

latter, although including anharmonic effects due to the expansion of the lattice, does not include anharmonic effects due to higher order terms in the interatomic potential (see Willis, 1969). Willis has estimated the increase in the temperature factors for KCl at 293°K, resulting from inclusion of these higher order terms, to be about 10%. The present result would therefore indicate that a similar increase occurs for nickel.

The authors are grateful to Dr L.D.Jennings for the provision of the nickel powder used in this work and for his comments.

References

BARRON, H. W. T. & SMITH, T. (1966). *J. Phys. Chem. Solids*, **27**, 1951.  
 BIRGENEAU, R. J., CORDES, J., DOLLING, G. & WOODS, A. D. B. (1964). *Phys. Rev.* **136**, A 1359.  
 CHIPMAN, D. R. & PASKIN, A. (1959). *J. Appl. Phys.* **30**, 1998.  
 INKINEN, O. & SUORTTI, P. (1964). *Ann. Acad. Scient. Fenn.* **A 6**, 147.  
 JENNINGS, L. D. (1969). *Acta Cryst.* **A25**, 217.  
 MOOK, H. A. (1966). *Phys. Rev.* **148**, 495.  
 WILLIS, B. T. M. (1969). *Acta Cryst.* **A25**, 277.

*Acta Cryst.* (1969). **A25**, 715

**Symbolism of rhombohedral space groups in Miller axes.** By J. D. H. DONNAY, *The Johns Hopkins University, Baltimore, Maryland 21218, U. S. A.*

(Received 24 February 1969)

The point symmetry of the hexagonal lattice,  $6/m\ 2/m\ 2/m$ , possesses 3 kinds of symmetry directions (*Blickrichtungen*); that of the rhombohedral lattice,  $\bar{3}\ 2/m$ , has only two. The proposed extension of the Hermann-Mauguin symbolism rests on this fact. Examples:  $P311 = P3$ ,  $P31 = R3$ . The dummy 1s stand for lattice-symmetry directions, as in the well-known symbols  $P3m1$ ,  $P31m$ , etc.

The question has been raised of the desirability of having a dual symbolism capable of representing the seven rhombohedral space groups both in the Bravais and in the Miller system of coordinate axes. At the present time *International Tables for X-ray Crystallography* use the same symbols:

$$R\bar{3}m, R\bar{3}c, R32, R3m, R3c, R\bar{3}, R3 \quad (1)$$

whether the cell used to describe the lattice is the triple ('*R* centered') hexagonal cell (*hR*) or the rhombohedral primitive cell (*rP*).

An extremely simple method of referring the space-group symbol to the *rP* cell is already available in the Hermann-Mauguin notation itself: use *P* instead of *R* as lattice letter and no confusion can result in 5 cases out of the 7 listed in (1). Indeed the symbols

$$P\bar{3}m, P\bar{3}c, P32, P3m, P3c \quad (2)$$

are new symbols, distinctly different from the hexagonal symbols

$$P\bar{3}m1, P\bar{3}1m; P\bar{3}c1, P\bar{3}1c; P321, P312; P3m1, P31m\ P3c1, P31c, \quad (3)$$

that apply to other space groups. In the symbols of the rhombohedral space groups (2), the lattice letter (*R* or *P*) is followed by two symmetry-element symbols, whereas in the hexagonal space-group symbols (3) the lattice letter *P* is followed by three. The notation reflects the fundamental fact that the point symmetry of the rhombohedral lattice,  $\bar{3}\ 2/m$ , contains one primary axis, three secondary axes, but no tertiary axes (such as are present in the symmetry  $6/m\ 2/m\ 2/m$  of the hexagonal lattice). In Carl Hermann's terminology the *Blickrichtungen* are of two kinds in a rhombohedral lattice and of three kinds in a hexagonal lattice, for it is obvious that the *Blickrichtungen* are the symmetry directions of the lattice.

Table 1. *Symbols of trigonal space groups*

Proposed new symbols and additions to old symbols are shown in bold face.

		$\bar{3}m1$	321	3m1	$\bar{3}11$	311
		$\bar{3}1m$	312	31m		
Hexagonal lattice (point symmetry $6/m\ 2/m\ 2/m$ )	Bravais axes <i>hP</i>	$P\bar{3}m1$	<b><i>P321</i></b>	<i>P3m1</i>	<b><i>P\bar{3}11</i></b>	<b><i>P311</i></b>
		$P\bar{3}1m$	<b><i>P312</i></b>	<i>P31m</i>		<b><i>P31,211</i></b>
			<b><i>P31,221</i></b>			
			<b><i>P31,212</i></b>			
		$P\bar{3}c1$		<i>P3c1</i>		
		$P\bar{3}1c$		<i>P31c</i>		
		$\bar{3}m$	32	3m	$\bar{3}1$	31
Rhombohedral lattice (point symmetry $\bar{3}2/m$ )	Bravais axes <i>hR</i>	$R\bar{3}m$	<b><i>R32</i></b>	<i>R3m</i>	<b><i>R\bar{3}</i></b>	<b><i>R3</i></b>
		$R\bar{3}c$		<i>R3c</i>		
	Miller axes <i>rP</i>	<b><i>P3m</i></b>	<b><i>P32</i></b>	<b><i>P3m</i></b>	<b><i>P31</i></b>	<b><i>P31</i></b>
		<b><i>P3c</i></b>		<b><i>P3c</i></b>		

The only two cases in (1) where confusion must be avoided are the last two:  $P\bar{3}$  and  $P3$  are now used to designate hexagonal space groups and thus cannot be applied to the rhombohedral  $P$  cell. Indicating by 1s the secondary directions in the rhombohedral lattice ( $P\bar{3}1$  and  $P31$ ), and both secondary and tertiary directions in the hexagonal lattice ( $1P\bar{3}11$  and  $1P311$ ), removes the ambiguity. The old hexagonal symbols  $P\bar{3}$  and  $P3$  will still be understood, as synonyms of  $P\bar{3}11$  and  $P311$ . Only  $P\bar{3}1$  and  $P31$  can be the equivalent of  $R\bar{3}$  and  $R3$ .

As to the old  $P3_1$  and  $P3_2$ , they could be retained as such. (They can only represent hexagonal space groups, since screw axes are implicit in rhombohedral space groups.) But they would be the only trigonal  $hP$  symbols in which the secondary and tertiary directions would not be filled. For the sake of uniformity, it may be better to designate them  $P3_11$  and  $P3_211$ .

In the  $hR$  notation there is no need to change the symbols  $R\bar{3}$  and  $R3$  to  $R\bar{3}1$  and  $R31$ . The meaning of the letter  $R$  is by now well established. Everyone knows that the ' $R$ ' centering' of a  $P$  hexagonal lattice reduces the symmetry from  $6/m2/m2/m$  to  $\bar{3}2/m$ . (This, of course, is the reason why Bravais placed the  $hR$  ( $=rP$ ) crystals in a *rhombohedral system* and

the  $hP$  crystals in the *hexagonal system*, since the point symmetry of the lattice was the basis of his classification.)\*

The trigonal space groups are presented (Table 1) in such a way as to show the proposed modifications to the symbolism now in use.

The present proposal has been thoroughly reviewed by Professor E. Hellner, Dr H. Burzlaff, Dr W. Fischer and myself, preliminary to its adoption for use in our forthcoming Tables, *Space Groups and Lattice Complexes*. I am much indebted to my Marburg co-workers for this critical discussion. My thanks are also due to Professor A. Pabst for a critical reading of the manuscript.

\* In contrast the present subdivision into 'trigonal' and 'hexagonal' systems looks trivial indeed; the only information these terms convey refers to the nature of the symmetry axis — 3 or  $\bar{3}$  vs 6 or  $\bar{6}$  (if this were the point to emphasize, the names of other crystal systems would have to be recast: monoclinic to 'digonal', orthorhombic to 'tridigonal', cubic to 'tetradigonal'). In our age of crystal-structure determinations, Bravais' classification based on the lattice acquires an enhanced significance, stressing as it does the triperiodicity, which is the dominant feature of a structure.

*Acta Cryst.* (1969). A25, 716

**Spurious peaks in electron-density maps.** By EFFI HUBER-BUSER, *Institut für Kristallographie und Petrographie, Eidgenössische Technische Hochschule, Zürich, Switzerland*

(Received 11 November 1968 and in revised form 20 January 1969)

Certain commonly used data-rejection procedures can cause specific patterns of prominent spurious peaks and holes in electron density maps.

In a recent structure analysis of the nine-coordinated thorium tetrakis( $\gamma$ -isopropyl tropolonate) monohydrate,\* the highest peak in our difference electron-density map with coefficients sign Th ( $F_{\text{obs}} - |F_{\text{calc Th}}|$ ) was eventually proved to be spurious. The positional parameters of the thorium atom were obtained from a three-dimensional Patterson map and were then subjected — together with an isotropic temperature factor,  $B$ , and a scale factor — to three cycles of full-matrix least-squares refinement, treating the thorium as an anomalous scatterer. Because of the microscopic size of the crystal no absorption corrections were applied. (A comparison of the final calculated structure amplitudes with the observed values confirmed that absorption was indeed negligible.) After this refinement the thorium atom settled within  $0.02 \text{ \AA}$  of its final position and the temperature parameter  $B$  deviated from the final average isotropic  $\bar{B}_{\text{Th}}$  ( $= 4.28 \text{ \AA}^2$ ) by  $0.3 \text{ \AA}^2$ . The spurious peak and an additional hole of approximately  $-17 \text{ e. \AA}^{-3}$  could therefore not be explained by an inaccuracy in the heavy atom parameters used in the calculation of the structure factor ( $F_{\text{calc Th}}$ ) entering the difference Fourier synthesis. Also these features were only slightly attenuated after the inclusion of all the light atoms in the structure factor calculation.

We then noted that the sites of the hole and the spurious peak are connected to the heavy atom site: their coordinates are three- and fivefold multiples respectively of the thorium

coordinates and a hole-peak pattern at odd multiples of the heavy atom position could be traced throughout the unit cell up to  $n=25$  (see Fig. 1).

In search of an explanation we found that in an electron-density map with one heavy atom per asymmetric unit and space group  $P\bar{1}$  one can produce such a pattern with the

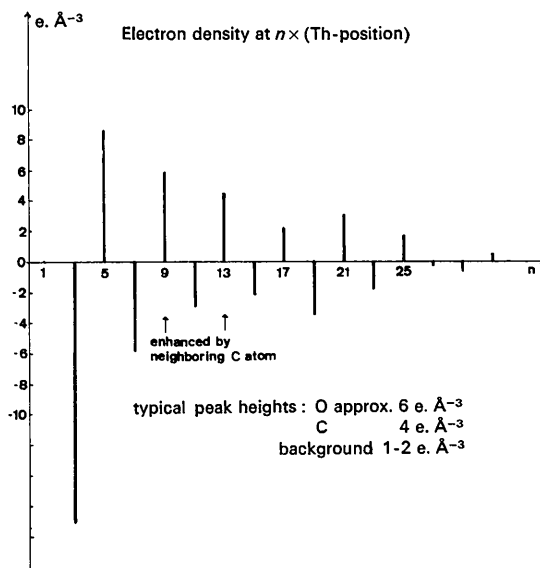


Fig. 1

\*  $\text{Th}(\text{C}_{10}\text{H}_{11}\text{O}_2)_4 \cdot \text{H}_2\text{O}$  plus one molecule of crystal solvent, either  $\text{H}_2\text{O}$  or a disordered  $\text{CH}_3\text{OH}$ ; space group  $P\bar{1}$ ; one molecule per asymmetric unit; detailed description not yet published.