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Pr_3InO: re-assessment of the cubic Pr_3In structure

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Key indicators: single-crystal X-ray study; T = 120 K; mean σ(Pr–Pr) = 0.001 Å; R factor = 0.023; wR factor = 0.057; data-to-parameter ratio = 8.3.

Single crystals of the title compound, tripraseodinium indium oxide, have been synthesized from a high-temperature reaction using a Pr–Cu eutectic mixture as flux. Based on its powder X-ray diffraction pattern, the product of the reaction was believed to be Pr_3In with the long known cubic $AuCu_3$ structure. However, structure refinements from single-crystal X-ray diffraction data confirmed that it is rather an oxygen-stabilized Pr_3InO with the inverse perovskite structure (Pearson's code *cP*5). The latter structure can be described as being built of corner-sharing Pr_6O octahedra with the In atoms occupying the cube–octahedral cavities. All three atoms in the asymmetric unit are in special positions: Pr $4/mm.m$, In $m\overline{3}m$ and O $m\overline{3}m$.

Related literature

For the previous model of Pr_3In, reported to adopt the $AuCu_3$ structure type (Villars & Calvert, 1991), see: Delfino *et al.* (1979). For re-determinations of other intermetallic phases where light elements such as N, C and O were found to occupy the interstices, see: Eisenmann *et al.* (1980); Gesing *et al.* (1995); Haschke *et al.* (1966); Leon-Escamilla & Corbett (2001); Röhr (1995); Schuster (1985); Widera & Schäfer (1980); Xia & Bobev (2007). For characterization of polycrystalline 'Pr_3In' samples, see: Christianson *et al.* (2005, 2007). Ionic radii were taken from Shannon (1976).

Experimental

Crystal data

Pr_3InO	$Z = 1$
$M_r = 553.55$	Mo $K\alpha$ radiation
Cubic, $Pm\overline{3}m$	$\mu = 33.45\ \text{mm}^{-1}$
$a = 4.9822$ (7) Å	$T = 120$ (2) K
$V = 123.67$ (3) Å^3	0.08 × 0.04 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer	1353 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	50 independent reflections
$T_{\min} = 0.188$, $T_{\max} = 0.368$	47 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$	6 parameters
$wR(F^2) = 0.057$	$\Delta\rho_{\max} = 1.43$ e Å^{-3}
$S = 1.29$	$\Delta\rho_{\min} = -1.21$ e Å^{-3}
50 reflections	

Table 1
Selected bond lengths (Å).

In—Pr	3.5229 (5)	Pr—Pr^{i}	3.5229 (5)
Pr—O	2.4911 (4)		

Symmetry code: (i) $y, z, x + 1$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XP* in *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2146).

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supplementary materials

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Pr_3InO: re-assessment of the cubic Pr_3In structure

A. D. Christianson and **S. Bobev**

Comment

"Pr_3In" has been known since 1979 (Delfino *et al.*, 1979) to crystallize in the $AuCu_3$ structure type (Villars & Calvert, 1991). A wide variety of other isotypic gallides, indides, germanides, stannides, and plumbides of the alkaline-earth and rare-earth metals are also known to crystallize with this cubic type (Villars & Calvert, 1991).

For many of these phases, subsequent structure re-determinations have proven that they are not true binary compounds and that light non-metallic elements such as carbon (Haschke *et al.*, 1966; Gesing *et al.*, 1995), nitrogen (Schuster, 1985), and oxygen (Widera & Schäfer, 1980; Röhr, 1995) fill the octahedral holes. Stabilization of the parent structures by utilizing well characterized interstitial holes is observed not only for the above-named cubic compounds with the inverse perovskite structure. Similar interstitial stabilization by oxygen for example is also reported for the layered pnictides of the alkaline-earth metals, such as Ca_4Sb_2O (Eisenmann *et al.*, 1980) and Ca_4Bi_2O (Xia & Bobev, 2007). Corbett's group has documented numerous examples of hydrogen impurity effects in A_5B_3-phases (A = alkaline-earth metals; B = Ge, Sn, Pb, Sb) with the Cr_5B_3 or Mn_5Si_3 structure types (Leon-Escamilla & Corbett, 2001).

In our previous studies of "Pr_3In" (Christianson *et al.*, 2005; Christianson *et al.*, 2007), we noticed that polycrystalline samples of this compound indicated the existence of an antiferromagnetic transition in the range 10–20 K. These results based on neutron diffraction, magnetic susceptibility and specific heat for a single-crystal of "Pr_3In" confirmed that antiferromagnetic order occurs in this material below $T_N = 12$ K with propagation vector $0, 0, 0.5 \pm \delta$, where $\delta = 1/12$ (Christianson *et al.*, 2005). Even though these studies were carried out using single crystals grown by the Bridgeman method, we noticed a subtle sample-dependence of the results, which pointed our attention at the possibility for an unrecognized impurity.

To study this in greater detail, we undertook a different synthetic approach (flux growth) and synthesized good quality crystals of the desired material, suitable for singe-crystal X-ray diffraction. This work confirmed that the product of the latter reaction crystallizes in the primitive cubic space group $Pm\bar{3}m$ with a cell parameter in excellent agreement with the previously reported value of 4.99 Å (Delfino *et al.*, 1979). Based on this information and surveying the Pearson's handbook (Villars & Calvert, 1991) one might conclude that "Pr_3In" is indeed a member of the cubic $AuCu_3$ structure type (Pearson's code *cP*4), in which the Pr atoms occupy the 3*c* Wyckoff site ((4/*mm.m* symmetry) and the In atoms are at the 1*a* Wyckoff site ($m\bar{3}m$ symmetry).

The presented structure refinements and the corresponding analyses of the Fourier and difference Fourier maps clearly indicate that the crystals we grew are not "Pr_3In" but its "stuffed" ternary variant Pr_3InO. A view of this structure, which is best described as an inverse cubic perovskite type (aka $CaTiO_3$), is shown in Figure 1. A s can be seen, the interstitial oxygen atoms are found at Wyckoff site 1*b* ($m\bar{3}m$ symmetry). The resultant $[OPr_6]$ octahedron is shown in Figure 2. The Pr—O distance of 2.4911 (4) Å is well within the expected range for trivalent Pr, according to the sum of the ionic radii (0.99 + 1.40 Å; Shannon, 1976).

Although the herein presented results are just a limiting case, this study calls the attention to the fact that many of recurring problems with "sample-dependence" in the literature on related intermetallic phases are most likely due to different types and amounts of interstitials occupying the octahedral holes in these structures.

Experimental

The reaction was carried out in an alumina crucible. The metallic elements, Pr (Alfa, ingot, 99.9%), In (Alfa, shot, 99.99%), and Cu (Alfa, shot, 99.99%) were loaded in a ratio of 7:1:2. The eutectic Pr–Cu (m.p. 715 K) mixture was intended to serve as a metal flux. The crucible with the reaction mixture was then flame sealed under vacuum in a silica ampoule, which was then placed in a furnace and heated to 1373 K at a rate of 300 K/h. The reaction proceeded at this temperature for 4 h before being cooled to 973 K at a rate of 4 K/h. At 973 K the ampoule was removed from the furnace and the flux was decanted. The main product of the reaction consisted of dark to black crystals with irregular shapes, which were later determined to be the title compound. The source of oxygen is unknown. Most likely a small, inadvertent crack in the fused silica ampoule is the cause for the partial oxidation of the molten intermetallic mixture during the reaction. However, we note that although the crystals were handled with care due to their air-sensitivity, diffusion of atmospheric oxygen through them cannot be ruled out.

Refinement

Structure refinements using the old Pr_3In model (Delfino *et al.*, 1979) proved a large residual peak in the difference Fourier map. The peak was located approximately 2.5 Å away from Pr. Such an interatomic distance is too short for a metal–metal bond and this ruled out the possibility for partially occupied In and/or Cu to be at that site. Since there were precedents in the literature for C, N, and O-atoms occupying this site, test refinements were performed with C, N, and O at the 1*b* site (hydrogen is too light to be even considered) and the results were as follows: 1) Pr_3InC (R1 = 0.0338, wR2 = 14.21); 2) Pr_3InN (R1 = 0.0284, wR2 = 0.0867); and 3) Pr_3InO (R1 = 0.0230, wR2 = 0.0590). The overall improvement in the refinement parameters, as well as the improved anisotropic displacement parameters confirmed that this octahedral site is indeed occupied by oxygen atoms. The full occupancies for all three crystallographic positions were verified by freeing the site occupation factor for an individual atom, while other remaining occupation parameters were kept fixed. This proved that all positions are fully occupied with corresponding deviations from full occupancy within 3σ. The maximum peak and deepest hole are located 0.90 Å away and 0.27 Å away from In, respectively.

Figures

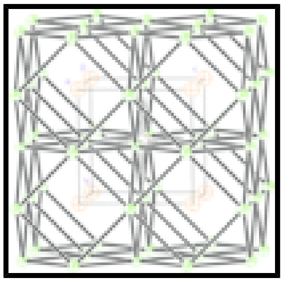

Fig. 1. A view of the structure of Pr_3InO, projected approximately along the [100] direction. Thermal ellipsoids are drawn at the 95% probability level. The Pr, In and O atoms are represented in green, yellow and red color, respectively.

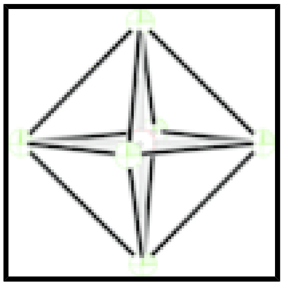

Fig. 2. A close view of the Pr_6O octahedron in the structure of Pr_3InO. The viewing projection and the color coding of the atoms is the same as in Fig. 1.

tripraseodinium indium oxide

Crystal data

Pr_3InO

$M_r = 553.55$

Cubic, $Pm\bar{3}m$

Hall symbol: -P 4 2 3

$a = 4.9822$ (7) Å

$b = 4.9822$ (7) Å

$c = 4.9822$ (7) Å

$\alpha = 90°$

$\beta = 90°$

$\gamma = 90°$

$V = 123.67$ (3) Å^3

$Z = 1$

$F_{000} = 234$

$D_x = 7.433$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 1353 reflections

$\theta = 4.1–27.9°$

$\mu = 33.45$ mm^{-1}

$T = 120$ (2) K

Irregular, black

0.08 × 0.04 × 0.03 mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 120(2)$ K

ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2003)

$T_{\min} = 0.188$, $T_{\max} = 0.368$

1353 measured reflections

50 independent reflections

47 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

$\theta_{\max} = 27.9°$

$\theta_{\min} = 4.1°$

$h = -6 \rightarrow 6$

$k = -6 \rightarrow 6$

$l = -6 \rightarrow 6$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.057$

$w = 1/[\sigma^2(F_o^2) + (0.031P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.43$ e Å^{-3}

$\Delta\rho_{\min} = -1.21$ e Å^{-3}

$S = 1.29$	Extinction correction: SHELXTL (Bruker, 2002), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
50 reflections	Extinction coefficient: 0.0026 (3)
6 parameters	

Special details

Experimental. Crystals were selected from the reaction and cut in a Paratone N oil bath to the desired dimensions. A suitable crystal was then chosen mounted on the tip of a glass fiber and quickly placed under the cold nitrogen stream (*ca* 120 K) in a Bruker *SMART* CCD-based diffractometer.

Data collection was performed with four batch runs at φ = 0.00 ° (450 frames), at φ = 90.00 ° (450 frames), at φ = 180.00 ° (450 frames), and at φ = 270.00 (450 frames). Frame width was = 0.40 ° in ω. Data were merged, corrected for decay, and treated with multi-scan absorption corrections.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}*/U_{\rm eq}$
Pr	0.0000	0.5000	0.5000	0.0090 (6)
In	0.0000	0.0000	0.0000	0.0129 (6)
O	0.5000	0.5000	0.5000	0.010 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr	0.0078 (7)	0.0097 (7)	0.0097 (7)	0.000	0.000	0.000
In	0.0129 (6)	0.0129 (6)	0.0129 (6)	0.000	0.000	0.000
O	0.010 (3)	0.010 (3)	0.010 (3)	0.000	0.000	0.000

Geometric parameters (Å, °)

In—Pr^{i}	3.5229 (5)	Pr—Pr^{xiii}	3.5229 (5)
In—Pr	3.5229 (5)	Pr—Pr^{xi}	3.5229 (5)
In—Pr^{ii}	3.5229 (5)	Pr—In^{xiv}	3.5229 (5)
In—Pr^{iii}	3.5229 (5)	Pr—Pr^{vii}	3.5229 (5)
In—Pr^{iv}	3.5229 (5)	Pr—Pr^{xv}	3.5229 (5)
In—Pr^{v}	3.5229 (5)	Pr—In^{xvi}	3.5229 (5)
In—Pr^{vi}	3.5229 (5)	Pr—Pr^{xvii}	3.5229 (5)

In—Pr^{vii}	3.5229 (5)	Pr—Pr^{iv}	3.5229 (5)
In—Pr^{viii}	3.5229 (5)	Pr—Pr^{i}	3.5229 (5)
In—Pr^{ix}	3.5229 (5)	O—Pr^{xiii}	2.4911 (4)
In—Pr^{x}	3.5229 (5)	O—Pr^{xviii}	2.4911 (4)
In—Pr^{xi}	3.5229 (5)	O—Pr^{iv}	2.4911 (4)
Pr—O^{xii}	2.4911 (4)	O—Pr^{xv}	2.4911 (4)
Pr—O	2.4911 (4)	O—Pr^{i}	2.4911 (4)
?···?	?		
Pr^{i}—In—Pr	60.0	In—Pr—Pr^{xi}	60.0
Pr^{i}—In—Pr^{ii}	120.0	Pr^{xiii}—Pr—Pr^{xi}	180.0
Pr—In—Pr^{ii}	180.0	O^{xii}—Pr—In^{xiv}	90.0
Pr^{i}—In—Pr^{iii}	180.0	O—Pr—In^{xiv}	90.0
Pr—In—Pr^{iii}	120.0	In—Pr—In^{xiv}	180.0
Pr^{ii}—In—Pr^{iii}	60.0	Pr^{xiii}—Pr—In^{xiv}	60.0
Pr^{i}—In—Pr^{iv}	60.0	Pr^{xi}—Pr—In^{xiv}	120.0
Pr—In—Pr^{iv}	60.0	O^{xii}—Pr—Pr^{vii}	45.0
Pr^{ii}—In—Pr^{iv}	120.0	O—Pr—Pr^{vii}	135.0
Pr^{iii}—In—Pr^{iv}	120.0	In—Pr—Pr^{vii}	60.0
Pr^{i}—In—Pr^{v}	120.0	Pr^{xiii}—Pr—Pr^{vii}	120.0
Pr—In—Pr^{v}	120.0	Pr^{xi}—Pr—Pr^{vii}	60.0
Pr^{ii}—In—Pr^{v}	60.0	In^{xiv}—Pr—Pr^{vii}	120.0
Pr^{iii}—In—Pr^{v}	60.0	O^{xii}—Pr—Pr^{xv}	135.0
Pr^{iv}—In—Pr^{v}	180.0	O—Pr—Pr^{xv}	45.0
Pr^{i}—In—Pr^{vi}	60.0	In—Pr—Pr^{xv}	120.0
Pr—In—Pr^{vi}	90.0	Pr^{xiii}—Pr—Pr^{xv}	60.0
Pr^{ii}—In—Pr^{vi}	90.0	Pr^{xi}—Pr—Pr^{xv}	120.0
Pr^{iii}—In—Pr^{vi}	120.0	In^{xiv}—Pr—Pr^{xv}	60.0
Pr^{iv}—In—Pr^{vi}	120.0	Pr^{vii}—Pr—Pr^{xv}	180.0
Pr^{v}—In—Pr^{vi}	60.0	O^{xii}—Pr—In^{xvi}	90.0
Pr^{i}—In—Pr^{vii}	120.0	O—Pr—In^{xvi}	90.0
Pr—In—Pr^{vii}	60.0	In—Pr—In^{xvi}	90.0
Pr^{ii}—In—Pr^{vii}	120.0	Pr^{xiii}—Pr—In^{xvi}	120.0
Pr^{iii}—In—Pr^{vii}	60.0	Pr^{xi}—Pr—In^{xvi}	60.0
Pr^{iv}—In—Pr^{vii}	90.0	In^{xiv}—Pr—In^{xvi}	90.0
Pr^{v}—In—Pr^{vii}	90.0	Pr^{vii}—Pr—In^{xvi}	120.0
Pr^{vi}—In—Pr^{vii}	120.0	Pr^{xv}—Pr—In^{xvi}	60.0
Pr^{i}—In—Pr^{viii}	60.0	O^{xii}—Pr—Pr^{xvii}	45.0
Pr—In—Pr^{viii}	120.0	O—Pr—Pr^{xvii}	135.0
Pr^{ii}—In—Pr^{viii}	60.0	In—Pr—Pr^{xvii}	120.0
Pr^{iii}—In—Pr^{viii}	120.0	Pr^{xiii}—Pr—Pr^{xvii}	120.0

Pr^{iv}—In—Pr^{viii}	90.0
Pr^{v}—In—Pr^{viii}	90.0
Pr^{vi}—In—Pr^{viii}	60.0
Pr^{vii}—In—Pr^{viii}	180.0
Pr^{i}—In—Pr^{ix}	120.0
Pr—In—Pr^{ix}	90.0
Pr^{ii}—In—Pr^{ix}	90.0
Pr^{iii}—In—Pr^{ix}	60.0
Pr^{iv}—In—Pr^{ix}	60.0
Pr^{v}—In—Pr^{ix}	120.0
Pr^{vi}—In—Pr^{ix}	180.0
Pr^{vii}—In—Pr^{ix}	60.0
Pr^{viii}—In—Pr^{ix}	120.0
Pr^{i}—In—Pr^{x}	90.0
Pr—In—Pr^{x}	120.0
Pr^{ii}—In—Pr^{x}	60.0
Pr^{iii}—In—Pr^{x}	90.0
Pr^{iv}—In—Pr^{x}	60.0
Pr^{v}—In—Pr^{x}	120.0
Pr^{vi}—In—Pr^{x}	120.0
Pr^{vii}—In—Pr^{x}	120.0
Pr^{viii}—In—Pr^{x}	60.0
Pr^{ix}—In—Pr^{x}	60.0
Pr^{i}—In—Pr^{xi}	90.0
Pr—In—Pr^{xi}	60.0
Pr^{ii}—In—Pr^{xi}	120.0
Pr^{iii}—In—Pr^{xi}	90.0
Pr^{iv}—In—Pr^{xi}	120.0
Pr^{v}—In—Pr^{xi}	60.0
Pr^{vi}—In—Pr^{xi}	60.0
Pr^{vii}—In—Pr^{xi}	60.0
Pr^{viii}—In—Pr^{xi}	120.0
Pr^{ix}—In—Pr^{xi}	120.0
Pr^{x}—In—Pr^{xi}	180.0
O^{xii}—Pr—O	180.0
O^{xii}—Pr—In	90.0
O—Pr—In	90.0
O^{xii}—Pr—Pr^{xiii}	135.0
O—Pr—Pr^{xiii}	45.0
In—Pr—Pr^{xiii}	120.0
O^{xii}—Pr—Pr^{xi}	45.0
Pr^{xi}—Pr—Pr^{xvii}	60.0
In^{xiv}—Pr—Pr^{xvii}	60.0
Pr^{vii}—Pr—Pr^{xvii}	90.0
Pr^{xv}—Pr—Pr^{xvii}	90.0
In^{xvi}—Pr—Pr^{xvii}	60.0
O^{xii}—Pr—Pr^{iv}	135.0
O—Pr—Pr^{iv}	45.0
In—Pr—Pr^{iv}	60.0
Pr^{xiii}—Pr—Pr^{iv}	60.0
Pr^{xi}—Pr—Pr^{iv}	120.0
In^{xiv}—Pr—Pr^{iv}	120.0
Pr^{vii}—Pr—Pr^{iv}	90.0
Pr^{xv}—Pr—Pr^{iv}	90.0
In^{xvi}—Pr—Pr^{iv}	120.0
Pr^{xvii}—Pr—Pr^{iv}	180.0
O^{xii}—Pr—Pr^{i}	135.0
O—Pr—Pr^{i}	45.0
In—Pr—Pr^{i}	60.0
Pr^{xiii}—Pr—Pr^{i}	90.0
Pr^{xi}—Pr—Pr^{i}	90.0
In^{xiv}—Pr—Pr^{i}	120.0
Pr^{vii}—Pr—Pr^{i}	120.0
Pr^{xv}—Pr—Pr^{i}	60.0
In^{xvi}—Pr—Pr^{i}	60.0
Pr^{xvii}—Pr—Pr^{i}	120.0
Pr^{iv}—Pr—Pr^{i}	60.0
Pr^{xiii}—O—Pr	90.0
Pr^{xiii}—O—Pr^{xviii}	90.0
Pr—O—Pr^{xviii}	180.0
Pr^{xiii}—O—Pr^{iv}	90.0
Pr—O—Pr^{iv}	90.0
Pr^{xviii}—O—Pr^{iv}	90.0
Pr^{xiii}—O—Pr^{xv}	90.0
Pr—O—Pr^{xv}	90.0
Pr^{xviii}—O—Pr^{xv}	90.0
Pr^{iv}—O—Pr^{xv}	180.0
Pr^{xiii}—O—Pr^{i}	180.0
Pr—O—Pr^{i}	90.0
Pr^{xviii}—O—Pr^{i}	90.0
Pr^{iv}—O—Pr^{i}	90.0
Pr^{xv}—O—Pr^{i}	90.0

O—Pr—Pr$^{\mathrm{xi}}$	135.0

Symmetry codes: (i) y, z, x; (ii) $x, y-1, z-1$; (iii) $y-1, z-1, x$; (iv) z, x, y; (v) $z-1, x, y-1$; (vi) $x, y, z-1$; (vii) $z-1, x, y$; (viii) $z, x, y-1$; (ix) $x, y-1, z$; (x) $y, z-1, x$; (xi) $y-1, z, x$; (xii) $x-1, y, z$; (xiii) $y, z, x+1$; (xiv) $x, y+1, z+1$; (xv) $z, x+1, y$; (xvi) $x, y+1, z$; (xvii) $z-1, x+1, y$; (xviii) $x+1, y, z$.

Fig. 1

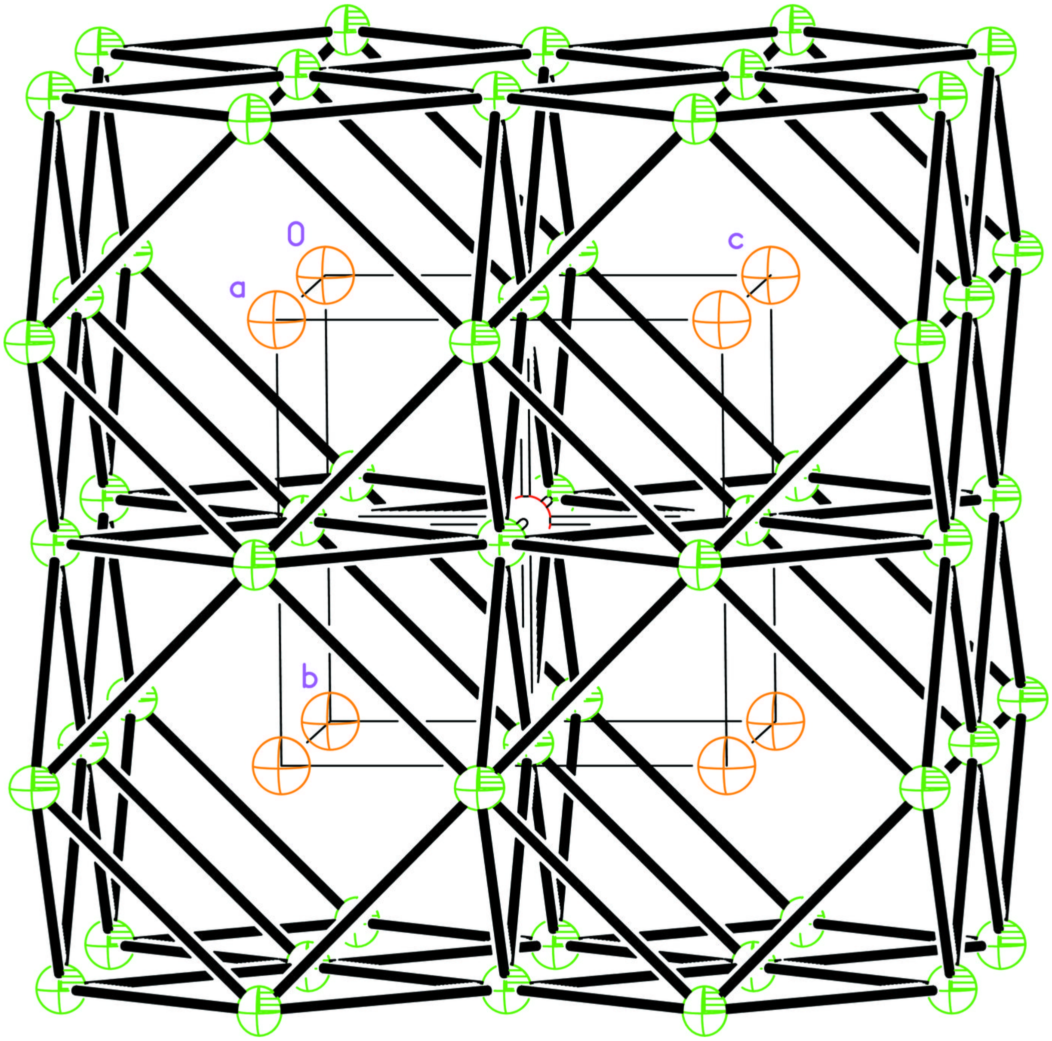

Fig. 2