Redetermination of the crystal structure of pentastrontium trisilicide, Sr_5Si_3

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Received August 28, 1998, transferred to 1st update of database ICSD in 1999, CSD-No. 409376

Abstract

Si_3Sr_5 , tetragonal, $I4/mcm$ (No. 140), $a = 8.089(4) \text{ \AA}$, $c = 15.733(8) \text{ \AA}$, $V = 1029.4 \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.029$, $R_w(F^2) = 0.055$, $T = 298 \text{ K}$.

Source of material

Sr_5Si_3 was prepared by heating a stoichiometric mixture of the elements at 1363 K (2 d, cooling down within 10 h). Sr_5Si_3 forms grey-black, plate-like crystals with a metallic lustre.

Table 2. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sr(1)	4c	0	0	0	0.0182(3)	U_{11}	0.0498(7)	0	0	0
Sr(2)	16l	0.17815(4)	$x+1/2$	0.14162(3)	0.0211(2)	U_{11}	0.0227(2)	0.0003(2)	-0.0030(2)	U_{13}
Si(1)	4a	0	0	1/4	0.0233(9)	U_{11}	0.023(1)	0	0	0
Si(2)	8h	0.3919(2)	$x+1/2$	0	0.0172(6)	U_{11}	0.0200(9)	-0.0003(7)	0	0

Discussion

Sr_5Si_3 crystallises with the Cr_5B_3 structure type in the space group $I4/mcm$, and not in $I4cm$ as previously published [1]. The refinement in $I4cm$ did not lead to any improvements of the R factors and the Sr1 atom hardly moves away from the mirror plane ($z = 0.0003$). Furthermore, strong correlations of positions that are symmetrically equivalent in $I4/mcm$ are observed when the structure is refined in $I4cm$. Therefore, we chose $I4/mcm$ to describe Sr_5Si_3 , in contrast to the previously published structure [1]. Sr_5Si_3 contains Si_2^{6-} dumb-bells and isolated Si^{4-} Zintl anions. It can be described, according to the Zintl-Klemm concept, by the formulation $(\text{Sr}^{2+})_5[\text{Si}_2^{6-}][\text{Si}^{4-}]$. The Si-Si bond distance in the dumb-bell is 2.47 Å. Sr1 is coordinated by four equatorial Si2 dumb-bells and two axial Si1 atoms forming a very elongated octahedron. This may be the reason for the large U_{33} displacement parameter of Sr1.

Table 1. Data collection and handling.

Crystal:	black piece, size 0.10 x 0.15 x 0.20 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	260.08 cm^{-1}
Diffractometer, scan mode:	Stoe STADI4, ω/θ
$2\theta_{\text{max}}$:	59.88°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2900, 425
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 336
$N(\text{param})_{\text{refined}}$:	16
Programs:	SHELXS-96 [2], SHELXL-96 [3], ORTEPII [4]

Acknowledgment. This work was supported by the Swiss National Foundation.

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