

Bond distances and their e.s.d.'s (program *DISTAN*; E. Prince, private communication) are presented in Table 3. A plot of the observed and calculated intensity data over the region $17 \leq 2\theta \leq 82^\circ$ is presented in Fig. 1. An examination of the plot output indicates a good fit of the data throughout the entire spectrum. A Hamilton's (1965) test of the *R* values obtained with and without all thermal parameters anisotropic (0.0773 vs 0.0786, respectively) indicated the isotropic case could be rejected at the 0.995 confidence level.

Related literature. The positional parameters are in excellent agreement with those derived for BaBrCl by a Rietveld line-profile fit of X-ray powder diffraction data (Hodorowicz, Hodorowicz & Eick, 1983), substantiating the previous report that even though a Rietveld treatment of X-ray powder diffraction data may give erroneous thermal parameters, it yields accurate positional parameters (Malmros & Thomas, 1977). The positional parameters differ somewhat from

those expected from a comparison with parameters reported for BaCl₂ and BaBr₂ (Brackett, Brackett & Sass, 1963).

Support of the NSF Division of Materials Research, Solid State Chemistry grant DMR 84-00739, the help of Mr Zhenchuan Kang in obtaining the electron diffraction patterns, the NSF Regional Instrumentation Center for High Resolution Electron Microscopy at Arizona State University, and the NBS Reactor Division are gratefully acknowledged.

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Acta Cryst. (1986). **C42**, 917–918

Structure of Mercury Tellurate(IV)

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(Received 10 May 1985; accepted 7 February 1986)

Abstract. HgTeO₃, $M_r = 376.2$, triclinic, $P\bar{1}$, $a = 6.139$ (1), $b = 7.361$ (8), $c = 7.459$ (3) Å, $\alpha = 84.76$ (3), $\beta = 65.72$ (4), $\gamma = 87.11$ (2)°, $V = 305.94$ Å³, $Z = 4$, $D_x = 8.154$ g cm⁻³, $\lambda(\text{Ag } K\alpha) = 0.56083$ Å, $\mu = 333.4$ cm⁻¹, $F(000) = 624$, room temperature, final $R = 0.065$ for 2318 independent observed reflections. The structure consists of slightly distorted trigonal TeO₃ pyramids (mean Te–O distance 1.89 Å) with single connective bonds to each of three adjacent pyramids [Te–O distances 2.54 (2)–3.13 (2) Å]; with these longer bonds a framework of edge-sharing distorted TeO₆ octahedra is formed, in which the mercury atoms are incorporated. The resulting Hg–O coordination polyhedra are an octahedron [Hg–O 2.07 (2)–2.74 (2) Å] and a mono-capped trigonal prism [Hg–O 2.15 (2)–2.94 (2) Å], both distorted.

Experimental. Colourless single crystals prepared by annealing a mixture of HgO + TeO₂ in an evacuated quartz ampoule for two days at 770 K. Irregular-shaped crystal of 0.0032 mm³ selected; D_m not measured. Enraf–Nonius CAD-4 diffractometer; graphite-monochromatized Ag $K\alpha$ radiation; lattice parameters from refinement of 16 reflections in range $9 < \theta < 23^\circ$; scan width 1.2°, ω – 2θ scan mode; max. $\sin\theta/\lambda = 0.837$ Å⁻¹; hkl range: h 0 to 12, k –12 to 12, l –11 to 12. *SHELX76* (Sheldrick, 1976) and *XRAY* systems (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976); two standard reflections: no significant variation; 3828 total reflections, 3015 independent, 2318 with $I > 3\sigma(I)$; $R_{\text{int}} = 0.061$ (on F , 639 contributors); corrections for Lorentz–polarization, absorption (numerical integration with subprogram *ABSORB*: A^* 9.92 to 44.58) and ex-

inction effects [Lorentz distribution, $g = 5.2(2) \times 10^{-5}$]. Starting set of heavy atoms selected from E map calculated with direct methods (*SHELX76*); remaining atoms from successive Fourier syntheses; $\sum w(\Delta F^2)$ minimized, unit weights. Refinement of positional and anisotropic thermal parameters resulted in final $R = 0.065$; * unit weights; least squares based on F ; $S = 12.8$; 91 parameters refined; max. $\Delta/\sigma = 3.2 \times 10^{-5}$; max. $\Delta\rho = 10.5$, min. $\Delta\rho = -9.8 \text{ e } \text{\AA}^{-3}$ close to heavy atoms; scattering factors of neutral atoms (Cromer & Mann, 1968) used and corrected for anomalous dispersion (Cromer & Liberman, 1970).

Atomic coordinates are listed in Table 1, bond lengths in Table 2; Fig. 1 displays a perspective view of the structure, Fig. 2 the mercury–oxygen coordination polyhedra.

Related literature. For further information see Brandt & Moritz (1985) and Krämer & Brandt (1985).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42821 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

| | x | y | z | $U_{\text{eq}}(\text{\AA}^2)$ |
|-------|------------|------------|------------|-------------------------------|
| Hg(1) | 0.7926 (2) | 0.0557 (1) | 0.7664 (1) | 0.0133 (5) |
| Hg(2) | 0.2066 (2) | 0.2794 (1) | 0.8416 (1) | 0.0147 (5) |
| Te(1) | 0.6863 (2) | 0.1596 (2) | 0.3192 (2) | 0.0106 (8) |
| Te(2) | 0.2346 (2) | 0.4808 (2) | 0.2433 (2) | 0.0110 (8) |
| O(1) | 0.661 (3) | 0.016 (2) | 0.138 (3) | 0.02 (1) |
| O(2) | 0.268 (3) | 0.043 (2) | 0.528 (3) | 0.02 (1) |
| O(3) | 0.029 (3) | 0.186 (2) | 0.188 (3) | 0.02 (1) |
| O(4) | 0.644 (3) | 0.302 (2) | 0.715 (3) | 0.02 (1) |
| O(5) | 0.089 (3) | 0.439 (2) | 0.642 (3) | 0.02 (1) |
| O(6) | 0.730 (3) | 0.449 (2) | 0.017 (3) | 0.02 (1) |

Table 2. Bond distances (\AA), e.s.d. 0.02 \AA

| | | | |
|------------|------|------------|------|
| Hg(1)–O(4) | 2.07 | Hg(2)–O(5) | 2.15 |
| O(3) | 2.12 | O(1) | 2.30 |
| O(1) | 2.54 | O(3) | 2.40 |
| O(2) | 2.54 | O(4) | 2.46 |
| O(1') | 2.65 | O(6) | 2.47 |
| O(2') | 2.74 | O(2) | 2.93 |
| | | O(6') | 2.94 |
| Te(1)–O(1) | 1.85 | Te(2)–O(6) | 1.89 |
| O(2) | 1.88 | O(5) | 1.89 |
| O(3) | 1.93 | O(4) | 1.90 |
| O(2') | 2.54 | O(3) | 2.71 |
| O(6) | 2.89 | O(5') | 2.72 |
| O(4) | 3.13 | O(6') | 2.82 |

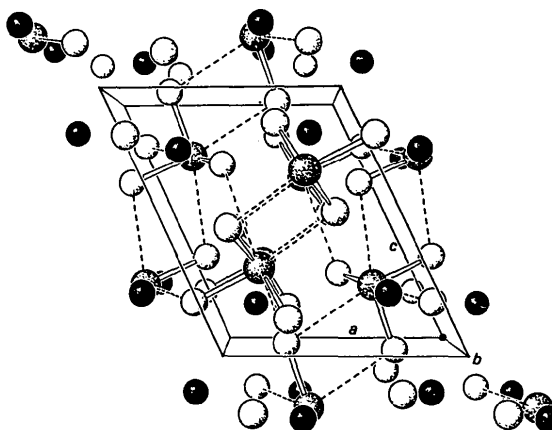


Fig. 1. Perspective view of the unit cell with surrounding atoms showing TeO_3 pyramids, connective bonds between them (broken lines) and Hg atoms (black); drawn with *SCHAKAL* (Keller, 1984).

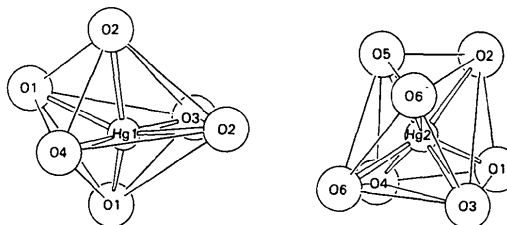


Fig. 2. The oxygen coordination of Hg(1) and Hg(2) [*SCHAKAL* (Keller, 1984)].

The authors thank Dr E. Keller for the intensity collection and for *SCHAKAL* plots. Numerical calculations were performed on the Sperry 1100/82 computer of the Rechenzentrum der Universität Freiburg.

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