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Structures of Calcium Tellurate, CaTeO$_4$, and Strontium Tellurate, SrTeO$_4$

By D. Hottentot and B. O. Loopstra

Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands

Abstract. CaTeO$_4$, orthorhombic, *Pbcn*, $a = 5.231$ (1), $b = 12.676$ (2), $c = 4.977$ (1) Å, $V = 330.0$ Å^3, $Z = 4$, $D_c = 4.66$ Mg m^{-3}. SrTeO$_4$, orthorhombic, *Pbcn*, $a = 5.574$ (2), $b = 13.114$ (3), $c = 5.001$ (1) Å, $V = 365.6$ Å^3, $Z = 4$, $D_c = 5.07$ Mg m^{-3}. The structures of the isostructural compounds CaTeO$_4$ and SrTeO$_4$ were determined from X-ray powder data. They contain strings of Te–O octahedra similar to those in Na$_2$TeO$_4$.

Introduction. The investigation of the title compounds was undertaken because little is known about the tellurates and tellurites of Ca and Sr, the only known structure being Ca$_3$TeO$_6$ (Baglio & Natansohn, 1969; Trömel, 1972). Cell constants of CaTeO$_4$ and SrTeO$_4$ have been given by Sleight, Foris & Licis (1972), who stated the space group to be *Pca2$_1$* or *Pcam*.

Powder samples of CaTeO$_4$ and SrTeO$_4$ were prepared by dissolving equimolar amounts of CaCl$_2$.2H$_2$O or SrCl$_2$.6H$_2$O and H$_6$TeO$_6$ in water. After evaporation, yellow-white flocculent precipitates were obtained which were powdered and heated in air at 873 K for 3 d. Powder patterns (Cu *Kα* radiation, Guinier camera, internal standard: *α*-quartz) were indexed in accordance with the cell dimensions given by Sleight, Foris & Licis (1972). From the systematic absences 0*kl* with $k = 2n + 1$, *h0l* with $l = 2n + 1$ and *hk*0 with $h + k = 2n + 1$ the space group was found to be *Pbcn*.

The structures were determined from step-scanned Cu *Kα* data, obtained on a Philips PW 1100 diffractometer. The coordinates of the Te and Ca atoms of CaTeO$_4$ were deduced from Patterson maps; the O atoms were placed on positions equivalent to those in Na$_2$TeO$_4$ (Kratochvil & Jensovsky, 1977). They were refined by a modified version of *SFLS* (Rutten-Keulemans, 1973). Non-observed reflections were omitted from the refinement. A final R of 0.074 was obtained for 73 observed (groups of) reflections. R is defined as $\sum |\sum_j n_j F_j^2(\text{obs.}) - \sum_j n_j F_j^2(\text{calc.})| / \sum \sum_j n_j F_j^2(\text{obs.})$ where n_j is the multiplicity factor and $\sum_j$ is a summation over the reflections which together constitute an unresolved peak. The temperature factors were refined isotropically, one common factor being used for the O atoms. The Sr, Te and O atoms of

SrTeO$_4$ were initially placed on the positions of the Ca, Te and O atoms in CaTeO$_4$ and were refined in the same way as those of CaTeO$_4$. A final R of 0.035 was obtained for 49 observed (groups of) reflections.*

Atomic parameters are given in Table 1, selected bond lengths and angles in Table 2.

Table 1. *Coordinates and thermal parameters*

	x	y	z	B (Å^2)
CaTeO$_4$				
Ca	0	0.6682 (8)	$\frac{1}{4}$	0.3 (2)
Te	$\frac{1}{2}$	0.4280 (3)	$\frac{3}{4}$	0.8 (1)
O(1)	0.299 (6)	0.544 (3)	0.570 (7)	0.1 (4)
O(2)	0.276 (6)	0.322 (3)	0.619 (5)	0.1 (4)
SrTeO$_4$				
Sr	0	0.6665 (4)	$\frac{1}{4}$	1.3 (2)
Te	$\frac{1}{2}$	0.4296 (3)	$\frac{3}{4}$	0.4 (1)
O(1)	0.318 (6)	0.542 (3)	0.549 (7)	1.8 (7)
O(2)	0.268 (6)	0.328 (4)	0.644 (4)	1.8 (7)

Table 2. *Selected bond lengths* (Å) *and angles* (°) *for* CaTeO$_4$ *and* SrTeO$_4$

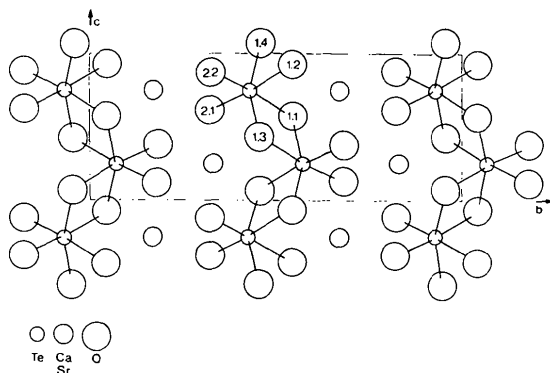|	CaTeO$_4$	SrTeO$_4$
Te–O(1.1)	2.02 (4)	2.05 (4)
Te–O(1.1)		
Te–O(1.3)	1.94 (3)	1.85 (4)
Te–O(1.4)		
Te–O(2.1)	1.89 (3)	1.93 (4)
Te–O(2.2)		
O(1.1)–Te–O(1.3)	78 (1)	74 (1)
O(1.3)–Te–O(2.1)	100 (1)	107 (1)
O(2.1)–Te–O(2.2)	90 (1)	93 (2)
O(2.2)–Te–O(1.4)	92 (1)	92 (2)
O(1.1)–Te–O(1.4)	87 (1)	89 (2)
O(1.1)–Te–O(1.2)	86 (1)	88 (1)
O(1.3)–Te–O(2.2)	94 (1)	90 (1)

Fig. 1. The structure projected along a.

Discussion. The structure of these compounds is given in Fig. 1. It exhibits octahedrally coordinated Te atoms in infinite chains along c, similar to those in Na_2TeO_4 (Kratochvil & Jensovsky, 1977).

The Ca and Sr atoms are also octahedrally coordinated by O atoms with Ca—O ranging from 2·34 (3) to 2·39 (4) Å and Sr—O from 2·47 (3) to 2·61 (4) Å.

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Bis{μ-[bromo(pentacarbonylmanganio)germanium(IV)]}-octacarbonyldimanganese

BY HANS PREUT AND HANS-JÜRGEN HAUPT

Lehrstuhl für Anorganische Chemie II der Universität, Postfach 500500, D-4600 Dortmund 50, Federal Republic of Germany

Abstract. $Ge_2Mn_4Br_2(CO)_{18}$, $M_r = 1028\cdot94$, monoclinic, $P2_1/c$, $a = 8\cdot762$ (4), $b = 12\cdot124$ (4), $c = 15\cdot425$ (4) Å, $\beta = 62\cdot82$ (9)°, $U = 1458$ Å³, $Z = 2$, $D_c = 2\cdot343$ Mg m⁻³; $F(000) = 972$; Mo $K\alpha$ radiation, $\lambda = 0\cdot71069$ Å, μ(Mo $K\alpha$) = 6·37 mm⁻¹. The structure was refined to an R of 0·0325 for 1397 unique diffractometer data. The central fragment of the molecule consists of a planar Mn_2Ge_2 rhombus with a Mn—Mn bond [r(Mn—Mn) = 2·923 (2) Å] across the metal ring.

Introduction. We have recently reported the structures of $Mn_2(CO)_8[\mu\text{-Sn(Br)Mn(CO)}_5]_2$ (Preut & Haupt, 1976) and $Mn_2(CO)_8[\mu\text{-Sn(Cl)Mn(CO)}_5]_2$ (Haupt, Preut & Wolfes, 1978). As part of our study of compounds with a covalent metal—metal bond we have determined the crystal structure of $Mn_2(CO)_8[\mu\text{-Ge(Br)Mn(CO)}_5]_2$. The crystal was prepared with the starting materials $Br_3GeMn(CO)_5$ and $BrMn(CO)_5$ (Ködel, Haupt & Huber, 1979).

Three-dimensional intensity data were collected using a crystal of dimensions 0·18 [100] × 0·07 [010]

× 0·09 [001] mm. Unit-cell parameters were determined by least-squares fits to the reflecting positions of 23 reflections on a Hilger & Watts Y 290 automatic four-circle diffractometer with graphite-monochromatized Mo $K\alpha$ radiation and a scintillation counter. The intensities of 1543 reflections ($I > 3\sigma$) with $2° \leq \theta \leq 24\cdot3°$ were measured by the $\omega/2\theta$ scan technique, with a scan width $\Delta 2\theta = (1\cdot34 + 0\cdot34 \tan \theta)°$ from background to background and a scan speed of 0·02° s⁻¹ in 2θ. Backgrounds were measured at each end of the scan range for a time of 7 s. Four standard reflections were measured after every fifty reflections during the data collection and showed only random deviations from their mean intensities. Lorentz and polarization corrections (but no correction for absorption) were applied and after the equivalent reflections were averaged the data set contained 1397 unique reflections for the structure analysis. The structure was solved by Patterson and Fourier methods and refined by a least-squares method (unit weights) with *SHELX* (Sheldrick, 1976). The refinement con-