

more sophisticated use of the data available and is far more efficient.

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## On Crystallography in Higher Dimensions. III. Results in $R_4$

BY H. WONDRA TSCH EK

*Kristallographisches Institut der Universität Karlsruhe, Germany*

AND R. BÜLOW AND J. NEUBÜSER

*Lehrstuhl D für Mathematik der Technischen Hochschule Aachen, Germany*

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(Dedicated to Wolfgang Gaschütz on the occasion of his 50th birthday)

An explicit classification of lattices and crystallographic groups of 4-dimensional space  $R_4$  is given. There are (in  $R_4$ ): 710 arithmetic crystal classes; 227 geometric crystal classes belonging to 118 isomorphism types of groups; 64 Bravais classes corresponding to 64 Bravais types of lattices; 33 crystal systems; 23 crystal families.

This paper presents some of the results obtained by the methods, explained in Bülow, Neubüser & Wondratschek (1971) (referred to as II). The definitions used are found in Neubüser, Wondratschek & Bülow (1971) (referred to as I).

### 1. Crystal classes and crystal systems

The 710 arithmetic crystal classes are not explicitly given. For each (geometric) crystal class the number of arithmetic crystal classes contained in it is included in Table 1.

The 227 (geometric) crystal classes, derived by Hurley (1951) (*cf.* also Hurley, Neubüser & Wondratschek, 1967), have been ordered into the 33 crystal systems in Table 1.

Within a crystal system the crystal classes are ordered by the following characteristics (common to all groups

in a crystal class) which apply in the sequence listed below:\*

- Group order. Smaller order precedes larger one.
- Determinants. Determinants only positive precede determinants both positive and negative.
- Crystal classes of groups containing  $I'$  precede those of groups not containing  $I'$ .
- Highest order of elements: Smaller order precedes higher order.

\* Of course there are other ordering schemes; this one seemed convenient to us. A nomenclature for the crystal classes corresponding to that of Hermann-Mauguin in  $R_2$  and  $R_3$  has not yet been developed. There are some difficulties in introducing such a nomenclature, as in  $R_4$  there are no symmetry axes in most cases and, therefore, the description of 'symmetry in certain directions' is not as easily used as in  $R_2$  and  $R_3$ .

Table 1. *List of the geometric crystal classes of  $R_4$* 

The Table contains for each crystal system its number and its name (*e.g.* 3, triclinic). For each crystal class belonging to this system one finds its number (*e.g.* 3/01), its place in Hurley's (1951) paper in parentheses [*e.g.* (2a, 2), *i.e.* the second entry in Hurley's Table 2a], and the number of arithmetic crystal classes belonging to it (*e.g.* 3 for this example). The last class in each crystal system is its holohedral one.

Generators for one representative of this holohedral class are listed by a denotation in Table 3. These denotations refer to the matrices tabulated in Table 4.

1, hexaclinic	1/01 (2a, 1) 1	1/02 (1a, I, 1) 1		
2, triclinic	2/01 (2b, 1) 2	2/02 (2b, 2) 2	2/03 (1b, XXXIII, 1) 2	
3, triclinic	3/01 (2a, 2) 3	3/02 (1a, I, 2) 3		
4, monoclinic	4/01 (2b, 3) 6	4/02 (2b, 4) 7	4/03 (2b, 5) 6	4/04 (1b, XXXIII, 2) 6
5, orthogonal <i>KU</i> -centred	5/01 (2a, 17) 13	5/02 (1a, XI, 1) 9		
6, orthorhombic	6/01 (2b, 32) 12	6/02 (2b, 33) 12	6/03 (1b, XXXV, 1) 8	
7, tetragonal monoclinic	7/01 (2a, 4) 2	7/02 (2a, 5) 2	7/03 (1a, I, 4) 2	7/04 (2b, 11) 2
	7/05 (2b, 12) 2	7/06 (2b, 20) 4	7/07 (1b, XXXIII, 7) 2	
8, rhombohedral monoclinic	8/01 (2a, 3) 2	8/02 (1a, I, 3) 2	8/03 (2b, 7) 3	8/04 (2b, 8) 3
	8/05 (1b, XXXIII, 5) 3			
9, hexagonal monoclinic	9/01 (2a, 7) 1	9/02 (2a, 8) 1	9/03 (1a, I, 6) 1	9/04 (2b, 13) 1
	9/05 (2b, 14) 1	9/06 (2b, 16) 1	9/07 (1b, XXXIII, 10) 1	
10, ditetragonal triclinic	10/01 (1a, I, 8) 1			
11, dihexagonal triclinic	11/01 (2a, 11) 1	11/02 (1a, I, 10) 1		
12, tetragonal orthorhombic <i>KG</i> -centred	12/01 (2b, 6) 7	12/02 (1b, XXXIII, 3) 6	12/03 (2b, 34) 13	12/04 (2b, 35) 13
	12/05 (1b, XXXV, 2) 11			
13, tetragonal orthorhombic	13/01 (2a, 19) 6	13/02 (2a, 20) 6	13/03 (2b, missing) 6	13/04 (2b, 21) 6
	13/05 (1a, XI, 3) 5	13/06 (1b, XXXIII, 6) 5	13/07 (2b, 52) 6	13/08 (2b, 53) 6
	13/09 (2b, 46) 12	13/10 (1b, XXXV, 4) 5		
14, rhombohedral orthorhombic	14/01 (2a, 18) 8	14/02 (2b, 10) 4	14/03 (2b, 9) 4	14/04 (1a, XI, 2) 4
	14/05 (1b, XXXIII, 4) 4	14/06 (2b, 38) 6	14/07 (2b, 37) 6	14/08 (2b, 36) 6
	14/09 (2b, 39) 6	14/10 (1b, XXXV, 3) 6		
15, hexagonal orthorhombic	15/01 (2a, 23) 2	15/02 (2a, 22) 4	15/03 (2b, 18) 2	15/04 (2b, 15) 2
	15/05 (2b, 17) 2	15/06 (1a, XI, 5) 2	15/07 (1b, XXXIII, 9) 2	15/08 (2b, 43) 4
	15/09 (2b, 40) 2	15/10 (2b, 41) 2	15/11 (2b, 42) 4	15/12 (1b, XXXV, 6) 2
16, ditetragonal monoclinic	16/01 (1a, III, 1) 3			
17, dihexagonal monoclinic	17/01 (2a, 15) 3	17/02 (1a, III, 2) 2		
18, ditetragonal orthorhombic <i>D</i> -centred	18/01 (1a, I, 12) 3	18/02 (1a, XI, 9) 5	18/03 (1b, XXXIII, 14) 5	18/04 (1b, XXXVI, 1) 7
	18/05 (1b, XXXV, 9) 7			
19, ditetragonal orthorhombic	19/01 (1a, I, 13) 2	19/02 (1b, XXXIII, 8) 2	19/03 (1a, XI, 10) 2	19/04 (1b, XXXV, 5) 4
	19/05 (1b, XXXIII, 15) 2	19/06 (1b, XXXV, 10) 2		

Table 1 (*cont.*)

20, hexagonal tetragonal			
20/01 (2a, 10) 1	20/02 (2a, 9) 1	20/03 (2b, 19) 2	20/04 (1a, I, 7) 1
20/05 (2a, 25) 2	20/06 (2a, 24) 2	20/07 (1b, XXXIII, 11) 1	20/08 (2b, 45) 4
20/09 (2b, 44) 4	20/10 (2b, 26) 2	20/11 (2b, 30) 2	20/12 (2b, 25) 1
20/13 (2b, 24) 1	20/14 (2b, 31) 2	20/15 (1a, XI, 6) 1	20/16 (1b, XXXV, 7) 2
20/17 (1b, XXXIII, 12) 1	20/18 (1b, XXXIII, 13) 1	20/19 (2b, 51) 2	20/20 (2b, 50) 2
20/21 (2b, 56) 4	20/22 (1b, XXXV, 8) 1		
21, dihexagonal orthogonal <i>D</i> -centred			
21/01 (2a, 12) 2	21/02 (1a, I, 11) 2	21/03 (2a, 26) 4	21/04 (1a, XI, 8) 2
22, dihexagonal orthogonal <i>RR</i> -centred			
22/01 (2a, 13) 2	22/02 (1a, I, 15) 2	22/03 (2a, 27) 5	22/04 (2b, 23) 4
22/05 (2b, 22) 3	22/06 (1a, XI, 12) 3	22/07 (1b, XXXIII, 16) 3	22/08 (2b, 48) 4
22/09 (2b, 49) 5	22/10 (2b, 47) 4	22/11 (1b, XXXV, 11) 4	
23, dihexagonal orthogonal			
23/01 (2a, 14) 1	23/02 (1a, I, 16) 1	23/03 (2a, 28) 2	23/04 (2b, 28) 1
23/05 (2b, 29) 2	23/06 (2b, 27) 1	23/07 (1a, XI, 13) 1	23/08 (1b, XXXIII, 17) 1
23/09 (2b, 55) 2	23/10 (2b, 54) 2	23/11 (1b, XXXV, 12) 1	
24, cubic <i>KU</i> -centred			
24/01 (2a, 30) 6	24/02 (1a, XXI) 6	24/03 (2b, missing) 6	24/04 (2b, missing) 6
24/05 (1b, XL) 6			
25, cubic			
25/01 (2a, 31) 5	25/02 (2a, missing) 5	25/03 (2b, 64) 5	25/04 (2b, 63) 5
25/05 (1a, XXVI) 5	25/06 (1b, XXXIX) 5	25/07 (2b, 66) 5	25/08 (2b, missing) 5
25/09 (2b, 65) 5	25/10 (2b, missing) 5	25/11 (1b, XLIV) 5	
26, octagonal			
26/01 (1a, I, 9) 1	26/02 (1a, XI, 7) 1		
27, decagonal			
27/01 (2a, 6) 1	27/02 (1a, I, 5) 1	27/03 (2a, 21) 2	27/04 (1a, XI, 4) 1
28, dodecagonal			
28/01 (1a, I, 14) 1	28/02 (1a, XI, 11) 1		
29, di-isohexagonal orthogonal <i>RR</i> -centred			
29/01 (2a, 16) 3	29/02 (1a, III, 6) 2	29/03 (2a, 29) 5	29/04 (2b, 62) 4
29/05 (1a, XIII', 3) 2	29/06 (1b, XXXVI, 5) 3	29/07 (2b, 61) 4	29/08 (2b, 60) 4
29/09 (1b, XIII', 2) 3			
30, di-isohexagonal orthogonal			
30/01 (1a, II, 2) 1	30/02 (1a, IV, 2) 2	30/03 (1a, II, 4) 1	30/04 (1a, III, 5) 1
30/05 (1a, II, 6) 1	30/06 (1a, XII, 2) 1	30/07 (1a, XII, 4) 1	30/08 (1a, IV, 4) 1
30/09 (1a, X, 3) 1	30/10 (1a, XIII, 2) 1	30/11 (1b, XXXVI, 6) 1	30/12 (1b, XXXIV, 2) 2
30/13 (1b, XXXVII, 3) 1			
31, icosahedral			
31/01 (2b, 59) 4	31/02 (1b, XXXVI, 2) 2	31/03 (2a, 32) 2	31/04 (1a, XXXII) 2
31/05 (2b, 57) 2	31/06 (2b, 58) 2	31/07 (1b, LI) 2	
32, hypercubic			
32/01 (1a, II, 1) 2	32/02 (1a, II, 3) 2	32/03 (1a, IV, 1) 2	32/04 (1a, III, 3) 2
32/05 (1a, VI) 3	32/06 (1a, X, 1) 2	32/07 (1a, XII, 1) 2	32/08 (1a, IV, 3) 2
32/09 (1a, XIII', 1) 2	32/10 (1b, XXXVI, 3) 5	32/11 (1a, XVIII) 3	32/12 (1a, XIII, 1) 2
32/13 (1b, XXXIV, 1) 4	32/14 (1b, XXXVI, 4) 2	32/15 (1b, XIII', 1) 4	32/16 (1a, XXII) 3
32/17 (1b, XXXVII, 2) 2	32/18 (1a, XXVII) 3	32/19 (1b, XLII) 3	32/20 (1b, XLI) 3
32/21 (1b, XLVII) 3			
33, hypercubic <i>Z</i> -centred			
33/01 (1a, V, 1) 1	33/02 (1a, III, 4) 1	33/03 (1a, II, 5) 1	33/04 (1a, VIII, 1) 1
33/05 (1a, XII, 3) 1	33/06 (1a, V, 2) 1	33/07 (1a, V, 3) 1	33/08 (1a, XVI, 1) 1
33/09 (1a, VIII, 2) 1	33/10 (1a, XIV) 1	33/11 (1a, XVI, 2) 1	33/12 (1a, XVII) 1
33/13 (1a, XX) 1	33/14 (1a, XXVIII) 1	33/15 (1b, XLIII) 2	33/16 (1b, XLV) 1

(e) Number of elements of highest order: Smaller number precedes higher number.

(f) Number of elements of highest order with positive determinant: Higher number precedes smaller one.

(g) For those crystal classes which have the same characteristics (a)–(f), an order of preference is established using the ‘simplicity of symmetry operations’.

Fig. 1 shows relations between the holohedries. To

explain its meaning we need two further definitions: A holohedry **B** is of *lower symmetry* than the holohedry **A** if for each group  $\mathcal{A}$  of **A** there is a group  $\mathcal{B}$  of **B** with  $\mathcal{B} \subset \mathcal{A}$ . The holohedry **B** is called *maximal* in **A** if it is of lower symmetry than **A**, but if there is no holohedry **C** different from **A** and **B** such that **B** is of lower symmetry than **C** and **C** is of lower symmetry than **A**.

In the Figure holohedries of lower symmetry are drawn at a lower level and each holohedry is connected

downward with all those that are maximal in it.

We may also distinguish holohedries – as well as geometric classes in general – with respect to their decomposability. An integral  $n \times n$  matrix group is called decomposable, if it is geometrically equivalent to a group of integral matrices of (common) block diagonal form  $\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$  where the  $A_i$  are  $n_i \times n_i$  matrices with  $n_i < n$ . Each group  $\mathcal{H}$  of integral  $n \times n$  matrices is geometrically equivalent to a group of integral matrices of

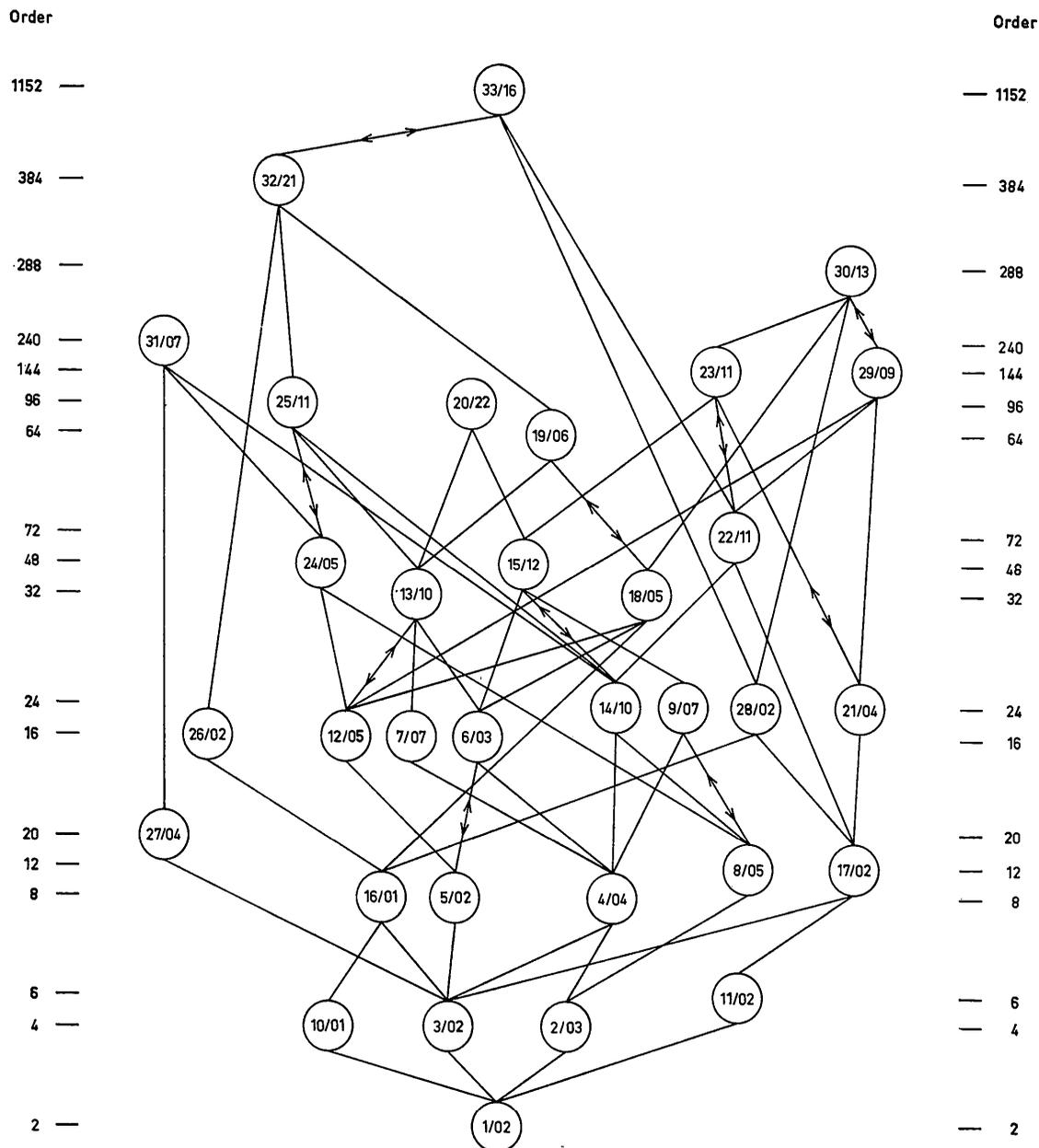


Fig. 1. Diagram of the relations between the holohedries. Each holohedry **A** is connected by lines with all other holohedries, which are of lower symmetry than **A** and are maximal in **A**.

block diagonal form  $\begin{pmatrix} A_1 & & 0 \\ & \ddots & \\ 0 & & A_k \end{pmatrix}$  where the  $A_i$  are  $n_i \times n_i$  matrices and where for each  $i$  the group of the  $A_i$  is not decomposable. If we impose the condition  $n_1 \geq \dots \geq n_k$  the  $n_i$  are uniquely determined by  $\mathcal{H}$ .  $(n_1, \dots, n_k)$  is called the decomposition type of  $\mathcal{H}$ . Clearly all groups of a geometric crystal class have the same decomposition type, which may therefore be assigned to the class.\*

The holohedries of  $R_4$  have the following decomposition types:

- (1,1,1,1): 01/02; 02/03; 03/02; 04/04; 05/02; 06/03;
- (2,1,1): 07/07; 08/05; 09/07; 12/05; 13/10; 14/10; 15/12;
- (2,2): 10/01; 11/02; 16/01; 17/02; 18/05; 19/06; 20/22; 21/04; 22/11; 23/11;
- (3,1): 24/05; 25/11;
- (4): 26/02; 27/04; 28/02; 29/09; 30/13; 31/07; 32/21; 33/16.

**2. The Bravais types and crystal families**

The concept of 'centrings' is familiar to crystallographers from  $R_2$  and  $R_3$ . It is also useful in  $R_4$ .

Here it suffices to explain this process as follows: from a Bravais type  $\mathbf{B}$  a lattice  $L$  and a lattice basis  $\mathbf{B}$  are chosen. Then a new basis  $\mathbf{B}'$  of the vector space is formed, such that all vectors of  $\mathbf{B}$  are linear combinations with integral coefficients† of the vectors of  $\mathbf{B}'$ . Let  $L'$  be the lattice consisting of all integral linear combinations of the vectors of  $\mathbf{B}'$  and let  $\mathbf{B}'$  be the Bravais type of  $L'$ . Then, if  $\mathbf{B}$  and  $\mathbf{B}'$  belong to the same family, we say that:

- (i)  $L'$  is obtained by centring from  $L$ ,
- (ii)  $\mathbf{B}'$  is obtained by centring from  $\mathbf{B}$ .

All Bravais types of the same family can be obtained from each other by the process of centring. If one restricts to centrings that do not change the 'point symmetry of the lattice', one obtains the Bravais types belonging to the same crystal system. This latter construction method has been used by Mackay & Pawley (1963).

In Table 2 are shown the different types of centrings which are used in the table (Table 3) of the Bravais types which follows. Of these  $I$ ,  $F$ , and  $R$  are known from  $R_3$ , for which  $S$  occurs in the form  $A$ ,  $B$  or  $C$ . In

\* If we restrict to arithmetic equivalence some decomposition into block-diagonal form may be obtained, that cannot be further decomposed. However, in contrast to the situation above the degrees  $n_i$  of the blocks thus obtained are no longer always an invariant of the arithmetic class (cf. Reiner, 1962).

† In crystallography the set of all linear combinations  $\sum_{i=1}^n x_i \mathbf{b}_i$  with  $0 \leq x_i < 1$ ,  $\mathbf{b}_i \in \mathbf{B}$  is called the cell of  $L$  with respect to  $\mathbf{B}$ . Those of these linear combinations which belong to  $L'$  are called centring points.

$R_4$  central centring of the cell belonging to  $\mathbf{B}$  is called  $Z$ . Simultaneous  $S$ -centring of two 2-dimensional faces of the cell intersecting in the origin only is denoted by  $D$ , centring of all 2-dimensional faces by  $U$ . The geometric description of the other types of centring is a little more complicated.

Table 2. Types of centring

The 'types of centring' are denoted by  $P, S, I, Z, R, RR, D, F, G, RS, KG, U, KU$  and  $SN$ . These are abbreviations of the German names of the corresponding centring types, e.g. seitenflächenzentriert.

If necessary, the numbers of those basis vectors (of the lattice to be centred) which play a distinguished role for the centring are given in ( , ), e.g.  $S(3, 4)$  means, that the  $c$ - $d$  face of the cell is centred.  $\mathbf{a}_i'$  are the chosen basis vectors of the centred lattice given as linear combinations of the basis vectors  $\mathbf{a}_i$  of the original lattice.  $\det$ =determinant of the transformation  $\mathbf{a}_i \rightarrow \mathbf{a}_i'$ ;  $N$ = $1/\det$  is the number of centring points. The coefficients (coordinates) of these centring points with respect to the basis of the original lattice are given explicitly, except for the  $SN$ -centring.

$S$ (seitenflächenzentriert)		
$S(3, 4)$		
$\mathbf{a}' = \mathbf{a}$	$\mathbf{b}$	$\det = \frac{1}{2}; N = 2$
$\mathbf{b}' =$	$\frac{1}{2}(\mathbf{c} - \mathbf{d})$	$0000; 00\frac{1}{2}\frac{1}{2}$
$\mathbf{c}' =$	$\frac{1}{2}(\mathbf{c} + \mathbf{d})$	
$\mathbf{d}' =$		
$S(2, 3)$		
$\mathbf{a}' = \mathbf{a}$	$\mathbf{b}$	$\det = \frac{1}{2}; N = 2$
$\mathbf{b}' =$	$\frac{1}{2}(\mathbf{b} - \mathbf{c})$	$0000; 0\frac{1}{2}\frac{1}{2}0$
$\mathbf{c}' =$	$\frac{1}{2}(\mathbf{b} + \mathbf{c})$	
$\mathbf{d}' =$	$\mathbf{d}$	
$S(1, 2)$		
$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$	$\mathbf{c}$	$\det = \frac{1}{2}; N = 2$
$\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$		$0000; \frac{1}{2}\frac{1}{2}00$
$\mathbf{c}' =$		
$\mathbf{d}' =$	$\mathbf{d}$	
<hr/>		
$I$ (innenzentriert)		
$I(2, 3, 4)$		
$\mathbf{a}' = \mathbf{a}$	$\mathbf{b}$	$\det = \frac{1}{2}; N = 2$
$\mathbf{b}' = \frac{1}{2}(-\mathbf{b} + \mathbf{c} + \mathbf{d})$		$0000; 0\frac{1}{2}\frac{1}{2}\frac{1}{2}$
$\mathbf{c}' = \frac{1}{2}(\mathbf{b} - \mathbf{c} + \mathbf{d})$		
$\mathbf{d}' = \frac{1}{2}(\mathbf{b} + \mathbf{c} - \mathbf{d})$		
<hr/>		
$Z$ (zentralzentriert)		
$Z$		
$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c} - \mathbf{d})$		$\det = \frac{1}{2}; N = 2$
$\mathbf{b}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c} - \mathbf{d})$		$0000; \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$
$\mathbf{c}' = \frac{1}{2}(-\mathbf{a} - \mathbf{b} + \mathbf{c} - \mathbf{d})$		
$\mathbf{d}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c} + \mathbf{d})$		
<hr/>		
$R$ (rhomboedrisch zentriert)		
$R(1, 2, 3)$		
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b} + \mathbf{c})$	$\mathbf{d}$	$\det = \frac{1}{3}; N = 3$
$\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$		$0000; \frac{2}{3}\frac{1}{3}\frac{1}{3}0; \frac{1}{3}\frac{2}{3}\frac{2}{3}0$
$\mathbf{c}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$		
$\mathbf{d}' =$		
<hr/>		
$RR$ (rhomboedrisch-rhomboedrisch-zentriert)		
$RR$		
$\mathbf{a}' = \frac{1}{3}(\mathbf{a} - \mathbf{b} + \mathbf{c} + 2\mathbf{d})$		$\det = \frac{1}{3}; N = 3$
$\mathbf{b}' = \frac{1}{3}(-2\mathbf{a} - \mathbf{b} + \mathbf{c} + 2\mathbf{d})$		$0000; \frac{1}{3}\frac{1}{3}\frac{1}{3}\frac{1}{3}; \frac{2}{3}\frac{2}{3}\frac{2}{3}\frac{2}{3}$
$\mathbf{c}' = \frac{1}{3}(\mathbf{a} + 2\mathbf{b} - 2\mathbf{c} - \mathbf{d})$		
$\mathbf{d}' = \frac{1}{3}(\mathbf{a} + 2\mathbf{b} + \mathbf{c} - \mathbf{d})$		

Table 2 (cont.)

*D* (doppelt seitenflächenzentriert)  
*D*(1, 4) (2, 3)  
 $a' = \frac{1}{2}(a - d)$   
 $b' = \frac{1}{2}(b - c)$   
 $c' = \frac{1}{2}(b + c)$   
 $d' = \frac{1}{2}(a + d)$

det =  $\frac{1}{4}$ ;  $N = 4$   
 0000;  $\frac{1}{2}00\frac{1}{2}$ ;  $0\frac{1}{2}\frac{1}{2}0$ ;  $\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$

*F* (flächenzentriert)  
*F*(2, 3, 4)  
 $a' = a$   
 $b' = \frac{1}{2}(c + d)$   
 $c' = \frac{1}{2}(b + d)$   
 $d' = \frac{1}{2}(b + c)$

det =  $\frac{1}{4}$ ;  $N = 4$   
 0000;  $00\frac{1}{2}\frac{1}{2}$ ;  $0\frac{1}{2}0\frac{1}{2}$ ;  $0\frac{1}{2}\frac{1}{2}0$

*G* (gemischt zentriert (*S*, *I*)) [Combination of an *S*- and two *I*-centrings. (, ) refers to *S*-centring involved]  
*G*(1, 2)  
 $a' = \frac{1}{2}(a + c + d)$   
 $b' = \frac{1}{2}(b + c + d)$   
 $c' = c$   
 $d' = d$

det =  $\frac{1}{4}$ ;  $N = 4$   
 0000;  $\frac{1}{2}0\frac{1}{2}\frac{1}{2}$ ;  $0\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ;  $\frac{1}{2}\frac{1}{2}00$

*RS* (rhomboedrisch-seitenflächenzentriert)  
*RS*(1, 2, 3) (3, 4)  
 $a' = \frac{1}{2}(2a + b + c)$   
 $b' = \frac{1}{2}(-a + b + c)$   
 $c' = \frac{1}{2}(-a - 2b + c)$   
 $d' = \frac{1}{2}(c + d)$

det =  $\frac{1}{8}$ ;  $N = 6$   
 0000;  $\frac{3}{4}\frac{1}{4}0$ ;  $\frac{1}{4}\frac{3}{4}0$   
 $00\frac{1}{2}\frac{1}{2}$ ;  $\frac{3}{8}\frac{5}{8}\frac{1}{2}$ ;  $\frac{1}{8}\frac{7}{8}\frac{1}{2}$

Table 2 (cont.)

*KG* (kombiniert gemischt zentriert) [Derived from *G*-centring; (, ) refers to *S*-centring involved]  
*KG*(1, 2)  
 $a' = \frac{1}{4}(a + b + 2d)$   
 $b' = \frac{1}{4}(a - b + 2c)$   
 $c' = \frac{1}{4}(a + b - 2d)$   
 $d' = \frac{1}{4}(a - b - 2c)$

det =  $\frac{1}{8}$ ;  $N = 8$   
 0000;  $\frac{1}{4}0\frac{1}{4}\frac{1}{4}$ ;  $0\frac{1}{4}\frac{1}{4}\frac{1}{4}$ ;  $\frac{1}{4}\frac{1}{4}00$   
 $\frac{1}{4}\frac{1}{4}0\frac{1}{4}$ ;  $\frac{3}{4}\frac{1}{4}0$ ;  $\frac{1}{4}\frac{3}{4}0$ ;  $\frac{3}{4}\frac{3}{4}0\frac{1}{4}$

*U* (überall seitenflächenzentriert)  
*U*  
 $a' = \frac{1}{2}(a - b)$   
 $b' = \frac{1}{2}(b - c)$   
 $c' = \frac{1}{2}(c + d)$   
 $d' = \frac{1}{2}(-a + d)$

det =  $\frac{1}{8}$ ;  $N = 8$   
 0000;  $\frac{1}{2}\frac{1}{2}00$ ;  $\frac{1}{2}0\frac{1}{2}0$ ;  $\frac{1}{2}00\frac{1}{2}$   
 $0\frac{1}{2}\frac{1}{2}0$ ;  $0\frac{1}{2}0\frac{1}{2}$ ;  $00\frac{1}{2}\frac{1}{2}$ ;  $\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$

*KU* (kombiniert überall seitenflächenzentriert)  
*KU*  
 $a' = \frac{1}{4}(a + b - c - d)$   
 $b' = \frac{1}{4}(a - b - c - d)$   
 $c' = \frac{1}{4}(a - b - c + d)$   
 $d' = \frac{1}{4}(a + b + c + d)$

det =  $\frac{1}{16}$ ;  $N = 16$   
 0000;  $\frac{1}{4}\frac{1}{4}00$ ;  $\frac{1}{4}0\frac{1}{4}0$ ;  $\frac{1}{4}00\frac{1}{4}$   
 $0\frac{1}{4}\frac{1}{4}0$ ;  $0\frac{1}{4}0\frac{1}{4}$ ;  $00\frac{1}{4}\frac{1}{4}$ ;  $\frac{1}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4}$   
 $\frac{1}{4}\frac{1}{4}\frac{1}{4}\frac{1}{4}$ ;  $\frac{3}{4}\frac{3}{4}\frac{1}{4}\frac{1}{4}$ ;  $\frac{1}{4}\frac{3}{4}\frac{3}{4}\frac{1}{4}$ ;  $\frac{3}{4}\frac{1}{4}\frac{3}{4}\frac{1}{4}$   
 $\frac{3}{4}\frac{3}{4}\frac{1}{4}\frac{1}{4}$ ;  $\frac{1}{4}\frac{3}{4}\frac{1}{4}\frac{3}{4}$ ;  $\frac{1}{4}\frac{1}{4}\frac{3}{4}\frac{3}{4}$ ;  $\frac{3}{4}\frac{1}{4}\frac{1}{4}\frac{3}{4}$

*SN* (seitenflächen-nebendiagonal zentriert)  
*SN*  
 $a' = \frac{1}{3}(-a - b - c - 2d)$   
 $b' = \frac{1}{3}(-a - b - 2c - d)$   
 $c' = \frac{1}{3}(-a - 2b - c - d)$   
 $d' = \frac{1}{3}(-2a - b - c - d)$

det =  $\frac{1}{125}$ ;  $N = 125$   
 0000;  $\frac{1}{5}\frac{1}{5}\frac{1}{5}$ ;  $\frac{1}{5}\frac{1}{5}\frac{1}{5}$   
 $\frac{1}{5}\frac{1}{5}\frac{1}{5}$ ;  $\frac{2}{5}\frac{2}{5}\frac{1}{5}$ ;  $\frac{1}{5}\frac{2}{5}\frac{2}{5}$   
 $\frac{2}{5}\frac{1}{5}\frac{2}{5}$ ;  $\frac{2}{5}\frac{2}{5}\frac{2}{5}$ ; *etc.*

Table 3. List of the Bravais types of  $R_4$ 

The listing of the Bravais types is given in the following way:

First heading: (Roman) number of family (*e.g.* Family III), name of family (*e.g.* diclinic), number of free parameters (*e.g.* 6 parameters).

Second heading: (Arabic) number of system (*e.g.* system 3), number of holohedral crystal class of this system (holohedry 3/02, *cf.* Table 1), order of this crystal class (*e.g.* order 4), Hurley's (1951) characteristics of this class (*e.g.*  $I + I' + 2E$ ), generators for a representative group in a notation referring to Table 4 (*e.g.* Generators  $I'$ ,  $E_1$ ).

Third heading: Bravais type: number within its family and number running from 1 to 64 (*e.g.* Bravais type III/3 = 6); Belov & Kuntsevich's (1969) number (*e.g.* B.K. No. 3.2) and Mackay & Pawley's (1963) number (*e.g.* M.P. No. 3.2) '–' means: missing in the corresponding list; type of centring (*e.g.*  $D(1, 4)$  (2, 3)-centred, *cf.* Table 2). Matrix of the scalar products of the chosen basis vectors ('metric tensor'); the letters in the matrix (*e.g.*  $A$ ,  $B$ ,  $C$ ,  $D$ ,  $E$ ,  $F$ ) denote parameters which may be chosen freely within certain restrictions (caused by the positive definiteness of the matrix).

FAMILY I, hexaclinic, 10 parameters

System 1, holohedry 1/02, order 2.  $I + I'$ . Generators:  $I'$

Bravais type I/1 = 1	primitive	<i>A</i>	<i>E</i>	<i>F</i>	<i>G</i>
B.K. No. 1	<i>P</i>		<i>B</i>	<i>H</i>	<i>J</i>
M.P. No. 1				<i>C</i>	<i>K</i>
					<i>D</i>

FAMILY II, triclinic, 7 parameters

System 2, holohedry 2/03, order 4.  $I + I' + T + T'$ . Generators  $I'$ ,  $T_1$

Bravais type II/1 = 2	primitive	<i>A</i>	<i>E</i>	<i>F</i>	0
B.K. No. 2.0	<i>P</i>		<i>B</i>	<i>G</i>	0
M.P. No. 2				<i>C</i>	0
					<i>D</i>
Bravais type II/2 = 3	$S(3, 4)$ -centred	<i>A</i>	<i>D</i>	<i>E</i>	<i>E</i>
B.K. No. 2.1			<i>B</i>	<i>F</i>	<i>F</i>
M.P. No. 2.1				<i>C</i>	<i>G</i>
					<i>C</i>

FAMILY III, diclinic, 6 parameters

System 3, holohedry 3/02, order 4.  $I + I' + 2E$ . Generators  $I'$ ,  $E_1$

Bravais type III/1 = 4	primitive	<i>A</i>	<i>E</i>	0	0
B.K. No. 3.0	<i>P</i>		<i>B</i>	0	0
M.P. No. 3				<i>C</i>	<i>F</i>
					<i>D</i>
Bravais type III/2 = 5	$S(2, 3)$ -centred	<i>A</i>	<i>D</i>	<i>D</i>	0
B.K. No. 3.1			<i>B</i>	<i>E</i>	<i>F</i>
M.P. No. 3.1				<i>B</i>	– <i>F</i>
					<i>C</i>

Table 3 (cont.)

Bravais type III/3=6 B.K. No. 3.2 M.P. No. 3.2	$D(1, 4) (2, 3)$ -centred	$A$	$C$ $B$	$D$ $F$ $B$	$E$ $D$ $C$ $A$
FAMILY IV, monoclinic, 5 parameters					
System 4, holohedry 4/04, order 8. $I+I'+2E+2T+2T'$ . Generators $I', E_1, T_1$					
Bravais type IV/1=7 B.K. No. 4.0 M.P. No. 4	primitive	$A$	$E$ $B$	0 0 $C$	0 0 0 $D$
Bravais type IV/2=8 B.K. No. 4.1 M.P. No. 4.1	$S(3, 4)$ -centred	$A$	$D$ $B$	0 0 $C$	0 0 $E$ $C$
Bravais type IV/3=9 B.K. No. 4.2 M.P. No. 4.2	$S(2, 3)$ -centred	$A$	$D$ $B$	$D$ $E$ $B$	0 0 0 $C$
Bravais type IV/4=10 B.K. No. 4.4 M.P. No. 4.3	$I(2, 3, 4)$ -centred	$A$	$C$ $B$	$-C$ $D$ $B$	$-C$ $E$ $-(B+D+E)$ $B$
Bravais type IV/5=11 B.K. No. 4.5 M.P. No. -	$D(1, 4) (2, 3)$ -centred	$A$	$C$ $B$	$C$ $E$ $B$	$D$ $C$ $C$ $A$
Bravais type IV/6=12 B.K. No. 4.3 M.P. No. 4.4	$F(2, 3, 4)$ -centred	$A$	0 $B$	$E$ $\frac{1}{2}(B+C-D)$ $C$	$E$ $\frac{1}{2}(B-C+D)$ $\frac{1}{2}(C-B+D)$ $D$
FAMILY V, orthogonal, 4 parameters					
System 5, holohedry 5/02, order 8. $I+I'+6E$ . Generators $I', E_3, E_6$					
Bravais type V/1=13 B.K. No. - M.P. No. -	$KU$ -centred	$A$	$B$ $A$	$C$ $D$ $A$	$D$ $C$ $B$ $A$
System 6, holohedry 6/03, order 16. $I+I'+6E+4T+4T'$ . Generators $I', E_1, T_1, T_6$					
Bravais type V/2=14 B.K. No. 5.0 M.P. No. 7	primitive	$A$	0 $B$	0 0 $C$	0 0 0 $D$
Bravais type V/3=15 B.K. No. 5.1 M.P. No. 7.1	$S(3, 4)$ -centred	$A$	0 $B$	0 0 $C$	0 0 $D$ $C$
Bravais type V/4=16 B.K. No. 5.2 M.P. No. 7.2	$I(2, 3, 4)$ -centred	$A$	0 $B$	0 $C$ $B$	0 $D$ $-(B+C+D)$ $B$
Bravais type V/5=17 B.K. No. 5.3 M.P. No. 7.3	$Z$ -centred	$A$	$B$ $A$	$C$ $(A-B+C)$ $A$	$D$ $(B+D-A)$ $(C+D-A)$ $A$
Bravais type V/6=18 B.K. No. 5.5 M.P. No. 7.6	$D(1, 4) (2, 3)$ -centred	$A$	0 $B$	0 $D$ $B$	$C$ 0 0 $A$
Bravais type V/7=19 B.K. No. 5.4 M.P. No. 7.4	$F(2, 3, 4)$ -centred	$A$	0 $B$	0 $\frac{1}{2}(B+C-D)$ $C$	0 $\frac{1}{2}(B-C+D)$ $\frac{1}{2}(C-B+D)$ $D$
Bravais type V/8=20 B.K. No. 5.6 M.P. No. 7.5	$G(1, 2)$ -centred	$A$	$\frac{1}{2}(C+D)$ $B$	$C/2$ $C/2$ $C$	$D/2$ $D/2$ 0 $D$

Table 3 (cont.)

Bravais type V/9=21	<i>U</i> -centred	<i>A</i>	<i>D</i>	0	$-(A+D)$
B.K. No. 5.7			<i>B</i>	$-(B+D)$	0
M.P. No. 7.7				<i>C</i>	$C-B-D$
					$A-B+C$
FAMILY VI, tetragonal monoclinic, 4 parameters					
<i>System 7</i> , holohedry 7/07, order 16. $I+I'+2E+2R+2R'+4T+4T'$ . Generators $I', R_1, T_1$					
Bravais type VI/1=22	primitive	<i>A</i>	<i>D</i>	0	0
B.K. No. 6.0	<i>P</i>		<i>B</i>	0	0
M.P. No. 6				<i>C</i>	0
					<i>C</i>
Bravais type VI/2=23	$I(2, 3, 4)$ -centred	<i>A</i>	<i>C</i>	$-C$	$-C$
B.K. No. 6.1			<i>B</i>	<i>D</i>	<i>D</i>
M.P. No. 6.1				<i>B</i>	$-(B+2D)$
					<i>B</i>
FAMILY VII, hexagonal monoclinic, 4 parameters					
<i>System 8</i> , holohedry 8/05, order 12. $I+I'+2K+2K'+3T+3T'$ . Generators $I', K_1, T_{14}$					
Bravais type VII/1=24	$R(1, 2, 3)$ -centred	<i>A</i>	<i>C</i>	<i>C</i>	<i>D</i>
B.K. No. 10	(rhombohedral)		<i>A</i>	<i>C</i>	<i>D</i>
M.P. No. -				<i>A</i>	<i>D</i>
					<i>B</i>
<i>System 9</i> , holohedry 9/07, order 24. $I+I'+2E+2K+2K'+6T+6T'+2Z+2Z'$ . Generators $I', Z, T_{14}$					
Bravais type VII/2=25	primitive	<i>A</i>	$-A/2$	0	0
B.K. No. 9	<i>P</i>		<i>A</i>	0	0
M.P. No.5				<i>B</i>	<i>D</i>
					<i>C</i>
FAMILY VIII, ditetragonal diclinic, 4 parameters					
<i>System 10</i> , holohedry 10/01, order 4. $I+I'+2D$ . Generators $D_1$					
Bravais type VIII/1=26	primitive	<i>A</i>	0	<i>C</i>	<i>D</i>
B.K. No. 17	<i>P</i>		<i>A</i>	$-D$	<i>C</i>
M.P. No. -				<i>B</i>	0
					<i>B</i>
FAMILY IX, dihexagonal diclinic, 4 parameters					
<i>System 11</i> , holohedry 11/02, order 6. $I+I'+2S+2S'$ . Generators $S_1$					
Bravais type IX/1=27	primitive	<i>A</i>	$-A/2$	<i>C</i>	<i>D</i>
B.K. No. 18	<i>P</i>		<i>A</i>	<i>D</i>	$-(C+D)$
M.P. No. -				<i>B</i>	$-B/2$
					<i>B</i>
FAMILY X, tetragonal orthogonal, 3 parameters					
<i>System 12</i> , holohedry 12/05, order 16. $I+I'+6E+4F+2T+2T'$ . Generators $I', F_1, T_{15}$					
Bravais type X/1=28	$KG(1, 2)$ -centred	<i>A</i>	<i>B</i>	<i>C</i>	<i>B</i>
B.K. No. 8			<i>A</i>	<i>B</i>	<i>C</i>
M.P. No. -				<i>A</i>	<i>B</i>
					<i>A</i>
<i>System 13</i> , holohedry 13/10, order 32. $I+I'+10E+2R+2R'+4F+6T+6T'$ . Generators $I', R_1, T_1, T_6$					
Bravais type X/2=29	primitive	<i>A</i>	0	0	0
B.K. No. 7.0	<i>P</i>		<i>B</i>	0	0
M.P. No. 10				<i>C</i>	0
					<i>C</i>
Bravais type X/3=30	$S(1, 2)$ -centred	<i>A</i>	<i>C</i>	0	0
B.K. No. 7.1			<i>A</i>	0	0
M.P. No. 10.1				<i>B</i>	0
					<i>B</i>
Bravais type X/4=31	$I(2, 3, 4)$ -centred	<i>A</i>	0	0	0
B.K. No. 7.2			<i>B</i>	<i>C</i>	<i>C</i>
M.P. No. 10.2				<i>B</i>	$-(B+2C)$
					<i>B</i>
Bravais type X/5=32	<i>Z</i> -centred	<i>A</i>	<i>B</i>	<i>C</i>	$\frac{1}{2}(A-C)$
B.K. No. 7.4			<i>A</i>	$(A-B+C)$	$\frac{1}{2}(2B-A-C)$
M.P. No. 10.3				<i>A</i>	$\frac{1}{2}(C-A)$
					<i>A</i>
Bravais type X/6=33	$G(1, 2)$ -centred	<i>A</i>	$C/2$	$C/2$	$C/2$
B.K. No. 7.3			<i>B</i>	$C/2$	$C/2$
M.P. No. 10.4				<i>C</i>	0
					<i>C</i>

Table 3 (cont.)

## FAMILY XI, hexagonal orthogonal, 3 parameters

*System 14*, holohedry 14/10, order 24.  $I+I'+6E+2K+2K'+2N+2N'+4T+4T'$ . Generators  $I', K_1, T_{14}, T_1$   
(rhombohedral orthogonal)

Bravais type XI/1=34	$R(1, 2, 3)$ -centred	$A$	$C$	$C$	0
B.K. No. 12.0			$A$	$C$	0
M.P. No. 9				$A$	0
					$B$
Bravais type XI/2=35	$RS(1, 2, 3)$ (3, 4)-centred	$A$	$C$	$C$	$\frac{1}{2}(A+2C)$
B.K. No. 12.1			$A$	$C$	$\frac{1}{2}(A+2C)$
M.P. No. 9.1				$A$	$\frac{1}{2}(A+2C)$
					$B$

*System 15*, holohedry 15/12, order 48.  $I+I'+14E+2K+2K'+4N+4N'+8T+8T'+2Z+2Z'$ . Generators  $I', Z, T_{14}, T_1$

Bravais type XI/3=36	primitive	$A$	$-A/2$	0	0
B.K. No. 11.0	$P$		$A$	0	0
M.P. No. 11				$B$	0
					$C$
Bravais type XI/4=37	$S(3, 4)$ -centred	$A$	$-A/2$	0	0
B.K. No. 11.1			$A$	0	0
M.P. No. 11.1				$B$	$C$
					$B$

## FAMILY XII, ditetragonal monoclinic, 3 parameters

*System 16*, holohedry 16/01, order 8.  $I+I'+2D+4E$ . Generators  $D_1, E_6$

Bravais type XII/1=38	primitive	$A$	0	$C$	0
B.K. No. 19.0	$P$		$A$	0	$C$
M.P. No. 8				$B$	0
					$B$
Bravais type XII/2=39	$S(3, 4)$ -centred	$A$	0	$C$	$C$
B.K. No. 19.1			$A$	$-C$	$C$
M.P. No. 8.1				$B$	0
					$B$
Bravais type XII/3=40	$D(1, 4)$ (2, 3)-centred	$A$	$B$	0	$C$
B.K. No. 19.2			$A$	$C$	0
M.P. No. 8.2				$A$	$-B$
					$A$

## FAMILY XIII, dihexagonal monoclinic, 3 parameters

*System 17*, holohedry 17/02, order 12.  $I+I'+6E+2S+2S'$ . Generators  $S_1, E_6$

Bravais type XIII/1=41	primitive	$A$	$-A/2$	$C$	$-2C$
B.K. No. 20	$P$		$A$	$-2C$	$C$
M.P. No. -				$B$	$-B/2$
					$B$
Bravais type XIII/2=42	$RR$ -centred	$A$	$C$	$-B/2$	$-A/2$
B.K. No. -			$B$	$-B/2$	$-B/2$
M.P. No. -				$B$	$(B/2-C)$
					$A$

## FAMILY XIV, ditetragonal orthogonal, 2 parameters

*System 18*, holohedry 18/05, order 32.  $I+I'+4D+10E+8F+4T+4T'$ . Generators  $D_2, E_6, F_2$

Bravais type XIV/1=43	$D(1, 4)$ (2, 3)-centred	$A$	0	0	$B$
B.K. No. -			$A$	$B$	0
M.P. No. -				$A$	0
					$A$

*System 19*, holohedry 19/06, order 64.  $I+I'+4D+18E+16F+4R+4R'+8T+8T'$ . Generators  $R_1, D_1, T_1, T_6$

Bravais type XIV/2=44	primitive	$A$	0	0	0
B.K. No. 21.0	$P$		$A$	0	0
M.P. No. 14				$B$	0
					$B$
Bravais type XIV/3=45	$Z$ -centred	$A$	$B$	$(2B-A)$	$(A-B)$
B.K. No. 21.1			$A$	$B$	0
M.P. No. 14.1				$A$	$(B-A)$
					$A$

## FAMILY XV, hexagonal tetragonal, 2 parameters

*System 20*, holohedry 20/22, order 96.  $I+I'+26E+12F+2K+2K'+4M+4M'+8N+8N'+2R+2R'+10T+10T'+2Z+2Z'$   
Generators  $Z, R_1, T_{14}, T_1$

Bravais type XV/1=46	primitive	$A$	$-A/2$	0	0
B.K. No. 15	$P$		$A$	0	0
M.P. No. 13				$B$	0
					$B$

Table 3 (cont.)

## FAMILY XVI, dihexagonal orthogonal, 2 parameters

System 21, holohedry 21/04, order 24.  $I+I'+4B+14E+2S+2S'$ . Generators  $S_1, E_6, E_3$ 

Bravais type XVI/1=47	$D(1, 4)$ (2, 3)-centred	$A$	$-A/2$	$B$	$-2B$
B.K. No. -			$A$	$-2B$	$B$
M.P. No. -				$A$	$-A/2$
					$A$

System 22, holohedry 22/11, order 72.  $I+I'+18E+4K+4K'+12N+12N'+4S+4S'+6T+6T'$ . Generators  $S_2, S_3, E_{11}, T_{19}$ 

Bravais type XVI/2=48	$RR$ -centred	$A$	$B$	$-A/2$	$-A/2$
B.K. No. -			$A$	$-A/2$	$-A/2$
M.P. No. -				$A$	$\frac{1}{2}(A-2B)$
					$A$

System 23, holohedry 23/11, order 144.  $I+I'+8B+38E+4K+4K'+24N+24N'+4S+4S'+12T+12T'+4Z+4Z'$ . Generators  $S_1, Z, T_2, T_{14}$ 

Bravais type XVI/3=49	primitive	$A$	$-A/2$	0	0
B.K. No. 16	$P$		$A$	0	0
M.P. No. 15				$B$	$-B/2$
					$B$

## FAMILY XVII, cubic orthogonal, 2 parameters

System 24, holohedry 24/05, order 48.  $I+I'+6E+12F+8K+8K'+6T+6T'$ . Generators  $I', F_1, F_2$ 

Bravais type XVII/1=50	$KU$ -centred	$A$	$B$	$B$	$B$
B.K. No. 14			$A$	$B$	$B$
M.P. No. 16				$A$	$B$
					$A$

System 25, holohedry 25/11, order 96.  $I+I'+18E+12F+8K+8K'+8N+8N'+6R+6R'+10T+10T'$ . Generators  $I', T_1, T_2, E_2$ 

Bravais type XVII/2=51	primitive	$A$	0	0	0
B.K. No. 13.0	$P$		$B$	0	0
M.P. No. 12				$B$	0
					$B$
Bravais type XVII/3=52	$I(2, 3, 4)$ -centred	$A$	0	0	0
B.K. No. 13.1			$B$	$-B/3$	$-B/3$
M.P. No. 12.1				$B$	$-B/3$
					$B$
Bravais type XVII/4=53	$Z$ -centred	$A$	$B$	$\frac{1}{3}(2B-A)$	$\frac{1}{3}(2A-B)$
B.K. No. 13.2			$A$	$\frac{1}{3}(2A-B)$	$\frac{1}{3}(2B-A)$
M.P. No. 12.2				$A$	$\frac{1}{3}(B-2A)$
					$A$
Bravais type XVII/5=54	$F(2, 3, 4)$ -centred	$A$	0	0	0
B.K. No. 13.3			$B$	$B/2$	$B/2$
M.P. No. 12.3				$B$	$B/2$
					$B$
Bravais type XVII/6=55	$U$ -centred	$A$	$-B/2$	0	$\frac{1}{2}(B-2A)$
B.K. No. 13.4			$B$	$-B/2$	0
M.P. No. 12.4				$B$	$B/2$
					$A$

## FAMILY XVIII, octagonal, 2 parameters

System 26, holohedry 26/02, order 16.  $I+I'+4A+2D+8E$ . Generators  $A_1, E_3$ 

Bravais type XVIII/1=56	primitive	$A$	0	$B$	$B$
B.K. No. -	$P$		$A$	$-B$	$B$
M.P. No. -				$A$	0
					$A$

## FAMILY XIX, decagonal, 2 parameters

System 27, holohedry 27/04, order 20.  $I+I'+10E+4L+4L'$ . Generators  $L_1, E_3$ 

Bravais type XIX/1=57	primitive	$A$	$B$	$-\frac{1}{2}(A+2B)$	$-\frac{1}{2}(A+2B)$
B.K. No. -	$P$		$A$	$B$	$-\frac{1}{2}(A+2B)$
M.P. No. -				$A$	$B$
					$A$

## FAMILY XX, dodecagonal, 2 parameters

System 28, holohedry 28/02, order 24.  $I+I'+4C+2D+12E+2S+2S'$ . Generators  $C_1, E_{14}$ 

Bravais type XX/1=58	primitive	$A$	$-A/2$	0	$B$
B.K. No. 24 (their holohedry is incorrect)	$P$		$A$	$B$	$-B$
M.P. No. 17				$A$	$-A/2$
					$A$

Table 3 (cont.)

## FAMILY XXI, di-isohexagonal orthogonal, 1 parameter

System 29, holohedry 29/09, order 144.  $I+I'+24B+30E+36F+4K+4K'+12N+12N'+4S+4S'+6T+6T'$ . Generators  $S_2, S_3, T_{19}, E_3$

Bravais type XXI/1=59	RR-centred	A	A/4	-A/2	-A/2
B.K. No. -			A	-A/2	-A/2
M.P. No. -				A	A/4
					A

System 30, holohedry 30/13, order 288.  $I+I'+32B+24C+12D+50E+72F+4K+4K'+24N+24N'+4S+4S'+12T+12T'+4Z+4Z'$ . Generators  $Z, T_{14}, E_{14}$

Bravais type XXI/2=60	primitive	A	-A/2	0	0
B.K. No. 25	P		A	0	0
M.P. No. 19				A	-A/2
					A

## FAMILY XXII, icosahedral, 1 parameter

System 31, holohedry 31/07, order 240.  $I+I'+30E+20K+20K'+24L+24L'+60F+20N+20N'+10T+10T'$ . Generators  $L_1, T_{14}$

Bravais type XXII/1=61	primitive	A	-A/4	-A/4	-A/4
B.K. No. 26	P		A	-A/4	-A/4
M.P. No. 21.1				A	-A/4
					A

Bravais type XXII/2=62	SN-centred	A	A/2	A/2	A/2
B.K. No. -			A	A/2	A/2
M.P. No. 21				A	A/2
					A

## FAMILY XXIII, hypercubic, 1 parameter

System 32, holohedry 32/21, order 384.  $I+I'+48A+12D+42E+96F+32K+32K'+32N+32N'+12R+12R'+16T+16T'$ . Generators  $T_1, T_2, K_1$

Bravais type XXIII/1=63	primitive	A	0	0	0
B.K. No. 22	P		A	0	0
M.P. No. 20				A	0
					A

System 33, holohedry 33/16, order 1152.  $I+I'+144A+96C+12D+90E+144F+64K+64K'+192N+192N'+36R+36R'+16S+16S'+24T+24T'$ . Generators  $T_7, K_2, T_{20}, K_{11}'$

Bravais type XXIII/2=64	Z-centred	A	A/2	0	A/2
B.K. No. 23			A	A/2	0
M.P. No. 18 and 20.1				A	-A/2
					A

The 64 Bravais types have been assigned to the 33 crystal systems as well as to the 23 crystal families.

The families are ordered by some invariants which can be assigned to them. For this purpose we refer back to the space  $\Omega(\mathcal{H})$  of symmetric matrices defined in II for any integral group  $\mathcal{H}$ . If  $\mathcal{H}$  and  $\mathcal{H}'$  are geometrically equivalent groups then  $\Omega(\mathcal{H})$  and  $\Omega(\mathcal{H}')$  have the same dimensions. Hence this dimension may be attributed to the arithmetic as well as geometric class of  $\mathcal{H}$ . Moreover, this number is the same for all arithmetic classes of a Bravais type and hence for all arithmetic and geometric classes of a family. We shall call it the number of free parameters of the Bravais type or family.

It can further be shown that all groups of all arithmetic classes of a family are of the same decomposition type, which we can, therefore, also assign to the family.

In Table 3 the crystal families are in the first place arranged according to decreasing number of free parameters varying from 10 to 1 with omission of 9 and 8. Families with equal numbers of free parameters are arranged according to their decomposition type [(1,1,1,1), (2,1,1), (2,2), (3,1), (4)] and then according to the highest of the orders of the Bravais classes in the

family. One exception has been made: family XXI has been thought to be more related to families in lower dimensions than family XXII in spite of the orders of corresponding Bravais classes.

The Bravais types are ordered within one family under special headings 'system...'. As explained in I, a Bravais type may be attributed to more than one system. Among these there is one with holohedry of highest order. In Table 3 a Bravais type is listed only under this system. The systems of the same family are arranged according to increasing order of their holohedral classes, by which, in  $R_4$ , the different crystal systems of a family can be distinguished.

The Bravais types of the same crystal system are listed according to increasing complexity, taking into consideration first of all the number of 'centring points'. We use the sequence  $P, S, I, Z, R, RR, D, F, G, RS, KG, U, KU, SN$ , in Table 3.

Combining the information of Tables 1 and 3 one notices that groups  $\mathcal{H}$  of the same order belong to a great variety of Bravais types, which even have considerably different numbers of free parameters; e.g. groups of order 8 belong to Bravais types with 5, 4, 3, 2, and 1 free parameters. The last figure is particularly

striking. It is caused by the fact that a lattice, left fixed by a group of motions isomorphic to the quaternion group of order 8, must be a hypercubic  $P$  or  $Z$  lattice. The Bravais groups of these lattices are of orders 384 and 1152 respectively. For comparison in  $R_3$  the cubic lattices have Bravais groups of order 48, but to force a lattice to be cubic needs at least the tetrahedral group of order 12.

Bravais types XV/1, XVII/3, XVII/5, XXI/1, XXI/2, XXII/1, XXII/2, XXIII/1, and XXIII/2 correspond to the 9 groups of Dade (1965), (*cf.* also Hermann, 1951.)

In  $R_4$  there are 9 Bravais types belonging to the orthogonal family; one of them is attributed only to crystal system 5. Half of the other 8 Bravais types have analogues in  $R_3$  ( $P$ ,  $S$ ,  $I$ , and  $F$ ). The other 4 ( $Z$ ,  $D$ ,  $G$ , and  $U$ ) have no analogues in spaces of lower dimensions.

For  $n=1,2,3,4$  there are  $2^{n-1}$  Bravais types with Bravais class of order  $2^n$  belonging to the orthogonal family of  $R_n$ . For general  $n$  neither a proof of this rule nor a counter-example is known to us.

The three Bravais types of family XVI, each of which determines its own crystal system, are very interesting. Here for the first time a family contains three crystal

systems, the holohedries of which are of orders 24, 72 and 144. The holohedries 21/04 and 22/11 are of lower symmetry than holohedry 23/11, but 21/04 is not of lower symmetry than 22/11.

### 3. Sphere packings in $R_4$

Sphere packing in  $R_3$  can be generalized to packings of 4-dimensional spheres. Only a few results will be given here concerning sphere packings for which the centres of the spheres form a lattice belonging to a Bravais type with one free parameter. These correspond to sphere packings  $Pm3m$ ,  $Im3m$ , and  $Fm3m$  in  $R_3$  with packing densities  $D$  of 0.52, 0.68 and 0.74 and coordination numbers (CN) of 6, 8 and 12 respectively.

There are 6 such sphere packings in  $R_4$ : XXI/1, XXI/2, XXII/1, XXII/2, XXIII/1, XXIII/2 with coordination numbers 18, 12, 10, 20, 8 and 24 respectively (*cf.* Table 5). The 'nearest neighbouring points' of the origin are given with respect to the basis  $B'$  for which the matrix of scalar products is given in Table 3:

$$\text{XXI/1} = 59: \begin{matrix} 8[1000], 2[1010], 2[1001], 2[0110], \\ 2[0101], 2[1111] \end{matrix}$$

Table 4. Matrices of generators occurring in Table 3

$$\begin{array}{llll} I' = \begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & \bar{1} \end{pmatrix} & A_1 = \begin{pmatrix} 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & \bar{1} \\ 0 & 1 & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} & C_1 = \begin{pmatrix} 0 & 0 & 1 & \bar{1} \\ 0 & 0 & 0 & \bar{1} \\ 0 & 1 & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} & D_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & \bar{1} & 0 \end{pmatrix} \\ D_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} & E_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & \bar{1} \end{pmatrix} & E_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \bar{1} \end{pmatrix} & E_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \\ E_6 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} & E_{11} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & \bar{1} & 0 \\ 0 & \bar{1} & 0 & 0 \\ 1 & 0 & 1 & 0 \end{pmatrix} & E_{14} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} & F_1 = \begin{pmatrix} 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \\ F_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} & K_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & K_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & \bar{1} & 1 & 0 \\ 1 & \bar{1} & 0 & \bar{1} \\ 0 & 0 & 0 & 1 \end{pmatrix} & K_{11}' = \begin{pmatrix} 1 & 0 & 0 & \bar{1} \\ 1 & \bar{1} & 0 & \bar{1} \\ 0 & 0 & \bar{1} & \bar{1} \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \\ L_1 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \end{pmatrix} & R_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & \bar{1} & 0 \end{pmatrix} & S_1 = \begin{pmatrix} 1 & 1 & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{1} \\ 0 & 0 & 1 & 1 \end{pmatrix} & S_2 = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 1 & 1 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \\ S_3 = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix} & T_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \bar{1} \end{pmatrix} & T_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} & T_6 = \begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ T_7 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ \bar{1} & 1 & 0 & 1 \\ \bar{1} & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} & T_{14} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & T_{15} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & T_{19} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ \bar{1} & 0 & 0 & \bar{1} \\ \bar{1} & 0 & \bar{1} & 0 \end{pmatrix} \\ T_{20} = \begin{pmatrix} 0 & 0 & \bar{1} & 0 \\ \bar{1} & 1 & \bar{1} & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & Z = \begin{pmatrix} 1 & 1 & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & & & \end{array}$$

Table 5. Coordination numbers CN, packing densities  $D$ , the quotient  $100D/CN$ , and the relative densities  $D/D_w$  ( $D_w=D_{63}$  in  $R_4$ ,  $D_w=D_P$  in  $R_3$ ,  $D_w=D_T$  in  $R_2$ ) for all lattices of  $R_4$ ,  $R_3$ , and  $R_2$  belonging to Bravais types, having one free parameter only

Bravais type	$R_4$	59	60	61	62	63	64
CN		18	12	10	20	8	24
$D$		0.55	0.41	0.44	0.55	0.31	0.62
$100D/CN$		3.06	3.42	4.40	2.75	3.88	2.58
$D/D_w$		1.77	1.32	1.42	1.77	1	2.00
Bravais type	$R_3$	cubic $P$	cubic $I$	cubic $F$	$R_2$ :	qua- dratic $T$	hex- agonal $H$
CN		6	8	12		4	6
$D$		0.52	0.68	0.74		0.785	0.907
$100D/CN$		8.67	8.50	6.17		19.6	15.1
$D/D_w$		1	1.31	1.42		1	1.16

XXI/2=60: 8[1000], 2[1100], 2[0011]  
 XXII/1=61: 8[1000], 2[1111]  
 XXII/2=62: 8[1000], 12[1 $\bar{1}$ 00]  
 XXIII/1=63: 8[1000]  
 XXIII/2=64: 8[1000], 2[1 $\bar{1}$ 00], 2[100 $\bar{1}$ ], 2[0110],  
 2[001 $\bar{1}$ ], 2[ $\bar{1}$ 101], 2[ $\bar{1}$ 10], 2[ $\bar{1}$ 011],  
 2[0 $\bar{1}$ 11].

8[1000] and 12[1 $\bar{1}$ 00]: all permutations and simultaneous sign changes in the symbols have to be performed to obtain all neighbouring points; analogously 2[1100] stands for [1100] and [ $\bar{1}\bar{1}$ 00] etc.

From Table 5 the following tendencies are seen in the material of  $R_2$ ,  $R_3$  and  $R_4$ .

- The coordination numbers (CN) increase in spaces of higher dimensions; at the same time they show an increasing variation.
- The packing density  $D$  decreases in spaces of higher dimensions; at the same time it also shows an increasing variation.
- The quotient of  $100 D/(CN)$  decreases in spaces of higher dimensions; the variation again increases.
- The value  $D/D_w$  means the density of a sphere packing compared with the density of the hypercubic  $P$ -sphere packing of this space. In  $R_2$ ,  $R_3$  and  $R_4$  this  $D_w$  is the minimal density; in  $R_4$  the densest packing based on a lattice has twice the value of  $D_w$ .
- Nothing seems to be known about the 'densest packings' of  $R_4$ . Possibly the packing based on XXIII/2=64 is one of them.
- CN and  $D$  do not always vary in the same directions; Bravais types 60 and 61 have CN=12 and 10, but  $D=0.41$  and  $0.44$  respectively.

#### 4. Black-white, colour, and other generalized symmetries

As all subgroups are known for a set of representatives of the crystal classes of  $R_4$ , the corresponding possible black-white, colour, and other generalized groups of  $R_4$  can be derived easily by inspection, using the method of Niggli & Wondratschek (1960) and Wondratschek & Niggli (1961).

Great care has been taken to avoid mistakes in the Tables of this paper. However, the authors would appreciate being informed of any errors that may be found.

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