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The Crystal Structure of a Tellurium(IV,VI) Oxyhydroxide, $\text{H}_2\text{Te}_2\text{O}_6$

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Single crystals of $\text{H}_2\text{Te}_2\text{O}_6$ have been prepared by hydrothermal synthesis. The space group is $Pbn2_1$ and the cell dimensions are $a = 8.037$, $b = 12.070$, $c = 4.735$ Å, and $Z = 4$. The structure was solved from three-dimensional Patterson and electron density calculations and the structure parameters, excluding those of the hydrogen atoms, were refined to an R value of 0.036 using 2480 independent reflexions. The structure contains Te(VI)O_6 octahedra and four-coordinated Te(IV) units with Te(VI)-O and Te(IV)-O bond distances in the ranges 1.864–1.952 Å and 1.861–2.107 Å, respectively. The Te(VI) octahedra are

linked through corners to form chains, which are connected *via* $-\text{Te(IV)-O}-\text{Te(IV)-O}-$ chains to form

infinite sheets. These sheets are held together by hydrogen bonds and van der Waals forces only, resulting in cleavage planes in the crystals. The $\text{H}_2\text{Te}_2\text{O}_6$ structure is closely related to that of Te_2O_5 , the three-dimensional structure of which can be regarded as a condensation of $\text{H}_2\text{Te}_2\text{O}_6$ layers.

Introduction

Phases of composition Te_2O_5 have been known for some years to exist as microcrystalline powders (Rosicky, Loub & Pavel, 1965; Moret & Maurin, 1968). Recently, single crystals of Te_2O_5 have been prepared and the crystal structure determined by X-ray methods (Lindqvist & Moret, 1973). The Te_2O_5 single crystals were obtained in a hydrothermal investigation of the TeO_2 - TeO_3 - H_2O system. In the same series of experiments it was also possible to isolate a new compound of composition $\text{H}_2\text{Te}_2\text{O}_6$ and to determine the conditions required for the growth of single crystals. Formally, $\text{H}_2\text{Te}_2\text{O}_6$ ought to be obtained by the reac-

tion of Te_2O_5 with water, and the present investigation was undertaken to examine the structural relationship between Te_2O_5 and $\text{H}_2\text{Te}_2\text{O}_6$.

Experimental

The hydrothermal synthesis of crystals of $\text{H}_2\text{Te}_2\text{O}_6$ and the analysis of the compound have been described elsewhere (Moret, 1972). Cell dimensions, as obtained from measurements with a calibrated Siemens powder diffractometer, and possible space groups have been given previously (Moret & Lindqvist, 1972) and a summary of the crystallographic data is given in Table 1.

Table 1. *Crystallographic data for H₂Te₂O₆*

Unit cell	Orthorhombic with $a = 8.037 (5) \text{ \AA}$ $b = 12.070 (5)$ $c = 4.735 (5)$ $V = 460.0 (0.5) \text{ \AA}^3$ $Z = 4$
F.W.	263.2
Density	$\rho_o = 5.1 \text{ g cm}^{-3}$ $\rho_c = 5.107 \text{ g cm}^{-3}$
Systematic absences	$0kl$ when $k = 2n + 1$ $h0l$ when $h + l = 2n + 1$
Space group	$Pbn2_1$
General point positions	$4(a): x, y, z; \frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z;$ $\bar{x}, \bar{y}, \frac{1}{2} + z; \frac{1}{2} - x, \frac{1}{2} + y, z$
Crystal habit	Colourless, rod-shaped with cleavage along (010).
$\mu(\text{Mo } K\alpha)$	130.4 cm^{-1} .

A crystal of the dimensions given in Table 2 was mounted along the c axis on a Philips PAILRED diffractometer. Using graphite monochromated, Mo $K\alpha$ radiation, the intensities of the $hk0$ – $hk9$ reflexions ($h, k \geq 0$) with $\sin \theta/\lambda$ up to approximately 1.5 were measured. The ω -scan technique with a scan speed of 2.5° per min was used and the background was measured for 40 sec at both ends of the scan interval.

Table 2. *Limiting surfaces of the crystal used for data collection and distances to these surfaces from an internal origin*

h	k	l	d (mm)
0	1	0	0.016
0	-1	0	0.016
1	1	0	0.050
1	-1	0	0.044
-1	-1	0	0.048
0	0	1	0.125
0	0	-1	0.125

Crystal volume: $8.13 \times 10^{-2} \text{ mm}^3$.

Counting statistics and Lp corrections were calculated with the program DATAP1, written by O. Lindgren, Göteborg. 223 reflexions with $I/\sigma(I) < 2.5$ were regarded as unobserved, and the number of independent reflexions to be used in the calculations was 2480.

The intensity data were corrected for absorption effects using the program DATAP2 (Coppens, Leisero-witz & Rabinovich, 1965), the crystal being divided into a $6 \times 6 \times 8$ Gaussian grid. The transmission ratios varied from 0.28 to 0.66.

Structure determination and refinement

Using those reflexions with $\sin \theta/\lambda \leq 0.6$, a three-dimensional Patterson summation was performed. The most prominent peaks showed that the structure is acentric, and the tellurium atoms were found to occupy

two positions 4(a) in space group $Pbn2_1$ (cf. Table 1). The oxygen atoms were located after two successive difference electron density calculations. The Fourier summations were performed with the fast Fourier transform program, FFT, originally written by G. Sande (Gentleman & Sande, 1966), expanded to three-dimensional crystallographic problems by Ten Eyck (1973).

The initial least-squares refinement of the structure was based on the low-order reflexions only, the block-diagonal approximation program BLOCK, written by O. Lindgren, being used. The final isotropic and the anisotropic refinement were based on all observed reflexions, and were carried out with the program LINUS (Busing, Martin & Levy, 1962; Coppens & Hamilton, 1970). The last isotropic cycles also included the variation of separate scale factors for the ten layer lines and a secondary isotropic extinction parameter, g (Coppens & Hamilton, 1970). The F_o scale factors for the $hk0$ and $hk1$ layers deviated significantly from the others by -7% , as a result of a necessary replacement of the X-ray tube after the collection of these two zones, while the others were the same within $\pm 1\%$. The R value in the isotropic refinement converged to 0.040 and the corresponding B values are given in Table 3.

In the final cycles of refinement, anisotropic temperature factors for all atoms were introduced, the inter-layer scale factors being kept constant. The R value converged to 0.036, and the resulting parameters are given in Table 3. The observed and calculated structure factors are compared in Table 4. Weights for each reflexion were calculated according to a modification of Cruickshank's (1970) formula, $w = (a + F_o + c \cdot F_o^2 + d \cdot F_o^3)^{-1}$, with $a = 100.0$, $c = 0.005$ and $d = 0.0008$. The corresponding weight analysis is given in Table 5. Scattering factors due to Cromer & Waber (1965) were used for Te and those given by Doyle & Turner (1968) for O. The tellurium contribution to the calculated structure factors was corrected for anomalous dispersion (Cromer, 1965).

Interatomic distances and angles were calculated with program DISTAN, written by A. Zalkin, Berkeley, California, and are given in Tables 6 and 7.

Table 3. *Final atomic parameters*

Positional parameters are expressed as fractions of the cell edges, and the anisotropic temperature factor is of the form

$$\exp [-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23}) \times 10^{-4}].$$

	x	y	z	B (\AA^2)
Te(VI)	0.03361 (4)	0.10960 (2)	0	0.447 (5)
Te(IV)	0.14154 (4)	0.44092 (2)	0.13714 (11)	0.555 (5)
O(1)	0.2346 (5)	0.0765 (4)	0.1975 (11)	0.67 (4)
O(2)	0.0899 (6)	0.9847 (4)	0.7609 (11)	0.74 (5)
O(3)	0.1661 (7)	0.2066 (4)	0.7765 (12)	0.91 (5)
O(4)	0.1628 (5)	0.8543 (4)	0.3126 (11)	0.68 (5)
O(5)	0.0470 (6)	0.4516 (4)	0.4946 (14)	0.87 (5)
O(6)	0.0033 (6)	0.2305 (4)	0.2640 (11)	0.80 (5)

Table 3 (cont.)

Table with 7 columns: Te(VI), U11, U22, U33, U12, U13, U23. Rows list coordination numbers for Te(VI), Te(IV), O(1), O(2), O(3), O(4), O(5), O(6).

Isotropic extinction parameter (Coppens & Hamilton, 1970), g · 10^-4 = 0.70 (4).

Discussion

The H2Te2O6 structure contains equal numbers of 4-valent and 6-valent tellurium atoms. This is evident from the oxygen environment of the two independent Te positions: Te(VI) has the usual octahedral configuration, while Te(IV) has a well known four-coordination as a trigonal bipyramid with the Te(IV) free electron pair in an equatorial position. The Te(VI) octahedra are connected through the O(2)

corner to form chains of composition [TeO3(OH)2]n- (the hydrogen positions are discussed below) in the crystallographic c-axis direction. This type of Te(VI) chain resulting from the sharing of corners has previously only been found in KTeO2(OH)3 (Lammers & Zemann, 1965), in which the chains have the composition [TeO2(OH)3]n-. The Te(VI) chains in H2Te2O6 are connected by [Te(IV)O]n+ chains via the O(1) and O(4) octahedral corners, resulting in infinite covalent sheets perpendicular to the b axis. One such layer con-

Table 4. Observed and calculated structure factors

The columns are h, 10F_o, 10|F_c| and phi (in radians).

Large table of structure factors with columns for h, 10F_o, 10|F_c|, and phi. The table is organized into multiple sections for different h values (e.g., h = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 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1669, 1670, 1671, 1672, 1673, 1674, 1675, 1676, 1677, 1678, 1679, 1680, 1681, 1682, 1683, 1684, 1685, 1686, 1687, 1688, 1689, 1690, 1691, 1692, 1693, 1694, 1695, 1696, 1697, 1698, 1699, 1700, 1701, 1702, 1703, 1704, 1705, 1706, 1707, 1708, 1709, 1710, 1711, 1712, 1713, 1714, 1715, 1716, 1717, 1718, 1719, 1720, 1721, 1722, 1723, 1724, 1725, 1726, 1727, 1728, 1729, 1730, 1731, 1732, 1733, 1734, 1735, 1736, 1737, 1738, 1739, 1740, 1741, 1742, 1743, 1744, 1745, 1746, 1747, 1748, 1749, 1750, 1751, 1752, 1753, 1754, 1755, 1756, 1757, 1758, 1759, 1760, 1761, 1762, 1763, 1764, 1765, 1766, 1767, 1768, 1769, 1770, 1771, 1772, 1773, 1774, 1775, 1776, 1777, 1778, 1779, 1780, 1781, 1782, 1783, 1784, 1785, 1786, 1787, 1788, 1789, 1790, 1791, 1792, 1793, 1794, 1795, 1796, 1797, 1798, 1799, 1800, 1801, 1802, 1803, 1804, 1805, 1806, 1807, 1808, 1809, 1810, 1811, 1812, 1813, 1814, 1815, 1816, 1817, 1818, 1819, 1820, 1821, 1822, 1823, 1824, 1825, 1826, 1827, 1828, 1829, 1830, 1831, 1832, 1833, 1834, 1835, 1836, 1837, 1838, 1839, 1840, 1841, 1842, 1843, 1844, 1845, 1846, 1847, 1848, 1849, 1850, 1851, 1852, 1853, 1854, 1855, 1856, 1857, 1858, 1859, 1860, 1861, 1862, 1863, 1864, 1865, 1866, 1867, 1868, 1869, 1870, 1871, 1872, 1873, 1874, 1875, 1876, 1877, 1878, 1879, 1880, 1881, 1882, 1883, 1884, 1885, 1886, 1887, 1888, 1889, 1890, 1891, 1892, 1893, 1894, 1895, 1896, 1897, 1898, 1899, 1900, 1901, 1902, 1903, 1904, 1905, 1906, 1907, 1908, 1909, 1910, 1911, 1912, 1913, 1914, 1915, 1916, 1917, 1918, 1919, 1920, 1921, 1922, 1923, 1924, 1925, 1926, 1927, 1928, 1929, 1930, 1931, 1932, 1933, 1934, 1935, 1936, 1937, 1938, 1939, 1940, 1941, 1942, 1943, 1944, 1945, 1946, 1947, 1948, 1949, 1950, 1951, 1952, 1953, 1954, 1955, 1956, 1957, 1958, 1959, 1960, 1961, 1962, 1963, 1964, 1965, 1966, 1967, 1968, 1969, 1970, 1971, 1972, 1973, 1974, 1975, 1976, 1977, 1978, 1979, 1980, 1981, 1982, 1983, 1984, 1985, 1986, 1987, 1988, 1989, 1990, 1991, 1992, 1993, 1994, 1995, 1996, 1997, 1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020, 2021, 2022, 2023, 2024, 2025, 2026, 2027, 2028, 2029, 2030, 2031, 2032, 2033, 2034, 2035, 2036, 2037, 2038, 2039, 2040, 2041, 2042, 2043, 2044, 2045, 2046, 2047, 2048, 2049, 2050, 2051, 2052, 2053, 2054, 2055, 2056, 2057, 2058, 2059, 2060, 2061, 2062, 2063, 2064, 2065, 2066, 2067, 2068, 2069, 2070, 2071, 2072, 2073, 2074, 2075, 2076, 2077, 2078, 2079, 2080, 2081, 2082, 2083, 2084, 2085, 2086, 2087, 2088, 2089, 2090, 2091, 2092, 2093, 2094, 2095, 2096, 2097, 2098, 2099, 2100, 2101, 2102, 2103, 2104, 2105, 2106, 2107, 2108, 21

Table 4 (cont.)

Table with multiple columns of numerical data, organized into sections labeled M 1 through M 15. Each section contains several columns of values, likely representing atomic coordinates or displacement parameters for different atoms in the crystal structure.

tains all the crystallographically independent atoms, and thus corresponds to the stoichiometric formula H2Te2O6. A stereoscopic projection of a single layer, prepared with the program ORTEP (Johnson, 1965), is shown in Fig. 1, and a schematic projection in the direction of the Te(VI) chains is given in Fig. 2.

The hydrogen atoms, whose positions could not be located in the presence of the heavy tellurium atoms,

may be assumed to be attached to O(3) and O(6), since these are the only oxygen atoms with only one strong bond to tellurium. Furthermore, there are two independent distances between O(3) and O(6) of 2.773 Å and 2.818 Å, which are likely to correspond to hydrogen bonds (cf. Table 6). On this assumption, the only bonds between the sheets apart from van der Waals forces are hydrogen bonds corresponding to the O(3)-O(6)

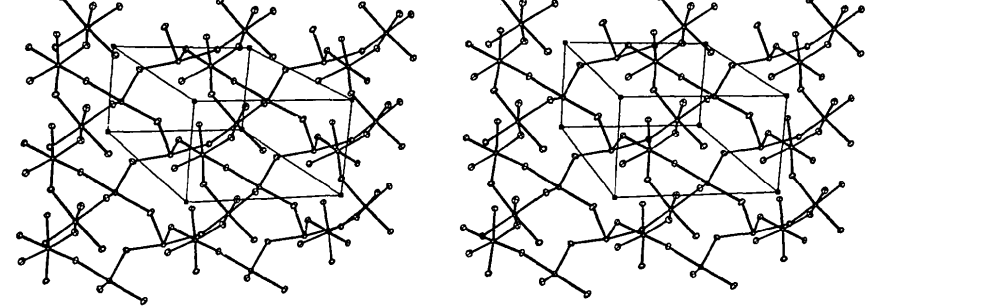


Fig. 1. Stereoscopic projection of one of the layers in the structure. The angle between the projection direction and the b axis is ~20°.

Table 4 (cont.)

2 122 125-1.81	5 263 233 2.62	8 906 399 1.72	9 131 99 2.40	M 1 3	6 181 179 -1.04	M 16 7	7 140 177 -2.97	9 598 593 -2.77	M 6 9
6 726 229 2.29	7 136 146 1.82	10 140 136 0.13	7 451 451 -1.02	2 328 308 -2.02	7 351 356 1.63	0 318 292 -1.30	7 168 178 0.62	7 168 178 0.62	0 450 450 0.00
9 215 185 -0.74	10 139 131 0.80	11 213 223 0.92	8 636 636 1.08	3 400 400 1.77	10 172 173 1.73	1 300 286 -1.45	6 426 426 2.60	6 426 426 2.60	2 425 212 -2.13
6 959 106 0.23	12 138 138 -0.00	13 230 240 -0.93	9 767 767 1.56	5 130 146 0.16	11 30 31 1.62	3 147 174 0.26	11 242 226 -0.11	11 242 226 -0.11	4 360 360 0.00
8 361 346 -0.16	1 137 137 0.00	13 240 240 -0.00	10 100 100 0.00	7 767 767 1.56	4 9 9 0.00	4 922 9 0.00	4 360 360 0.00	4 360 360 0.00	4 360 360 0.00
11 136 120 -2.18	3 507 512 0.24	M 0 0	11 211 211 0.00	8 136 128 1.00	8 7 7 0.00	1 403 393 -3.03	2 360 370 -0.31	2 360 370 -0.31	2 360 370 -0.31
11 128 119 -0.94	5 111 122 -1.12	M 0 0	1 361 321 -0.35	10 110 110 0.00	8 216 216 0.00	3 458 501 -0.96	3 458 501 -0.96	3 458 501 -0.96	3 458 501 -0.96
M 13 5	0 22 2 0.22	2 101 208 -3.01	4 205 206 -0.99	11 208 208 0.00	8 277 277 1.57	8 277 277 1.57	8 277 277 1.57	8 277 277 1.57	8 277 277 1.57
1 550 546 2.39	1 110 110 -0.29	4 318 316 -0.16	6 470 465 -0.51	12 663 671 1.58	8 958 808 1.58	6 958 808 1.58	6 958 808 1.58	6 958 808 1.58	6 958 808 1.58
7 256 239 -0.16	3 565 565 0.00	5 518 518 0.00	8 105 105 0.00	13 103 103 0.00	0 228 228 0.25	0 228 228 0.25	0 228 228 0.25	0 228 228 0.25	0 228 228 0.25
3 490 498 0.31	3 217 208 -1.75	6 110 110 0.00	10 105 105 0.00	M 2 7	M 10 1 7	M 10 1 7	M 10 1 7	M 10 1 7	M 10 1 7
3 187 182 -0.56	3 217 208 -1.75	6 110 110 0.00	10 105 105 0.00	0 228 228 0.25	0 228 228 0.25	0 228 228 0.25	0 228 228 0.25	0 228 228 0.25	0 228 228 0.25
5 102 105 0.00	3 309 318 -1.13	8 100 100 0.00	11 410 410 -0.09	1 152 151 0.07	1 152 151 0.07	1 152 151 0.07	1 152 151 0.07	1 152 151 0.07	1 152 151 0.07
6 478 472 -1.39	M 23 5	10 345 315 -0.50	11 237 247 0.99	4 122 129 0.77	4 122 129 0.77	4 122 129 0.77	4 122 129 0.77	4 122 129 0.77	4 122 129 0.77
7 463 466 2.85	1 147 148 -0.66	11 237 247 0.99	4 122 129 0.77	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25
8 248 248 0.00	2 291 298 -0.76	12 240 240 0.00	4 122 129 0.77	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25
10 285 293 -1.54	M 0 0	12 240 240 0.00	4 122 129 0.77	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25
11 408 407 -0.69	M 0 0	2 565 565 0.00	7 7 7 0.00	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25
12 271 218 -1.78	2 565 565 0.00	7 7 7 0.00	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25	1 408 408 -0.25

distance of 2.818 Å. The other O(3)–O(6) hydrogen bonds are situated within the same layer.

That H₂Te₂O₆ has this pronounced layer structure, with only weak links between the sheets, has the result that cleavage planes occur parallel to the (010) plane. These cleavage planes are readily visible in Fig. 3, which shows an electron microscope photograph of a broken surface of a small H₂Te₂O₆ single crystal.

Table 5. Weight analysis after the last cycle of refinement

The quantities $w\Delta^2$ are normalized sums, $K_{\text{norm}} \cdot (\sum w|F_o - |F_c||^2)$, and N is the number of reflexions within each F_o interval.

F_o interval	$w\Delta^2$	N
0.0—15.5	2.03	284
15.5—20.9	1.61	267
20.9—26.0	0.88	270
26.0—30.7	0.99	251
30.7—36.2	0.65	248
36.2—42.0	0.81	242
42.0—50.2	0.58	240
50.2—61.1	0.57	229
61.1—78.8	0.40	226
78.7—210.0	1.21	223

$$R = \frac{\sum |F_o - |F_c||}{\sum F_o} = 0.036$$

$$R_w = \frac{(\sum w|F_o - |F_c||^2 / \sum wF_o^2)^{1/2}}{\sum F_o} = 0.055.$$

Another interesting feature of the structure is its resemblance to the structure of Te₂O₃ (Lindqvist & Moret, 1973). A comparison of the cell dimensions shows that the a ($= 8.046 \text{ \AA}$) and the c ($= 4.735 \text{ \AA}$) axes in H₂Te₂O₆ have values very close to the c ($= 7.955 \text{ \AA}$) and the b ($= 4.696 \text{ \AA}$) axes in Te₂O₃. If the atomic x and z coordinates of all the non-hydrogen atoms in plane A, Fig. 2, are transformed as $y' = z$ and $z' = \frac{1}{2} - x$,

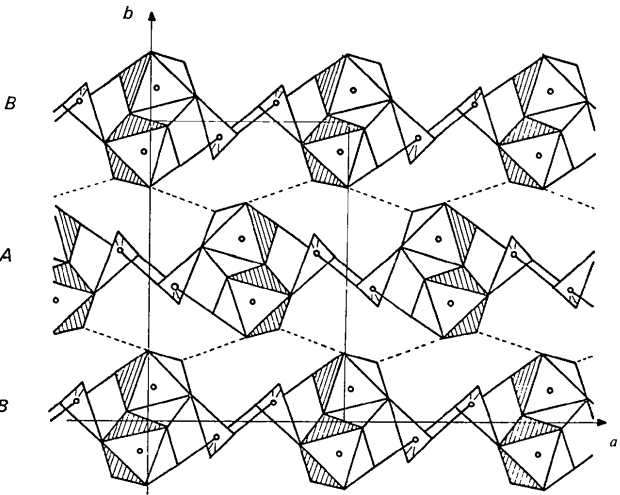


Fig. 2. Schematic projection along the c axis showing three layers in the structure. The interlayer hydrogen bonds are indicated as dotted lines.



Fig. 3. Electron microscope photograph (magnification: $4500\times$) showing the cleavage planes in an $\text{H}_2\text{Te}_2\text{O}_6$ single crystal.

it is found that $y' \cdot c$ and $z' \cdot a$ do not differ from the $y \cdot b$ and $z \cdot c$ values for corresponding atoms in Te_2O_5

Table 6. Oxygen–oxygen distances less than 3.67 Å and hydrogen bond angles

When both atoms are bonded to the same Te atom, this is indicated as =Te= or –Te=, where – corresponds to a weak interaction (*cf.* Fig. 5). For the other distances the position of atom 2 with respect to the position given in Table 3 is stated.

O(1)–O(3)	2.598 (7) Å	=Te(VI)=
O(1)–O(2)	2.619 (7)	=Te(VI)=
O(1)–O(6)	2.649 (7)	=Te(VI)=
O(3)–O(6)	2.670 (8)	=Te(VI)=
O'(2)–O'(6)	2.704 (6)	=Te(VI)=
O'(2)–O(4)	2.707 (7)	=Te(VI)=
O(1)–O(5)	2.709 (7)	=Te(IV)=
O(1)–O'(5)	2.713 (7)	=Te(IV)=
O(4)–O(6)	2.721 (7)	=Te(VI)=
O(1)–O'(2)	2.730 (6)	=Te(VI)=
O(5)–O'(5)	2.746 (5) (2×)	=Te(IV)=
O(2)–O(3)	2.748 (7)	=Te(VI)=
O(3)–O(4)	2.751 (7)	=Te(VI)=
O(4)–O(5)	2.753 (7)	=Te(IV)=
O(3)–O(6')	2.773 (8)	x, y, z
O(1)–O(4)	2.797 (6)	=Te(IV)=
O(2)–O'(2)	2.801 (5) (2×)	=Te(VI)=
O(3)–O(6 ¹¹)	2.818 (7)	$\frac{1}{2} + x, \frac{1}{2} - y, \bar{z}$
O(2)–O(4)	2.825 (6)	=Te(VI)=
O(5)–O(6)	2.905 (7)	=Te(IV)=
O(4)–O(6)	3.083 (7)	=Te(IV)–
O(3)–O(6)	3.096 (7)	$\bar{x}, 1 - y, z - \frac{1}{2}$
O(2)–O(4)	3.107 (7)	–Te(IV)=
O(1)–O(2)	3.114 (7)	$x, y - 1, z$
O(3)–O(4)	3.146 (7)	$\frac{1}{2} - x, y - \frac{1}{2}, z$
O(2)–O(5)	3.206 (7)	$\frac{1}{2} - x, \frac{1}{2} + y, z$
O(1)–O(3)	3.207 (7)	x, y, z
O(3)–O(5)	3.384 (7)	x, y, z
O(3)–O(4)	3.395 (7)	$\frac{1}{2} - x, y - \frac{1}{2}, 1 + z$
O(1)–O(4)	3.496 (6)	$\frac{1}{2} - x, y - \frac{1}{2}, z$
Te(VI)–O(6')–O(3)	115.3 (2)°	
Te(VI)–O(3)–O(6')	106.6 (2)	
Te(VI)–O(6 ¹¹)–O(3)	109.7 (2)	
Te(VI)–O(3)–O(6 ¹¹)	135.7 (3)	

by more than 0.2 Å for the tellurium and 0.8 Å for the oxygen atoms. This means that if the hydrogen atoms are disregarded, the $\text{H}_2\text{Te}_2\text{O}_6$ sheets (sheet *B* after 180° rotation around **b**) represent part of the three-dimensional Te_2O_5 structure. This is illustrated in Fig. 4. These close structural relationships between $\text{H}_2\text{Te}_2\text{O}_6$ and Te_2O_5 clearly indicate that Te_2O_5 is a true condensate of $\text{H}_2\text{Te}_2\text{O}_6$ according to the formal reaction $\text{H}_2\text{Te}_2\text{O}_6 = \text{Te}_2\text{O}_5 + \text{H}_2\text{O}$. However, since every second $\text{H}_2\text{Te}_2\text{O}_6$ sheet is rotated in Te_2O_5 , the condensation process cannot take place as a direct transformation of an $\text{H}_2\text{Te}_2\text{O}_6$ crystal, and the growth of crystals of either Te_2O_5 or $\text{H}_2\text{Te}_2\text{O}_6$ must be the result of the particular equilibrium state under the relevant hydrothermal conditions.

The similarities of the two structures are further emphasized when the coordination polyhedra of the tellurium atoms are compared (*cf.* Table 7). The bond distances agree very well, and the qualitative discussion in the Te_2O_5 paper (Lindqvist & Moret, 1973) as

to what influence the different types of 'axial' and 'equatorial' Te(IV)–O bonds might have on the bonds in the Te(VI) octahedron, is therefore also relevant for $\text{H}_2\text{Te}_2\text{O}_6$. In Te_2O_5 the Te(IV)–O(2) distance of 2.706 Å was considered to correspond to a weak bond resulting in a significant difference between the Te(VI)–O(2) and Te(VI)–O(3) bonds. Such a difference is also present in $\text{H}_2\text{Te}_2\text{O}_6$, but might here as well be considered to be an effect of the different roles of O(2) (bridge atom) and O(3) (hydroxyl group). It is thus difficult to come to any conclusion concerning the strength of the Te(IV)–O(2) interaction. That it is weaker than in Te_2O_5 is indicated not only by the longer distance (2.850 Å), but also by the fact that Te(IV) in $\text{H}_2\text{Te}_2\text{O}_6$ has another oxygen neighbour, O(6), at a distance of 2.837 Å. The position of O(6) (*cf.* Table 7) would seem to be more favourable for interaction with Te(IV) than that of O(2) [*cf.* discussion of CuTe_2O_5 , Hanke, Kupčik & Lindqvist (1973)].

Some of the differences in the coordination bond distances between $\text{H}_2\text{Te}_2\text{O}_6$ and Te_2O_5 , given in Table 7, may be regarded as being significant, *i.e.* Te(VI)–O(1), Te(VI)–O'(2), Te(VI)–O(4), Te(IV)–O(1),

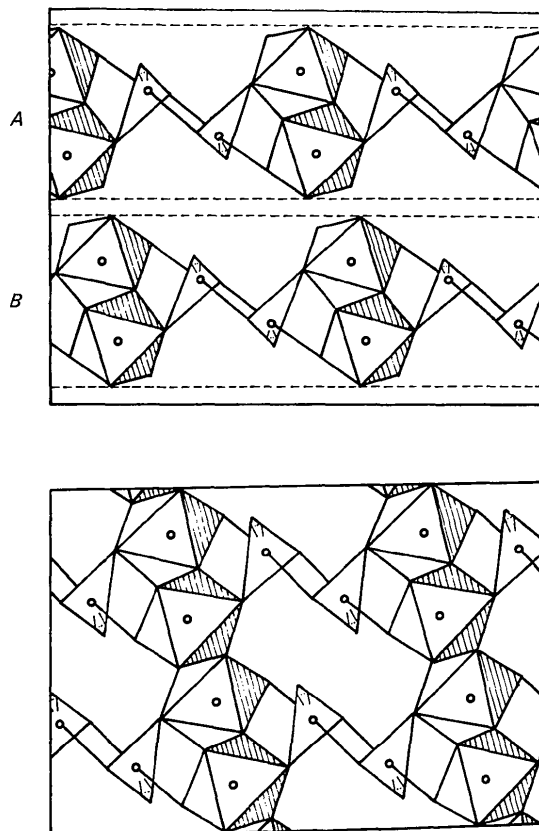


Fig. 4. Comparison between the $\text{H}_2\text{Te}_2\text{O}_6$ and the Te_2O_5 structures. In the upper part of the figure, plane *B* has been rotated 180° around the *b* axis (*cf.* Fig. 2) and translated along the *a* axis. The lower part of the figure shows a projection of the Te_2O_5 structure.

Te(IV)–O(5) and Te(IV)–O'(5). That these deviations are in fact significant is supported by the fact that there is a rational correspondence in all cases: The shortening of the Te(VI)–O(1) bond is accompanied by an elongation of the Te(IV)–O(1) bond; the weakened Te(IV)–O(1) bond is accompanied by a stronger Te(IV)–O(5) bond, which is to be expected, considering the Te(IV) 'equatorial' bonds to involve

Te(IV) sp^2 hybrid orbitals (Lindqvist, 1967). The Te(VI)–O(4) bond is longer in $H_2Te_2O_6$, which corresponds to a shorter, though not significantly so, Te(IV)–O(4) bond, and, in turn, to a longer Te(IV)–O'(5) bond, since both are 'axial'. The Te(VI)–O'(2) bond is shorter, and the assumed Te(IV)–O'(2) interaction corresponds to a longer distance. (*cf.* Fig. 5 in discussion of Te_2O_5).

Table 7. Distances (Å) and angles ($^\circ$) within the tellurium–oxygen polyhedra

The notation is in accordance with Fig. 5. Corresponding values for Te_2O_5 are given in parentheses.

Te(VI)–O(1)	1.911 (4)	(1.929)	Te(IV)–O(1)	1.937 (4)	(1.913)
Te(VI)–O(2)	1.940 (5)	(1.933)	Te(IV)–O(2)	2.850 (5)	(2.706)
Te(VI)–O'(2)	1.952 (5)	(1.972)	Te(IV)–O(4)	2.065 (5)	(2.072)
Te(VI)–O(3) (OH)	1.904 (5)	(1.907)	Te(IV)–O(5)	1.861 (6)	(1.892)
Te(VI)–O(4)	1.864 (5)	(1.848)	Te(IV)–O'(5)	2.107 (5)	(2.080)
Te(VI)–O(6) (OH)	1.937 (5)	(1.927)	Te(IV)–O(6) (OH)	2.837 (5)	
O(1)–Te(VI)–O(2)	85.7 (2)	(82.6)	O(1)–Te(IV)–O(2)	63.0 (2)	(64.3)
O(1)–Te(VI)–O'(2)	90.0 (2)	(87.2)	O(1)–Te(IV)–O(4)	88.6 (2)	(86.0)
O(1)–Te(VI)–O(3)	85.8 (2)	(86.4)	O(1)–Te(IV)–O(5)	91.0 (2)	(91.0)
O(1)–Te(VI)–O(4)	178.4 (2)	(175.9)	O(1)–Te(IV)–O'(5)	84.2 (2)	(81.8)
O(1)–Te(VI)–O(6)	87.0 (2)	(88.9)	O(2)–Te(IV)–O(4)	76.6 (2)	(80.0)
O(2)–Te(VI)–O'(2)	92.1 (1)	(91.5)	O(2)–Te(IV)–O(5)	150.0 (2)	(152.2)
O(2)–Te(VI)–O(3)	91.3 (2)	(88.8)	O(2)–Te(IV)–O'(5)	103.4 (2)	(100.8)
O(2)–Te(VI)–O(4)	95.9 (2)	(98.8)	O(4)–Te(IV)–O(5)	88.9 (2)	(86.0)
O(2)–Te(VI)–O(6)	172.7 (2)	(171.4)	O(4)–Te(IV)–O'(5)	171.8 (2)	(165.9)
O'(2)–Te(VI)–O(3)	174.4 (2)	(173.5)	O(5)–Te(IV)–O'(5)	87.4 (1)	(87.3)
O'(2)–Te(VI)–O(4)	90.3 (2)	(88.9)	O(1)–Te(IV)–O(6)	157.9 (2)	
O'(2)–Te(VI)–O(6)	88.1 (2)	(87.0)	O(2)–Te(IV)–O(6)	126.6 (1)	
O(3)–Te(VI)–O(4)	93.4 (2)	(97.5)	O(4)–Te(IV)–O(6)	76.1 (2)	
O(3)–Te(VI)–O(6)	88.1 (2)	(91.8)	O(5)–Te(IV)–O(6)	73.1 (2)	
O(4)–Te(VI)–O(6)	91.4 (2)	(89.6)	O'(5)–Te(IV)–O(6)	103.7 (2)	
Te(VI)–O(1)–Te(IV)	122.7 (2)	(121.7)			
Te(VI)–O(2)–Te(IV)	134.7 (3)	(133.8)			
Te(VI)–O(2)–Te(IV)	132.7 (3)	(131.2)			
Te(VI)–O(2)–Te(IV)	87.5 (2)	(91.1)			
Te(VI)–O(4)–Te(IV)	136.0 (2)	(136.4)			
Te(IV)–O(5)–Te(IV)	129.0 (3)	(128.7)			
Te(VI)–O(6)–Te(IV)	119.2 (2)				

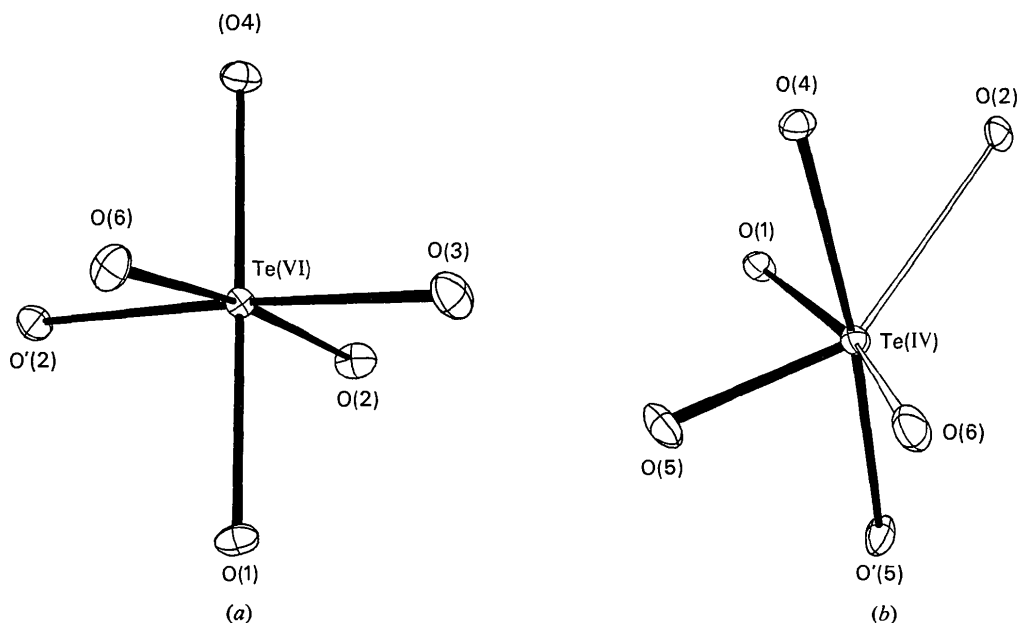


Fig. 5. Coordination of (a) the 6-valent and (b) the 4-valent tellurium atoms (probability level of the atomic ellipsoids: 50%).

These differences in bond distances and the deviations between the angles (*cf.* Table 7) may be a result of a higher degree of geometrical strain in the denser, three-dimensional Te₂O₅ structure. However, the differences are astonishingly small, and it is remarkable that there is no significant difference in the Te(VI)–O(3) and Te(VI)–O(6) bond distances, since O(3) and O(6) correspond to OH groups in H₂Te₂O₆, while they bridge two Te(VI) atoms in Te₂O₅.

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The Crystal Structure of CuTe₂O₅

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CuTe₂O₅ crystallizes in space group *P*2₁/*c*, with the following cell dimensions: *a* = 6·871(2), *b* = 9·322(2), *c* = 7·602(2) Å, β = 109·08(1)°, and with *Z* = 4. The phase problem was solved by direct methods and the final atomic parameters were obtained by full matrix least-squares refinement based on 3556 independent reflexions, an *R* value of 0·048 being obtained. The structure is a three-dimensional net resulting from copper and tellurium coordination polyhedra sharing oxygen atoms. Each oxygen atom interacts with three metal atoms, two of the interactions being strong and one weak. The Cu–O polyhedron may be described as a distorted octahedron with four strong bonds (Cu–O: 1·950–1·969 Å) and two weaker bonds (Cu–O: 2·305, 2·780 Å). Both independent tellurium atoms have three strong pyramidal bonds to oxygen (Te–O: 1·859–2·019 Å) and, in addition, one of them has a fourth interaction with an oxygen atom (Te–O: 2·402 Å), while the other has two weaker bonds (Te–O: 2·607, 2·733 Å).

Introduction

The structure of some double oxides of type MO_xTeO₂ where M = Zn or Cu have been investigated, *viz.* ZnTeO₃ (Hanke, 1967), CuTeO₃ (Lind-

qvist, 1972) and Zn₂Te₃O₈ (Hanke, 1966). The aim of this work was to determine the structure of another member of this series, CuTe₂O₅, which, like the above-mentioned oxides, has been prepared synthetically. Among the tellurium-containing minerals whose