

Lists of observed and calculated intensity data have been deposited with the IUCr (Reference: OH1097). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Bringley, J. F., Scott, B. A., La Placa, S. J., Boehme, R. F., Shaw, T. M., McElfresh, M. W., Trail, S. S. & Cox, D. E. (1990). *Nature (London)*, **347**, 263–265.
- Busing, W. R., Martin, K. O. & Levy, H. A. (1964). *ORFFE*. Report ORNL-TM-306. Oak Ridge National Laboratory, Tennessee, USA.
- Cava, R. J., Siegrist, T., Hesses, B., Krajewski, J. J., Peck, W. F. Jr, Batlogg, B., Takagi, H., Waszczak, J. V., Schneemeyer, L. F. & Zandbergen, H. W. (1991). *Physica C*, **177**, 115–121.
- Demazeau, G., Parent, C., Pouchard, M. & Hagenmuller, P. (1972). *Mater. Res. Bull.* **7**, 913–920.
- Dowty, E. (1995). *ATOMS*. Shape Software, 521 Hidden Valley Road, Kingsport, TN 37663, USA.
- Hiroi, Z. & Takano, M. (1995). *Nature (London)*, **377**, 41–43.
- Howard, C. J. (1982). *J. Appl. Cryst.* **15**, 615–620.
- Izumi, F. (1993). In *The Rietveld Method*, edited by R. A. Young, ch. 13. Oxford University Press.
- Kim, Y.-I. & Izumi, F. (1994). *J. Ceram. Soc. Jpn.* **102**, 401–404.
- La Placa, S. J., Bringley, J. F., Scott, B. A. & Cox, D. E. (1993). *Acta Cryst.* **C49**, 1415–1417.
- Norrestam, R., Nygren, M. & Bovin, J. O. (1991). *Angew. Chem.* **103**, 891–893.
- Poepelmeier, K. R., Lebnowicz, M. E., Scanlon, J. C., Longo, J. M. & Yelon, W. B. (1982). *J. Solid State Chem.* **45**, 71–79.
- Shannon, R. D. (1976). *Acta Cryst.* **A32**, 751–767.
- Thompson, P., Cox, D. E. & Hastings, J. M. (1987). *J. Appl. Cryst.* **20**, 79–83.
- Young, R. A. (1993). In *The Rietveld Method*, edited by R. A. Young, ch. 1. Oxford University Press.

Acta Cryst. (1996). **C52**, 2384–2385

CsAg_{0.64}Mn_{1.18}Te₂

ERIC J. WU, MICHAEL A. PELL AND JAMES A. IBERS

Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3113, USA. E-mail: ibers@chem.nwu.edu

(Received 29 January 1996; accepted 14 May 1996)

Abstract

The structure of CsAg_{0.64}Mn_{1.18}Te₂ has been determined from single-crystal X-ray data. It exhibits the ThCr₂Si₂ structure type, comprising layers of Ag- and Mn-centered tetrahedra that are stacked perpendicular to [001]. The Ag⁺ and Mn²⁺ cations are disordered over the same site.

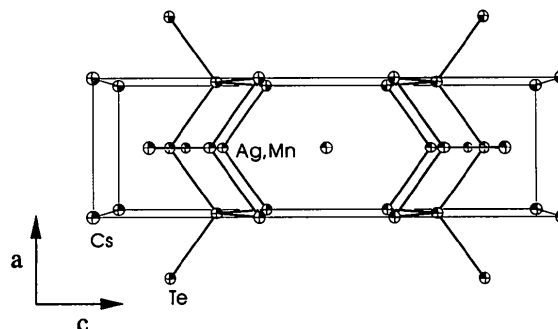


Fig. 1. View of the CsAg_{0.64}Mn_{1.18}Te₂ unit cell along *b* with 50% probability displacement ellipsoids.

Experimental

Cs₂Te₃, Ag (Aesar, 99.99%), Mn (Johnson Matthey, 99.9%), and Te (Aldrich, 99.8%) were combined in the molar ratio 1:1:2:1. Cs₂Te₃ was synthesized at 194 K from the stoichiometric reaction of Cs (Aldrich, 99.5%) and Te in liquid ammonia under an N₂ atmosphere. The reaction mixture was ground together, sealed under vacuum in a fused silica tube, heated to 1173 K for 8 days, then cooled to room temperature at 3 K h⁻¹. The red plates used for structure determination were manually extracted from the melt. Analysis of these crystals with an EDX-equipped Hitachi S-570 SEM showed the presence of Cs, Ag, Mn, and Te in the approximate ratio 1:0.5:1.5:2. We have also synthesized the potassium analogue of CsAg_{0.64}Mn_{1.18}Te₂ by a similar method, as confirmed by precession photographs.

Crystal data

CsAg_{0.64}Mn_{1.18}Te₂

M_r = 521.968

Tetragonal

I4/mmm

a = 4.520 (2) Å

c = 15.484 (8) Å

V = 316.3 (3) Å³

Z = 2

D_x = 5.469 Mg m⁻³

D_m not measured

Mo Kα₁ radiation

λ = 0.70930 Å

Cell parameters from 26 reflections

θ = 19.5–21.5°

μ = 18.88 mm⁻¹

T = 113 (2) K

Plate

0.431 × 0.319 × 0.078 mm

Red

Data collection

Picker diffractometer

θ–2θ scans

Absorption correction:

analytical

T_{min} = 0.037, *T_{max}* =

0.226

2621 measured reflections

245 independent reflections

R_{int} = 0.0600

θ_{max} = 34.97°

h = –7 → 7

k = –7 → 7

l = –24 → 24

6 standard reflections

monitored every 100

reflections

intensity decay: none

Refinement

Refinement on *F*²

R(*F*) = 0.0308

wR(*F*²) = 0.1182

S = 2.392

245 reflections

Extinction correction:

SHELXL93 (Sheldrick, 1993)

Extinction coefficient:

0.0103 (24)

11 parameters	Atomic scattering factors
$w = 1/[\sigma^2(F_o^2) + (0.04F_o^2)^2]$	from <i>International Tables</i>
$(\Delta/\sigma)_{\max} = 0.017$	for <i>Crystallography</i> (1992,
$\Delta\rho_{\max} = 3.75 \text{ e } \text{\AA}^{-3}$	Vol. C, Tables 4.2.6.8 and
$\Delta\rho_{\min} = -4.15 \text{ e } \text{\AA}^{-3}$	6.1.1.4)

Table 1. *Positional parameters, site occupancies and equivalent isotropic displacement parameters* (\AA^2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	Occupancy	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
Cs1	1.00	0	0	0	0.0176 (4)
Ag1	0.320 (8)	0	1/2	1/4	0.0151 (4)
Mn1	0.590 (5)	0	1/2	1/4	0.0151 (4)
Te1	1.00	0	0	0.35612 (4)	0.0154 (4)

Table 2. *Selected bond distances* (\AA) *and angles* ($^\circ$) (*M* = Ag, Mn)

Cs1—Te1 ⁱ	3.892 (2)	M—Te1 ⁱⁱ	2.794 (1)
Te1 ⁱⁱⁱ —M—Te1 ⁱⁱⁱⁱ	110.23 (2)	Te1 ^v —M—Te1 ^{vi}	107.96 (4)

Symmetry codes: (i) $x - \frac{1}{2}, y - \frac{1}{2}, z - \frac{1}{2}$; (ii) $-\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z$; (iii) $x, 1 + y, z$; (iv) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z$.

Initial cell parameters and symmetry information for $\text{CsAg}_{0.64}\text{Mn}_{1.18}\text{Te}_2$ were obtained from precession photographs taken at room temperature. Intensity data were processed (Waters & Ibers, 1977) and corrected for absorption (de Meulenaer & Tompa, 1965) on an IBM RS/6000 series computer. The initial Cs, Ag, Mn, and Te positional parameters were obtained from the structure of the isostructural compound CsLiMnS_2 (Schmitz & Bronger, 1987). The structure was refined with the program *SHELXL93* (Sheldrick, 1993). The Ag^+ and Mn^{2+} cations are disordered unequally over one site. The stoichiometry of these metals was determined by constraining the total charge of the Ag/Mn site to be +3 (to maintain charge balance) while refining the occupancies of the Ag^+ and Mn^{2+} cations. The refinement included anisotropic displacement parameters and an extinction parameter. The anisotropic displacement parameters of the Ag^+ and Mn^{2+} cations were constrained to be equal. The final difference electron density map shows no feature with a height greater than 1.3% that of a Cs atom.

$\text{CsAg}_{0.64}\text{Mn}_{1.18}\text{Te}_2$ exhibits the ThCr_2Si_2 structure type (Klepp & Boller, 1978) and comprises layers of edge-sharing *M*-centered tetrahedra (*M* = Ag/Mn) separated by Cs^+ cations.

Data collection: local program. Cell refinement: local program. Data reduction: local program. Molecular graphics: *SHELXTLPC* (Sheldrick, 1994). Software used to prepare material for publication: *SHELXTLPC*.

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: BR1142). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Klepp, K. & Boller, H. (1978). *Monatsh. Chem.* **109**, 1049–1078.
 Meulenaer, J. de & Tompa, H. (1965). *Acta Cryst.* **19**, 1014–1018.
 Schmitz, D. & Bronger, W. (1987). *Z. Anorg. Allg. Chem.* **553**, 248–260.
 Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Sheldrick, G. M. (1994). *SHELXTLPC*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Waters, J. M. & Ibers, J. A. (1977). *Inorg. Chem.* **16**, 3273–3277.

Acta Cryst. (1996). **C52**, 2385–2387

A New Europium Borosilicate, $\text{Eu}_3\text{BSi}_2\text{O}_{10}$

LISHENG CHI, HUAYANG CHEN, SHUIQUAN DENG, HONGHUI ZHUANG AND JINSHUN HUANG*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fujian, Fuzhou 350002, People's Republic of China

(Received 13 February 1996; accepted 18 April 1996)

Abstract

A single crystal of a new europium borosilicate, boron trieuropium disilicon decaoxide, was obtained by high-temperature solid-state reaction and chemical vapour transport methods. The structure is composed of layers of isolated BSiO_6^{5-} and $\text{Si}_2\text{O}_4^{4-}$ anions which alternate along the *c* axis. The layers are linked through three crystallographically independent Eu^{3+} ions to form a three-dimensional network structure.

Comment

Studies of rare earth borosilicates in the last ten years have shown these compounds to be promising phosphor and laser materials. The compounds LnBMO_5 (*M* = Si, Ge) with the stillwellite structure contain a distorted chain of tetrahedral BO_4 groups (Voronkov & Pyatenko, 1967; Ruimont & Tarte, 1988; Jsaryuk *et al.*, 1991); Eu^{3+} in these compounds shows relatively high luminescent efficiency (Antic-Fidancev, 1994). $\text{Nd}_3\text{BGe}_{1.08}\text{Si}_{0.92}\text{O}_{10}$ contains the planar BO_3 group (Serhan *et al.*, 1994) and the Ge and Si atoms are distributed statistically over the tetrahedral sites. The strong B—O bond in this compound influences the crystal field around the rare earth sites, which may be helpful in raising the fluorescence lifetime of the $^4F_{3/2}$ emitting state of Nd^{3+} . We have recently investigated the system $\text{Ln}_2\text{O}_3\text{—B}_2\text{O}_3\text{—SiO}_2$, and we report here the synthesis and crystal structure of $\text{Eu}_3\text{BSi}_2\text{O}_{10}$.

Fig. 1 shows the unit cell of $\text{Eu}_3\text{BSi}_2\text{O}_{10}$. It is apparent from this view that the structure consists of isolated BSiO_6^{5-} and $\text{Si}_2\text{O}_4^{4-}$ anion layers alternating along the *c* axis. The BSiO_6^{5-} anions consist of a BO_3 triangle and an SiO_4^{4-} tetrahedron linked by corner