	C_s I *h*	C_1 I *i*					
167	$R\bar{3}c$	L	D_3 I *a*	C_{3i} I *b*	C_3 I *c*	C_i I *d*	C_2 I *e*	C_1 I *f*					
168	$P6$	E	C_6 I *a*	C_3 I *b*	C_2 I *c*	C_1 I *d*							
169	$P6_1$	B	C_1 I *a*										
170	$P6_5$	B	C_1 I *a*										
171	$P6_2$	B	C_2 I *a* II *b*	C_1 I *c*									
172	$P6_4$	B	C_2 I *a* II *b*	C_1 I *c*									
173	$P6_3$	E	C_3 I *a* II *b*	C_1 I *c*									
174	$P\bar{6}$	G	C_{3h} I *a–f*	C_3 I *g–i*	C_s I *j–k*	C_1 I *l*							
175	$P6/m$	F	C_{6h} I *a–b*	C_{3h} I *c–d*	C_6 I *e*	C_{2h} I *f–g*	C_3 I *h*	C_2 I *i*	C_s I *j–k*	C_1 I *l*			
176	$P6_3/m$	F	C_{3h} I *a* II *c–d*	C_{3i} I *b*	C_3 I *e* II *f*	C_i I g	C_s I *h*	C_1 I I					
177	$P622$	F	D_6 I *a–b*	D_3 I *c–d*	C_6 I *e*	D_2 I *f–g*	C_3 I *h*	C_2 I *i* II *j–k* III *l–m*	C_1 I *n*				
178	$P6_122$	H	C_2 I *a* II *b*	C_1 I *c*									
179	$P6_522$	I	C_2 I *a* II *b*	C_1 I *c*									
180	$P6_222$	I	D_2 I *a–b* II *c–d*	C_2 I *e* II *f* III *g–h* IV *i–j*	C_1 I *k*								
181	$P6_422$	H	D_2 I *a–b* II *c–d*	C_2 I *e* II *f* III *g–h* IV *i–j*	C_1 I *k*								
182	$P6_322$	F	D_3 I *a* II *b* III *c–d*	C_3 I *e* II *f*	C_2 I *g* II *h*	C_1 I *i*							
183	$P6mm$	E	C_{6v} I *a*	C_{3v} I *b*	C_{2v} I *c*	C_s I *d* II *e*	C_1 I *f*						
184	$P6cc$	E	C_6 I *a*	C_3 I *b*	C_2 I *c*	C_1 I *d*							
185	$P6_3cm$	E	C_{3v} I *a*	C_3 I *b*	C_s I *c*	C_1 I *d*							
186	$P6_3mc$	E	C_{3v} I *a* II *b*	C_s I *c*	C_1 I *d*								
187	$P\bar{6}m2$	G	D_{3h} I *a–f*	C_{3v} I *g–i*	C_{2v} I *j–k*	C_s I *l–m* II *n*	C_1 I *o*						
188	$P\bar{6}c2$	G	D_3 I *a,c,e*	C_{3h} I *b*, *d*, *f*	C_3 I *g–i*	C_2 I *j*	C_s I *k*	C_1 I *l*					
189	$P\bar{6}2m$	F	D_{3h} I *a–b*	C_{3h} I *c–d*	C_{3v} I *e*	C_{2v} I *f–g*	C_3 I *h*	C_s I *i* II *j–k*	C_1 I *l*				
190	$P\bar{6}2c$	F	D_3 I *a*	C_{3h} I *b* II *c–d*	C_3 I *e* II *f*	C_2 I *g*	C_s I *h*	C_1 I *i*					
191	$P6/mmm$	F	D_{6h} I *a–b*	D_{3h} I *c–d*	C_{6v} I *e*	D_{2h} I *f–g*	C_{3v} I *h*	C_{2v} I *i* II *j–k* III *l–m*	C_s I *n* II *o* III *p–q*	C_1 I *r*			
192	$P6/mcc$	F	D_6 I *a*	C_{6h} I *b*	D_3 I *c*	C_{3h} I *d*	C_6 I *e*	D_2 I *f*	C_{2h} I *g*	C_3 I *h*	C_2 I *i* II *j* III *k*	C_1 I *m*	
193	$P6_3/mcm$	F	D_{3h} I *a*	D_{3d} I *b*	C_{3h} I *c*	D_3 I *d*	C_{3v} I *e*	C_{2h} I *f*	C_{2v} I *g*	C_3 I *h*	C_2 I *i*	C_s I *j* II *k*	C_1 I *l*
194	$P6_3/mmc$	F	D_{3d} I *a*	D_{3h} I *b* II *c–d*	C_{3v} I *e* II *f*	C_{2h} I *g*	C_{2v} I *h*	C_2 I *i*	C_s I *j* II *k*	C_1 I *l*			

Table 5
Normalizers and Wyckoff sets of cubic space groups.

Code: A: $Im3m$; B: $I_{222}m3m$; C: $P_{222}d3m$; D: $Ia3d$; E: $I4_132$; F: $P_{222}m3m$; G: $Ia3$.

Space group		Code	Wyckoff sets									
195	$P23$	A	T I *a–b*	D_2 I *c–d*	C_3 I *e*	C_2 I *f*, *i* II *g–h*	C_1 I *j*					
196	$F23$	B	T I *a–d*	C_3 I *e*	C_2 I *f–g*	C_1 I *h*						
197	$I23$	A	T I *a*	D_2 I *b*	C_3 I *c*	C_2 I *d* II *e*	C_1 I *f*					
198	$P2_13$	D	C_3 I *a*	C_1 I *b*								
199	$I2_13$	D	C_3 I *a*	C_2 I *b*	C_1 I *e*							
200	$Pm\bar{3}$	A	T_h I *a–b*	D_{2h} I *c–d*	C_{2v} I *e*, *h* II *f–g*	C_3 I *i*	C_s I *j–k*	C_1 I *l*				
201	$Pn\bar{3}$	A	T I *a*	C_{3i} I *b–c*	D_2 I *d*	C_3 I *e*	C_2 I *f* II *g*	C_1 I *h*				
202	$Fm\bar{3}$	F	T_h I *a–b*	T I *c*	C_{2h} I *d*	C_{2v} I *e*	C_3 I *f*	C_2 I *g*	C_s I *h*	C_1 I *i*		
203	$Fd\bar{3}$	C	T I *a–b*	C_{3i} I *c–d*	C_3 I *e*	C_2 I *f*	C_1 I *g*					
204	$Im\bar{3}$	A	T_h I *a*	D_{2h} I *b*	C_{3i} I *c*	C_{2v} I *d* II *e*	C_3 I *f*	C_s I *g*	C_1 I *h*			
205	$Pa\bar{3}$	G	C_{3i} I *a–b*	C_3 I *c*	C_1 I *d*							
206	$Ia\bar{3}$	D	C_{3i} I *a–b*	C_3 I *c*	C_2 I *d*	C_1 I *e*						
207	$P432$	A	O I *a–b*	D_4 I *c–d*	C_4 I *e–f*	C_3 I *g*	C_2 I *h* II *i–j*	C_1 I *k*				
208	$P4_232$	A	T I *a*	D_3 I *b–c*	D_2 I *d* II *e–f*	C_3 I *g*	C_2 I *h* II *i–j* III *k–l*	C_1 I *m*				
209	$F432$	F	O I *a–b*	T I *c*	D_2 I *d*	C_4 I *e*	C_3 I *f*	C_2 I *g–h* II *i*	C_1 I *j*			
210	$F4_132$	C	T I *a–b*	D_3 I *c–d*	C_3 I *e*	C_2 I *f* II *g*	C_1 I *h*					
211	$I432$	A	O I *a*	D_4 I *b*	D_3 I *c*	D_2 I *d*	C_4 I *e*	C_3 I *f*	C_2 I *g* II *h* III *i*	C_1 I *j*		
212	$P4_332$	E	D_3 I *a–b*	C_3 I *c*	C_2 I *d*	C_1 I *e*						
213	$P4_132$	E	D_3 I *a–b*	C_3 I *c*	C_2 I *d*	C_1 I *e*						
214	$I4_132$	D	D_3 I *a–b*	D_2 I *c–d*	C_3 I *e*	C_2 I *f* II *g–h*	C_1 I *i*					
215	$P\bar{4}3m$	A	T_d I *a–b*	D_{2d} I *c–d*	C_{3v} I *e*	C_{2v} I *f–g*	C_2 I *h*	C_s I *i*	C_1 I *j*			
216	$F\bar{4}3m$	B	T_d I *a–d*	C_{3v} I *e*	C_{2v} I *f–g*	C_s I *h*	C_1 I *i*					
217	$I\bar{4}3m$	A	T_d I *a*	D_{2d} I *b*	C_{3v} I *c*	S_4 I *d*	C_{2v} I *e*	C_2 I *f*	C_s I *g*	C_1 I *h*		
218	$P\bar{4}3n$	A	T I *a*	D_2 I *b*	S_4 I *c–d*	C_3 I *e*	C_2 I *f* II *g–h*	C_1 I *i*				
219	$F\bar{4}3c$	B	T I *a–b*	S_4 I *c–d*	C_3 I *e*	C_2 I *f–g*	C_1 I *h*					
220	$I\bar{4}3d$	D	S_4 I *a–b*	C_3 I *c*	C_2 I *d*	C_1 I *e*						
221	$Pm\bar{3}m$	A	O_h I *a–b*	D_{4h} I *c–d*	C_{4v} I *e–f*	C_{3v} I *g*	C_{2v} I *h* II *i–j*	C_s I *k–l* II *m*	C_1 I *n*			
222	$Pn\bar{3}n$	A	O I *a*	D_4 I *b*	C_{3i} I *c*	S_4 I *d*	C_4 I *e*	C_3 I *f*	C_2 I *g* II *h*	C_1 I *i*		
223	$Pm\bar{3}n$	A	T_h I *a*	D_{2h} I *b*	D_{2d} I *c–d*	D_3 I *e*	C_{2v} I *f* II *g–h*	C_3 I *i*	C_2 I *j*	C_s I *k*	C_1 I *l*	
224	$Pn\bar{3}m$	A	T_d I *a*	D_{3d} I *b–c*	D_{2d} I *d*	C_{3v} I *e*	D_2 I *f*	C_{2v} I *g*	C_2 I *h* II *i–j*	C_s I *k*	C_1 I *l*	
225	$Fm\bar{3}m$	F	O_h I *a–b*	T_d I *c*	D_{2h} I *d*	C_{4v} I *e*	C_{3v} I *f*	C_{2v} I *g* II *h–i*	C_s I *j* II *k*	C_1 I *l*		
226	$Fm\bar{3}c$	F	O I *a*	T_h I *b*	D_{2d} I *c*	C_{4h} I *d*	C_{2v} I *e*	C_4 I *f*	C_3 I *g*	C_2 I *h*	C_s I *i*	C_1 I *j*
227	$Fd\bar{3}m$	C	T_d I *a–b*	D_{3d} I *c–d*	C_{3v} I *e*	C_{2v} I *f*	C_s I *g*	C_2 I *h*	C_1 I *i*			
228	$Fd\bar{3}c$	C	T I *a*	D_3 I *b*	C_{3i} I *c*	S_4 I *d*	C_3 I *e*	C_2 I *f* II *g*	C_1 I *h*			
229	$Im\bar{3}m$	A	O_h I *a*	D_{4h} I *b*	D_{3d} I *c*	D_{2d} I *d*	C_{4v} I *e*	C_{3v} I *f*	C_{2v} I *g* II *h*	C_2 I *i*	C_s I *j* II *k*	C_1 I *l*
230	$Ia\bar{3}d$	D	C_{3i} I *a*	D_3 I *b*	D_2 I *c*	S_4 I *d*	C_3 I *e*	C_2 I *f* II *g*	C_1 I *h*			

Na 4 *b* $\frac{1}{2}$ 0 0 $\frac{1}{2}$ 0 $\frac{1}{2}$ 0 0 0
Cd 4 *c* .21 .25 .02   .21 .25 .52
P 4 *c* .40 .25 .57   .40 .25 .07
O1 4 *c* .39 .25 .26   .39 .25 .76
O3 4 *c* .03 .25 .83   .03 .25 .33
O2 8 *d* .33 .06 .69   .33 .06 .19   .33 .44 .19
PS = oP28, WS = *dc*4*b*.
Lattice parameters:
a = 10.83, b = 6.49, c = 5.06 Å.

According to Table 2, the fingerprint for both structures is 62: 28 4/16/8.

According to Lima-de-Faria *et al.* (1990), the structures are isotypic, they belong to the same symmetry class because positions *a* and *b* belong to the Wyckoff set C_i I *a–b*. The translation (0 0 $\frac{1}{2}$) is taken from the normalizer translations and maps structure 1 on structure 2. For position 8*d* 0.33 0.06 0.69, the equivalent position 0.33 0.44 0.69; for position 4*b* $\frac{1}{2}$ 0 $\frac{1}{2}$, the equivalent 0 0 0 is chosen.

(5) The following example deals with partial structures of more complicated modulated structures.

The structures of TiS_2(I) (Coll. code 56496), TiS_2(II) (Coll. code 41092) and VS_2(III) (Coll. code 153507), space group 2: $P\bar{1}$, occupy the following Wyckoff positions:

I: setting *C*-1
Ti 2 *a* 0 0 0
S 4 *b* .466 −.191 .127.
Lattice parameters:
a = 3.403 Å, α = 84.39°
b = 5.911 Å, β = 82.82°
c = 11.385 Å, γ = 90.01°

$(TiS_2)(SbS)_{1.15}$ sum formula
$Z = 2$, WS = *ia*
PS_{N1} = aP5, PS_{N2} = aP3,
II: setting *F*-1
Ti 4 *a* $\frac{1}{4}\,\frac{1}{4}$ 0
S 8 *b* .248 .559 −.062.
Lattice parameters:
$a = 3.412$ Å, $\alpha = 95.86°$
$b = 5.836$ Å, $\beta = 90.30°$
$c = 23.290$ Å, $\gamma = 90.00°$
$(TiS_2)(SnS)_{1.2}$ sum formula
$Z = 4$, WS = *ib*
PS_{N1} = aP5, PS_{N2} = aP3,

III: setting *C*-1
V 2 *a* $\frac{1}{4}\,\frac{1}{4}\,\frac{1}{2}$
S 4 *b* .285 .562 .374.
Lattice parameters:
$a = 3.410$ Å, $\alpha = 95.12°$
$b = 5.850$ Å, $\beta = 84.69°$
$c = 11.196$ Å, $\gamma = 90.00°$
$(VS_2)(LaS)_{1.196}$ sum formula
$Z = 2$, WS = *ig*
PS_{N1} = aP5, PS_{N2} = aP3.

The Pearson symbol taken from the database is aP5. The procedure (ii) (see above) leads to PS_{N2} = aP3 for all three structures.

According to Table 1, the fingerprint for the three structures is 2: 3 1/2.

Because of the relations among the structural parameters a closer relationship was supposed. Delaunay reductions (Burzlaff & Zimmermann, 1985) and hereby indicated transformations resulted in a monoclinic unit cell *mC* and closely related coordinates for all of them. The average lattice parameters are:

$a = 5.894$ (5), $b = 3.392$ (18), $c = 11.548$ (150) Å,
$\alpha = 90.38$ (130), $\beta = 101.59$ (137), $\gamma = 89.69$ (46)°.

The space group would be the supergroup 12: *C*2/*m*. The coordinates are

2 *a* 0 0 0 and 4 *b* .381 (4), −.012 (24) $\simeq$ 0, .126 (2).

The numbers in parentheses are maximal deviations related to the last digit.

The true symmetry can only be determined by a careful inspection of the experimental data. The authors did not give an indication that they discussed monoclinic or higher symmetry; the structures are isotypic in any case.

4. Applications

To test our considerations presented above, the ICSD database, version 2007 (ICSD, 2007), edition 2, was chosen. In a first step the complete database was reorganized according to space-group numbers. Since only a maximum of 50 space-group entries can be transferred at once from the 2007 database, this reorganization had to be done by hand, a very tedious procedure! For each item the 'fingerprint', *i.e.* the symmetry class of the crystal structure, was determined. In addition, the items were rearranged according to the number of sites in the primitive cell and their distribution on the Wyckoff sets. Table 6(*a*) shows a part of the fingerprint file for space group 15: *C*2/*c*. Column 1 contains a count after re-ordering. Column 2 gives the database collection code. Column 3 contains the number of sites. The next columns show their distribution on the Wyckoff sets. At the end follows the Wyckoff sequence. Table 6(*b*) gives a part of the list of symmetry classes for space group 15: *C*2/*c*. Each line refers to one symmetry class. Column 1 contains a running number, column 2 the number of items for this class. The following columns give the information as in Table 6(*a*).

Table 7 presents a survey of all monoclinic space groups. For each space group, column 2 contains the number of items in the database. Column 3 shows the number of symmetry classes. In columns 4 to 10 an indication of the frequency of items with respect to the different symmetry classes is presented.

Table 6
Part of the list of fingerprints and Wyckoff sequences for one space group: space group 15, *C*2/*c*.

	Wyckoff sets and Wyckoff positions	
1	C_i I	*a*, *b*, *c*, *d*
2	C_2 I	*e*
3	C_1 I	*f*

(*a*) Items: 3812; part of the list 724–742.

Item No.	Coll. code	Sites	Occupation numbers of Wyckoff sets and Wyckoff sequences			
724	86064	18	4	2	12	*f3eca*
725	85212	18	4	2	12	*f3eba*
726	64770	20	–	–	20	*f5*
727	38263	20	–	–	20	*f5*
728	68098	20	–	–	20	*f5*
729	9561	20	–	–	20	*f5*
730	31925	20	–	–	20	*f5*
731	200826	20	–	–	20	*f5*
732	410743	20	–	–	20	*f5*
733	16797	20	–	–	20	*f5*
734	2565	20	–	–	20	*f5*
735	16874	20	–	4	16	*f4e2*
736	20225	20	–	4	16	*f4e2*
737	20355	20	–	4	16	*f4e2*
738	10226	20	–	4	16	*f4e2*
739	20556	20	–	4	16	*f4e2*
740	35534	20	–	4	16	*f4e2*
741	20557	20	–	4	16	*f4e2*
742	62513	20	–	4	16	*f4e2*

(*b*) Symmetry classes: 463; part of the list 38–45.

			Occupation of Wyckoff sets		
No. of class	No. of items	No. of sites	C_i I	C_2 I	C_1 I
38	4	18	4	2	12
39	9	20	0	0	20
40	428	20	0	4	16
41	9	20	0	8	12
42	16	20	2	2	16
43	1	20	2	6	12
44	2	20	4	4	12
45	68	22	0	2	20

Table 7
Distribution of items and occupation of Wyckoff sets for monoclinic space groups.

No.	Space group	No. of items	Symmetry classes	No. N of items per class with $N \geq 100$	$N \geq 50$	$N \geq 20$	$N \geq 10$	$N \geq 5$	$N \geq 2$	$N = 1$
3	$P2$	36	29	0	0	0	0	0	7	22
4	$P2_1$	551	73	0	0	7	12	15	16	23
5	$C2$	315	136	0	0	0	3	12	47	74
6	Pm	41	27	0	0	0	0	1	4	22
7	Pc	239	59	0	0	1	3	11	21	23
8	Cm	270	137	0	0	1	2	5	47	82
9	Cc	489	74	0	0	6	12	14	18	24
10	$P2/m$	130	65	0	0	1	1	2	14	47
11	$P2_1/m$	1154	308	0	0	13	10	40	86	159
12	$C2/m$	3382	858	2	5	27	38	77	200	509
13	$P2/c$	461	162	0	1	0	3	14	60	84
14	$P2_1/c$	7281	264	20	16	26	27	28	69	78
15	$C2/c$	3812	463	3	15	32	30	53	127	203

Table 8
100 241 items and 15 325 symmetry classes for all space groups, 6811 with more than one item.

nc = number of classes per space group; nc+ = number of classes with more than one item.

Space group	Items	nc	nc+	Space group	Items	nc	nc+	Space group	Items	nc	nc+
1 $P1$	321	84	52	77 $P4_2$	7	5	1	154 $P3_221$	131	22	8
2 $P\bar{1}$	4017	408	255	78 $P4_3$	6	6	0	155 $R32$	138	68	23
3 $P2$	36	29	7	79 $I4$	37	20	11	156 $P3m1$	313	70	40
4 $P2_1$	551	73	50	80 $I4_1$	14	11	3	157 $P31m$	53	29	5
5 $C2$	315	136	62	81 $P\bar{4}$	34	26	4	158 $P3c1$	17	15	2
6 Pm	41	27	5	82 $I\bar{4}$	270	57	28	159 $P31c$	130	62	19
7 Pc	239	59	36	83 $P4/m$	34	18	8	160 $R3m$	661	166	71
8 Cm	270	137	55	84 $P4_2/m$	36	22	7	161 $R3c$	370	56	30
9 Cc	489	74	50	85 $P4/n$	126	55	20	162 $P\bar{3}1m$	120	37	16
10 $P2/m$	130	65	18	86 $P4_2/n$	93	40	16	163 $P\bar{3}1c$	150	62	19
11 $P2_1/m$	1154	308	149	87 $I4/m$	547	154	55	164 $P\bar{3}m1$	1011	139	64
12 $C2/m$	3382	858	349	88 $I4_1/a$	437	71	33	165 $P\bar{3}c1$	165	59	19
13 $P2/c$	461	162	78	89 $P422$	3	1	1	166 $R\bar{3}m$	2528	382	176
14 $P2_1/c$	7281	264	186	90 $P42_12$	11	8	3	167 $R\bar{3}c$	1720	178	76
15 $C2/c$	3812	463	260	91 $P4_122$	17	10	1	168 $P6$	1	1	0
16 $P222$	13	13	0	92 $P4_12_12$	190	42	21	169 $P6_1$	28	14	5
17 $P222_1$	26	14	6	93 $P4_222$	0	0	0	170 $P6_5$	12	6	3
18 $P2_12_12$	114	63	24	94 $P4_22_12$	5	4	1	171 $P6_2$	4	3	1
19 $P2_12_12_1$	741	67	56	95 $P4_322$	10	6	3	172 $P6_4$	1	1	0
20 $C222_1$	129	54	21	96 $P4_32_12$	59	32	11	173 $P6_3$	496	115	47
21 $C222$	34	21	7	97 $I422$	7	7	0	174 $P\bar{6}$	120	52	13
22 $F222$	25	14	6	98 $I4_122$	15	7	4	175 $P6/m$	22	12	3
23 $I222$	14	10	2	99 $P4mm$	221	24	11	176 $P6_3/m$	1156	314	122
24 $I2_12_12_1$	4	3	1	100 $P4bm$	85	19	12	177 $P622$	4	3	1
25 $Pmm2$	41	24	5	101 $P42cm$	2	2	0	178 $P6_122$	36	17	5
26 $Pmc2_1$	98	59	22	102 $P42nm$	18	9	3	179 $P6_522$	9	8	1
27 $Pcc2$	4	3	1	103 $P4cc$	6	2	1	180 $P6_222$	102	27	11
28 $Pma2$	25	17	5	104 $P4nc$	9	6	1	181 $P6_422$	34	12	8
29 $Pca2_1$	246	51	34	105 $P4_2mc$	5	4	1	182 $P6_322$	136	35	17
30 $Pnc2$	19	18	1	106 $P4_2bc$	4	2	2	183 $P6mm$	14	11	2
31 $Pmn2_1$	267	85	37	107 $I4mm$	83	37	12	184 $P6cc$	14	11	1
32 $Pba2$	33	21	6	108 $I4cm$	21	15	5	185 $P6_3cm$	126	33	14
33 $Pna2_1$	890	63	45	109 $I4_1md$	38	15	7	186 $P6_3mc$	848	122	62
34 $Pnn2$	45	29	7	110 $I4_1cd$	31	11	3	187 $P\bar{6}m2$	208	58	21
35 $Cmm2$	25	23	2	111 $P\bar{4}2m$	24	13	3	188 $P\bar{6}c2$	29	9	3
36 $Cmc2_1$	531	123	59	112 $P\bar{4}2c$	20	8	2	189 $P\bar{6}2m$	643	73	32
37 $Ccc2$	19	13	6	113 $P\bar{4}2_1m$	265	47	18	190 $P\bar{6}2c$	126	56	13
38 $Amm2$	149	71	21	114 $P\bar{4}2_1c$	69	45	14	191 $P6/mmm$	1698	144	65
39 $Abm2$	38	23	6	115 $P\bar{4}m2$	21	16	2	192 $P6/mcc$	158	23	11
40 $Ama2$	70	36	13	116 $P\bar{4}c2$	19	9	5	193 $P6_3/mcm$	412	63	32
41 $Aba2$	95	48	19	117 $I\bar{4}b2$	22	18	3	194 $P6_3/mmc$	3448	535	231
42 $Fmm2$	61	30	6	118 $P\bar{4}n2$	34	25	6	195 $P23$	14	13	1
43 $Fdd2$	233	60	34	119 $I\bar{4}m2$	58	31	7	196 $F23$	28	18	5
44 $Imm2$	116	46	19	120 $I\bar{4}c2$	30	15	7	197 $I23$	106	29	15
45 $Iba2$	19	11	4	121 $I\bar{4}2m$	143	33	14	198 $P2_13$	385	49	31
46 $Ima2$	127	29	12	122 $I\bar{4}2d$	409	65	28	199 $I2_13$	72	22	6
47 $Pmmm$	1002	65	25	123 $P4/mmm$	2015	304	148	200 $Pm\bar{3}$	79	38	12
48 $Pmmn$	9	8	1	124 $P4/mcc$	46	18	9	201 $Pn\bar{3}$	89	23	11

Table 8 (continued)

Space group	Items	nc	nc+	Space group	Items	nc	nc+	Space group	Items	nc	nc+
49 *Pccm*	6	6	0	125 *P4/nbm*	47	21	7	202 $Fm\bar{3}$	48	20	4
50 *Pban*	20	11	6	126 *P4/nnc*	65	29	11	203 $Fd\bar{3}$	155	100	27
51 *Pmma*	174	84	29	127 *P4/mbm*	578	111	38	204 $Im\bar{3}$	378	57	20
52 *Pnna*	128	51	16	128 *P4/mnc*	142	52	25	205 $Pa\bar{3}$	517	18	17
53 *Pmna*	65	38	11	129 *P4/nmm*	1197	100	51	206 $Ia\bar{3}$	290	20	9
54 *Pcca*	51	29	11	130 *P4/ncc*	139	42	18	207 *P*432	1	1	0
55 *Pbam*	562	141	54	131 $P4_2/mmc$	46	19	7	208 $P4_232$	9	4	2
56 *Pccn*	128	55	27	132 $P4_2/mcm$	19	16	2	209 *F*432	5	3	1
57 *Pbcm*	325	119	51	133 $P4_2/nbc$	25	9	5	210 $F4_132$	8	7	1
58 *Pnnm*	572	157	60	134 $P4_2/nnm$	20	11	5	211 *I*432	3	2	1
59 *Pmmn*	376	104	47	135 $P4_2/mbc$	88	24	9	212 $P4_332$	120	18	9
60 *Pbcn*	554	132	71	136 $P4_2/mnm$	861	79	39	213 $P4_132$	126	2 9	13
61 *Pbca*	961	91	65	137 $P4_2/nmc$	221	49	15	214 $I4_132$	25	9	3
62 *Pnma*	7472	398	213	138 $P4_2/ncm$	38	24	7	215 $P\bar{4}3m$	141	58	23
63 *Cmcm*	1943	432	165	139 *I4/mmm*	4051	367	176	216 $F\bar{4}3m$	1168	128	56
64 *Cmce*	676	191	69	140 *I4/mcm*	990	105	47	217 $I\bar{4}3m$	314	72	33
65 *Cmmm*	536	145	62	141 $I4_1/amd$	816	129	58	218 $P\bar{4}3n$	321	48	29
66 *Cccm*	137	48	22	142 $I4_1/acd$	276	70	35	219 $F\bar{4}3c$	44	18	7
67 *Cmme*	60	39	12	143 *P*3	77	56	16	220 $I\bar{4}3d$	291	51	29
68 *Ccce*	42	27	10	144 $P3_1$	74	25	12	221 $Pm\bar{3}m$	3002	219	79
69 *Fmmm*	235	99	32	145 $P3_2$	19	12	4	222 $Pn\bar{3}n$	4	2	1
70 *Fddd*	298	77	38	146 *R*3	166	82	33	223 $Pm\bar{3}n$	570	42	20
71 *Immm*	626	123	60	147 $P\bar{3}$	202	111	33	224 $Pn\bar{3}m$	96	25	12
72 *Ibam*	196	56	26	148 $R\bar{3}$	1386	227	122	225 $Fm\bar{3}m$	5587	233	106
73 *Ibca*	33	21	6	149 *P*312	26	10	4	226 $Fm\bar{3}c$	125	40	10
74 *Imma*	489	107	47	150 *P*321	198	40	19	227 $Fd\bar{3}m$	5081	216	112
75 *P*4	23	17	4	151 $P3_112$	29	11	5	228 $Fd\bar{3}c$	23	12	3
76 $P4_1$	38	11	6	152 $P3_121$	312	41	20	229 $Im\bar{3}m$	739	97	45
				153 $P3_212$	1	1	0	230 $Ia\bar{3}d$	633	42	18

Table 8 presents a compact survey of all 230 space groups. Column 2 contains the number of items for each space group. Column 3 presents the number of all symmetry classes and column 4 presents the number of symmetry classes with more than one item.

5. Results

One drawback of this procedure is evident: in most cases it is not possible to obtain metrical and geometrical information from this classification, the structure type must be evaluated separately. For the example of the pyrite family discussed by Allmann & Hinek (2007), no help is available using this method [*cf.* example (3)].

The advantages, however, are remarkable:

(i) The items of the database can be handled in this classification without changes, interpretation or any other manipulation.

(ii) The determination of the 'fingerprint' can be carried out easily and could be included in the item file in the Wyckoff-sequence line in the database.

(iii) The classification is highly suitable for further investigations, *e.g.* for the search of structural relations or the determination of structure types. All structures of one structure type belong to the same symmetry class. Moreover, structural relations that are based on symmetry are preserved, *e.g.* in Bärnighausen trees the search for isotypic structures can be restricted to symmetry classes of subgroups (Bärnighausen, 1975).

(iv) This concept is open-ended and independent of the number of new crystal structures determined in the future.

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