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Refinement of the crystal structure of diindium disilicate, $In_2(Si_2O_7)$

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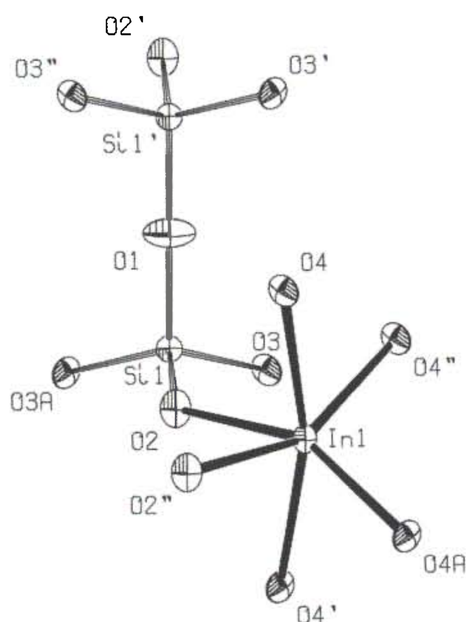

Abstract

$In_2O_7Si_2$, monoclinic, $C12/m1$ (No. 12), $a = 6.626(1)$ Å, $b = 8.604(1)$ Å, $c = 4.707(1)$ Å, $\beta = 102.94(2)°$, $V = 261.5$ Å^3, $Z = 2$, $R_{gt}(F) = 0.025$, $wR(F^2) = 0.059$, $T = 300$ K.

Source of material

Single crystals of indium disilicate were grown as a side product by chemical vapour transport of Ga_2O_3 and In_2O_3 in a closed quartz ampoule. Hydrogen chloride was used as transport agent and a mixture of Ga_2O_3 (3.3 mmol) and In_2O_3 (5.0 mmol) as source material. After two days of heating in a temperature gradient (1073 K $\rightarrow$ 1273 K), chemical transport was continued for 6 days using the inverted gradient. Gallium indium oxide was deposited as main product in the crystallization zone. Single crystals of indium disilicate were formed via reaction of In_2O_3 with the quartz wall in small amounts.

Discussion

The crystal structure of $In_2Si_2O_7$ is closely related to the thortveitite type which crystallizes in the monoclinic system (space group $C2/m$, $Z = 2$). Previous structural studies have been performed by Hagenmuller et al. [1] based on Rietveld refinements of X-ray powder diffraction data. The starting parameters for our refinement were taken from [1], which implies an origin shift of 0 0 1/2 compared to the original description of the thortveitite structure [2], but is in agreement with the TYPIX database [3].

The Si—O distances range from 161 pm to 164 pm, the In—O distances from 211 pm to 225 pm. The Si–O1–Si′ angle in the Si_2O_7 group is 180° forced by the centre of symmetry. It might be possible that we observe the average structure of a disordered Si_2O_7 group with a bonding angle unequal to 180°. But from the fact that the anisotropy of the displacement ellipsoid of O1 is rather moderate we conclude that the deviation of this angle from 180° is only small.

Table 1. Data collection and handling.

Crystal:	colourless rod, size 0.04 × 0.07 × 0.17 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	92.59 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 200 exposures, $\Delta\varphi = 1.5°$
$2\theta_{max}$:	56.04°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1296, 298
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 287
$N(param)_{refined}$:	32
Programs:	SHELXL-93 [4], CIF2SX [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	4*g*	0	0.30771(4)	0	0.0059(3)	0.0040(3)	0.0044(3)	0	0.0008(2)	0
Si(1)	4*i*	0.2203(2)	0	0.4101(3)	0.0049(7)	0.0048(8)	0.0016(8)	0	0.0007(5)	0
O(1)	2*c*	0	0	1/2	0.007(3)	0.020(4)	0.015(3)	0	0.005(2)	0
O(2)	4*i*	0.3902(6)	0	0.7177(9)	0.009(2)	0.007(2)	0.003(2)	0	-0.001(2)	0
O(3)	8*j*	0.2348(5)	0.1564(4)	0.2183(7)	0.008(1)	0.006(1)	0.006(1)	0.002(1)	0.002(1)	0.003(1)

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References

1. Gaewdang, T.; Chaminade, J. P.; Gravereau, P.; Garcia, A.; Fouassier, C.; Pouchard, M.; Jacquier, B.; Hagenmuller, P.: Structural Investigations and Luminescence of $In_2Ge_2O_7$ and $In_2Si_2O_7$. Z. Anorg. Allg. Chem. **620** (1994) 1965-70.
2. Zachariasen, W. H.: The structure of thortveitite, $Sc_2Si_2O_7$. Z. Kristallogr. **73** (1930) 1-6.
3. Cenzual, K.; Gladyshevskii, R.; Parthe, E.: TYPIX database. Gmelin-Institut, Frankfurt, 1995.
4. Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.
5. Farrugia, L. J.: CIF2SX, program to extract a SHELX-ins-file from a CIF. University of Glasgow, England 1997.

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