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Comments on the relationship between *The Archimedean truncated octahedron, and packing of geometric units in cubic crystal structures* by C. Chieh and *On the choice of origins in the description of space groups* by H. Burzlaff & H. Zimmermann.

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Abstract

The results of the investigation of the choice of origins in the description of space groups [Burzlaff & Zimmermann (1980). *Z. Kristallogr.* **153**, 151–179] can be used to give group-theoretical reasons for the classification of cubic space groups by the aid of Archimedean truncated octahedron as was proposed by Chieh [*Acta Cryst.* (1979), A**35**, 946–952]. The division into units is independent of the choice of origin; however, it is found to be advantageous to place the centers of the geometric units at proper or privileged origins in dealing with cubic space groups without the site of cubic point-group symmetry, so as to simplify description of the geometric units. A modification is proposed in the representations of geometric-unit sequences. If the new symbols for the sequences of geometric units are extended by the symmetry of the centers of the units, there is a one-to-one correspondence between these extended sequence symbols and the non-isomorphic space group. Moreover, the extension of this concept to orthorhombic space groups with 'cubic' affine normalizers may be useful.

It was recognized by one of the authors (Chieh, 1979) that it is possible to divide any cubic crystal structure into small units in the form of congruent semi-regular (Archimedean) truncated octahedra. He pointed out that for the description of any cubic crystal structure, it is sufficient to know the distribution of atoms within the non-equivalent polyhedra, which were defined as geometric units. Cubic crystal structures can be classified according to the arrangements of the geometric units. Representations of crystal structures were accomplished by listing the geometric units along the body diagonal of the unit cell. Examples in the application of this concept have been given by Chieh (1980, 1982). This method uses the advantage of origins with points of high symmetry of some space groups. Admittedly, in the classification of cubic space groups, difficulty was encountered in space groups $I2_13$, $P2_13$, $P4_132$ and $P4_332$. Therefore, sequences for these space groups were left in such a way that they correspond to the lattice type.

A useful choice of origin was developed from the group-theoretical point of view by Burzlaff & Zimmermann (1980). It was shown that the selection of the origins in *International Tables for X-ray Crystallography* (1969) follows the normalizer concept as far as possible, *i.e.* each space group uses the setting of its affine normalizer in which it can be embedded as a subgroup. Thus all settings of cubic space groups can be derived from $Im3m$ or $Ia3d$, the latter, however, is a subgroup of $Im3m$ of index 8. Following this subgroup relation, the equivalent origins of the supergroup [Wyckoff position $2(a)$] are transferred to the Wyckoff position $16(a)$ in $Ia3d$ without any decomposition, and it is most convenient to use this position as the set of equivalent origins.

The centers of the Archimedean truncated octahedra coincide with the set of origins which is an I lattice. Thus the space can be subdivided into the Dirichlet domains of an I lattice, *i.e.* into Archimedean truncated octahedra. This is also known as a Wigner–Seitz (1933) cell for an I lattice.

Following the subgroup relations among the cubic space groups, other possibilities of decomposing the space may be considered, *e.g.* by using $Pm3m$ or $Fm3m$ as the common supergroup. However, $Im3m$ seems to be particularly convenient because the set of origins common to all cubic space groups is minimal if $Im3m$ is used as a common supergroup.

Thus the group-theoretical advancement in the properties of space groups and the discussion on the choice of origins in the description of space groups led to a better treatment for the cubic space groups without site of cubic point-group symmetry than the one given in Chieh (1979). Thus we suggest a revision for Table 2 of Chieh (1979) as given in Table 1. There are two classes of sequences of geometric units, one with two (2) and one with four (4) letters, and these are the numbers of geometric units along the body diagonals of the cubic cell. Unchanged letters mean translation along [111] directions, and a different letter is used to represent an independent geometric unit. When the two units are related by a center of symmetry, they are represented by A and $\bar{A}$. Superscripts 2, n and d represent twofold axes parallel to $[1\bar{1}0]$, n- and d-glide planes perpendicular to $[1\bar{1}0]$. Symmetry operations along the same direction are used for those space groups that require four geometric units in the body diagonal of the cubic cell. Thus AA^dAA^d is used for $I\bar{4}3d$ and $Ia3d$ compared to $AA'/\bar{A}\bar{A}'$ in Chieh (1979). The latter designation indicates that not all the units in the [111] direction have the same orientations, and this was illustrated by diagrams in the paper just mentioned.

With the suitable choice of privileged origins, we have now placed the space groups $I4_132$, $P4_132$, $P4_332$ and $P2_13$ in the proper place in Table 1. Centers of geometric units A and B usually have the same rank in terms of privileged origins, *i.e.* they have the same point-group symmetry. Units represented by C in sequences $ACB\bar{C}$ or $ACBC^2$ have lower

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Table 1. *Classification of cubic space groups and their orthorhombic relatives by geometric units (g.u.)*

Sequence of g.u.		Cubic space groups					Orthorhombic space groups	
		*I*23	*Im*3	*I*432	$I\bar{4}3m$	*Im*3*m*	*I*222	*Immm*
AA	*A*:	2 *a* 23	2 *a m*3	2 *a* 432	2 *a* $\bar{4}3m$	2 *a m*3*m*	2 *a* 222	2 *a mmm*
		*Pn*3	*Pn*3*n*	*Pn*3*m*			*Pnnn*	
$A\bar{A}$	*A*:	2 *a* 23	2 *a* 432	2 *a* $\bar{4}3m$			2 *a* 222	
		$P\bar{4}3n$	*Pm*3*n*					
AA''	*A*:	2 *a* 23	2 *a m*3					
		$P4_232$						
$AA^{\neg}$	*A*:	2 *a* 23						
		*P*23	*Pm*3	*P*432	$P\bar{4}3m$	*Pm*3*m*	*P*222	*Pmmm*
AB	*A*:	1 *a* 23	1 *a m*3	1 *a* 432	1 *a* $\bar{4}3m$	1 *a m*3*m*	1 *a* 222	1 *a mmm*
	B:	1 *b* 23	1 *b m*3	1 *b* 432	1 *b* $\bar{4}3m$	1 *b m*3*m*	1 *h* 222	1 *h mmm*
		$I\bar{4}3d$*	*Ia*3*d**					
$AA^{d}AA^{d}$	*A*:	16 *c* 3†	16 *a* $\bar{3}$					
		$I4_132$*						
$AA^{\neg}AA^{\neg}$	*A*:	16 *e* 3†						
		*Fd*3*c*						
$AA^{\neg}A''\bar{A}$	*A*:	16 *a* 23						
		$I2_13$*	*Ia*3*				$I2_12_12_1$	*Ibca*
ABAB	*A*:	8 *a* 3†	8 *a* $\bar{3}$				8 *d* 1†	8 *a* $\bar{1}$
	B:	8 *b* 3†	8 *b* $\bar{3}$				8 *d* 1†	8 *b* $\bar{1}$
		*F*43*c*	*Fm*3*c*					
$ABA''B''$	*A*:	8 *a* 23	*A*: 8 *a* 43					
	B:	8 *b* 23	*B*: 8 *b m*3					
		*Fd*3	*Fd*3*m*				*Fddd*	
$A\bar{A}B\bar{B}$	*A*:	8 *a* 23	8 *a* $\bar{4}3m$				8 *a* 222	
	B:	8 *b* 23	8 *b* $\bar{4}3m$				8 *b* 222	
		$F4_132$	$P4_132$*	$P4_332$*				
$AA^{\neg}BB^{\neg}$	*A*:	8 *a* 23	8 *c* 3†	8 *c* 3†				
	B:	8 *b* 23	8 *c* 3†	8 *c* 3†				
		*Fm*3	*Fm*3*m*	*Pa*3*			*Fmmm*	*Pbca*
$ACB\bar{C}$	*A*:	4 *a m*3	4 *a m*3*m*	4 *a* $\bar{3}$			4 *a mmm*	4 *a* $\bar{1}$
	B:	4 *b m*3	4 *b m*3*m*	4 *b* $\bar{3}$			4 *b mmm*	4 *b* $\bar{1}$
	C:	8 *c* 23	8 *c* $\bar{4}3m$	8 *c* 3			8 *f* 222	8 *c* 1
		*F*432						
$ACBC^2$	*A*:	$\bar{4}$ *a* 432						
	B:	4 *b* 432						
	C:	8 *c* 23						
		*F*23	$F\bar{4}3m$	$P2_13$*			*F*222	$P2_12_12_1$
ACBD	*A*:	4 *a* 23	$\bar{4}$ *a* 43*m*	4 *a* 3†			4 *a* 222	4 *a* 1†
	C:	4 *c* 23	$\bar{4}$ *c* 43*m*	4 *a* 3†			4 *c* 222	4 *a* 1†
	B:	4 *b* 23	$\bar{4}$ *b* 43*m*	4 *a* 3†			4 *b* 222	4 *a* 1†
	D:	4 *d* 23	$\bar{4}$ *d* 43*m*	4 *a* 3†			4 *d* 222	4 *a* 1†

* Cubic space groups without cubic site symmetry.
† Singular points, 0,0,0; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{3}{4},\frac{3}{4},\frac{3}{4}$, of Wyckoff sites.

symmetry than those of *A* and *B*. There are four units each of *A* and *B*, but eight units of *C* per unit cell. The usage of *A*, *B* or *C* to represent geometric units related to the multiplicity factor was derived from the way of setting up Wyckoff notations.

Following the group-theoretical consideration it may be convenient to discuss also the orthorhombic structures in space groups *F*222, $P2_12_12_1$, $I2_12_12_1$, *Ibca*, *Pbca*, *P*222, *I*222, *Pmmm*, *Pnnn*, *Fmmm*, *Immm* and *Fddd* (*cf.* Table 1) because they also have 'cubic' affine normalizers. In this case, the geometric units do not have the shape of an Archimedean truncated octahedron, but they do have to fill the entire space without leaving gaps. The shapes of these polyhedra are being investigated and they will be published in the future.

References

BURZLAFF, H. & ZIMMERMANN, H. (1980). *Z. Kristallogr.* **153**, 151–179.

CHIEH, C. (1979). *Acta Cryst.* A**35**, 946–952.

CHIEH, C. (1980). *Acta Cryst.* A**36**, 819–826.

CHIEH, C. (1982). *Acta Cryst.* A**38**, 346–349.

International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.

WIGNER, E. & SEITZ, F. (1933). *Phys. Rev.* **43**, 804–810.