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The structures of $Bi_6O_7FCl_3$ and $Bi_{12}O_{15}Cl_6$ in relation to the hypothetical non-stoichiometric parent structure $Bi_6X_{7+n}Cl_3$.

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The structures of $Bi_6O_7FCl_3$ and $Bi_{12}O_{15}Cl_6$ can both be derived from a hypothetical non-stoichiometric parent structure with the composition $Bi_6X_{7+n}Cl_3$. The method for deriving the structures is a building operation at the unit-cell level named 'chemical twinning'.

Introduction

A useful method for deriving a great number of structures from a few parent ones is regular, polysynthetic twinning at the unit-cell level. This is obtained in the same way as macroscopic twinning with the same definitions of twin plane and twin axis. Unit-cell twinning simply means that the periodicity of the twin planes determines the size of the unit cell. This type of structure-building operation was introduced by Andersson & Hyde (1974) and given the name 'chemical twinning'.

Chemical twinning of $Bi_6X_{7+n}Cl_3$

The structures of $Bi_6O_7FCl_3$ (Hopfgarten, 1975) and $Bi_{12}O_{15}Cl_6$ (Hopfgarten, 1976) can both be derived by a twinning operation from a parent structure with the composition $Bi_6X_{7+n}Cl_3$ for $0 \le n \le 1$. In Fig. 1 the hypothetical structure of $Bi_6X_{7+n}Cl_3$ has been depicted in projection along y with square pyramids, octahedra and trigonal prisms as coordination polyhedra. The twin planes are marked with arrows. The twin operation consists of a rotation around a two-fold axis parallel to x and a glide plane parallel to y. The space between two twin planes is the common building block in the named structures.

The parent structure consists of one planar $(BiX^+)_\infty$ sheet, one zigzag $(Bi_3X_5)_\infty$ sheet, and trigonal-prismatic $(Cl_3^{3-})_\infty$ columns. The structure of $Bi_6O_7FCl_3$ can be derived from a twin operation on a single block. Fig. 2 shows the structure of $Bi_6O_7FCl_3$. The nets of formula $(Bi_6O_7F^{3+})_\infty$ run zigzag through the structure and are parallel to y. Between them there are trigonal-prismatic columns of formula $(Cl_3^{3-})_\infty$. If one five-coordinated Bi atom in the $(Bi_3X_5)_\infty$ sheet has a 'vacancy' in one of its corners, the same twin operation on a double block (two single blocks) would give $Bi_{12}O_{15}Cl_6$ (Fig. 3). The nets of formula $(Bi_{12}O_{15}^{6+})_\infty$ run zigzag through the

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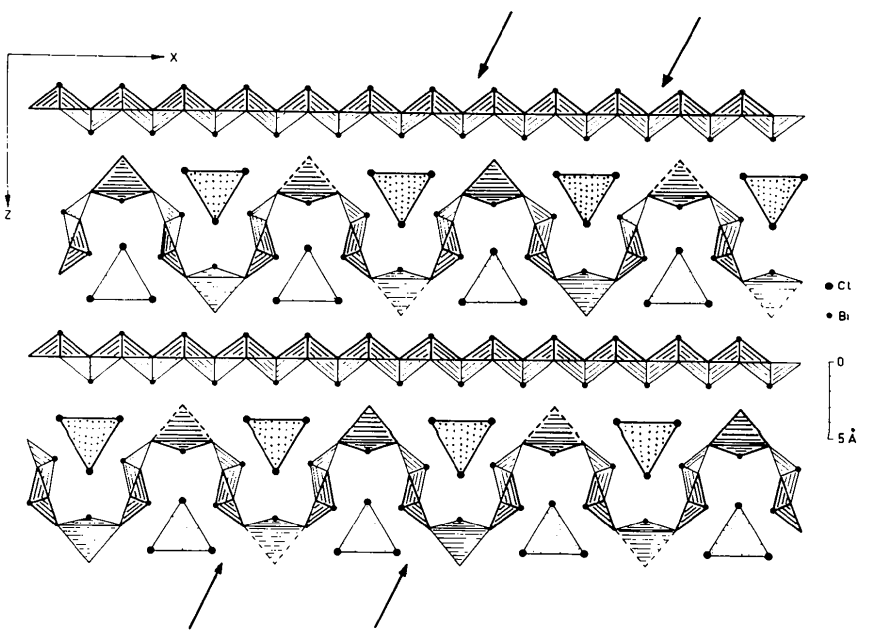

Fig. 1. The hypothetical non-stoichiometric parent structure $Bi_6X_{7+n}Cl_3$ projected along y. The coordination polyhedra of Bi, described as square pyramids and octahedra, are connected to one planar sheet and one zigzag sheet parallel to [010]. The Cl ions form trigonal-prismatic columns running along [010]. The polyhedra drawn in heavy and thin lines are $b/2$ apart.

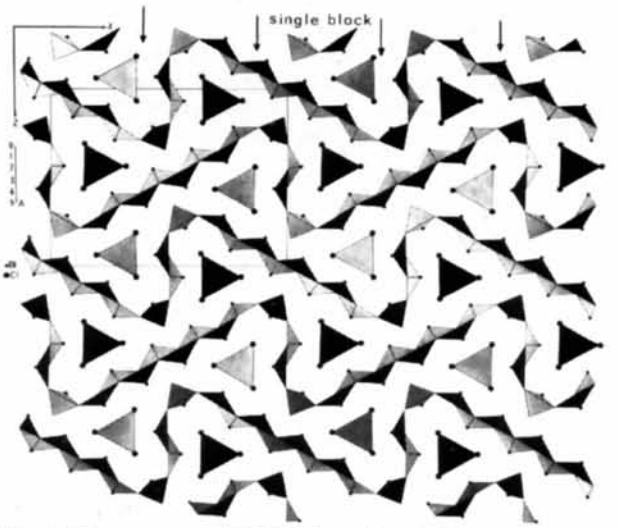

Fig. 2. The structure of $Bi_6O_7FCl_3$ projected along y. The coordination polyhedra of Bi, described as square pyramids and octahedra, are connected in infinite zigzag layers parallel to [010]. The Cl ions form trigonal-prismatic columns running along [010]. The polyhedra drawn in heavy and thin lines are $b/2$ apart.

structure and are parallel to y. Between them are trigonal-prismatic columns of formula $(Cl_3^{3-})_\infty$. These 'vacancies' are marked by dotted lines in Fig. 1, and the parent structure has the composition $Bi_6X_{7+0.5}Cl_3$.

It is clear that the number of single blocks upon which the twin operation acts varies with the composition. The intensities from $Bi_6O_7FCl_3$ and $Bi_{12}O_{15}Cl_6$ indicate a small variation in their composition.

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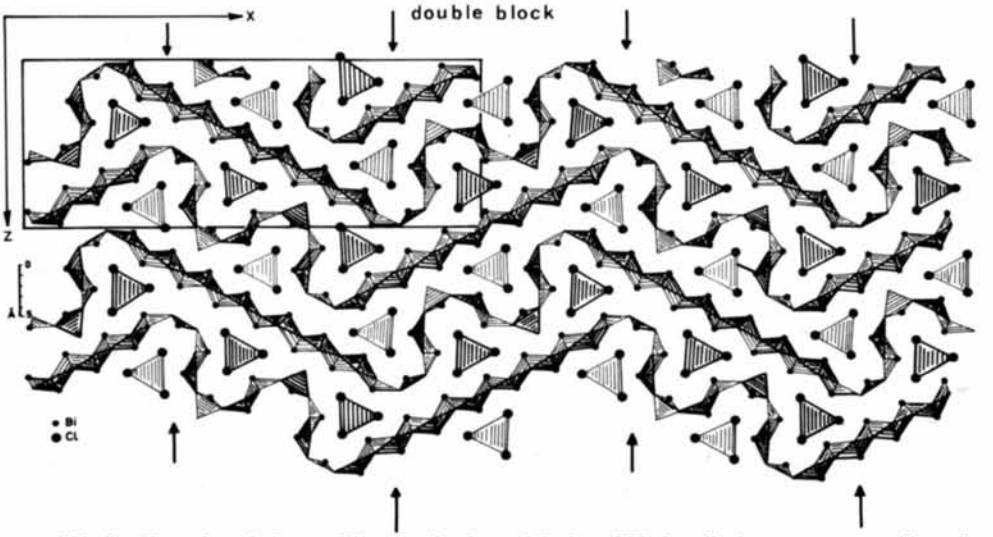

Fig. 3. The structure of $Bi_{12}O_{15}Cl_6$ projected along y. The coordination polyhedra of Bi, described as square pyramids and octahedra, are connected in infinite zigzag layers parallel to [010]. The Cl ions form trigonal-prismatic columns running along [010]. The polyhedra drawn in heavy and thin lines are $b/2$ apart.

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Deposition of Tables of Anisotropic Thermal Parameters

In its report to the IUCr Executive Committee and Tenth General Assembly of the Union which was held in Amsterdam, 7–15 August 1975, the Working Party on Information Services proposed that tables of anisotropic thermal parameters should, in general, be deposited together with structure factor tables.

With the agreement of the Executive Committee and the Chairman of the Commission on Journals, this proposal has now been implemented. All tables of anisotropic thermal parameters (except for very short tables) will be deposited, unless the Co-editor accepting the paper specifically requires that they be published. If a table gives both