

substance: WO₃

property: structural and related data of β -WO₃

space group $P\bar{1} - C_1^1$, $Z = 8$. The detailed structure is derived from ReO₃ with the corner-shared octahedra tilted (Figs. 1, 2).

lattice parameters

| | | | | |
|----------|------------|----|--|-------------|
| <i>a</i> | 7.309(2) Å | RT | data collected from a single domain crystal found by repeated thermal cycling of WO ₃ | 78D, 60T |
| <i>b</i> | 7.522(2) Å | | | |
| <i>c</i> | 7.678(2) Å | | | |
| α | 88.81° | | | |
| β | 90.92° | | | |
| γ | 90.93° | | | |

bond lengths and angles of the independent WO₆ octahedra

(distances in Å, angles in °, at RT [78D]) (see Fig. 2 for numbering of atoms)

W(1) O₆ octahedron

| | | |
|------------------------|-------|-------------|
| $d(W(1) - O(5))$ | | 1.751(21) |
| | O(12) | 1.756(22) |
| | O(4) | 1.826(21) |
| | O(1) | 1.952(23) |
| | O(6) | 2.056(23) |
| | O(9) | 2.215(23) |
| angle (O(5)–W(1)–O(9)) | | 87.62(90) |
| | O(1) | 93.34(96) |
| | O(4) | 98.89(96) |
| | O(12) | 100.22(100) |
| O(9) | O(1) | 80.69(90) |
| | O(4) | 83.52(90) |
| | O(6) | 79.72(85) |
| O(1) | O(6) | 82.43(93) |
| | O(12) | 95.20(98) |
| O(4) | O(6) | 82.06(92) |
| | O(12) | 98.63(98) |
| O(6) | O(12) | 92.29(95) |
| O(5) | O(6) | 167.13(96) |
| O(9) | O(12) | 171.39(88) |
| O(1) | O(4) | 159.57(102) |

W(2) O₆ octahedron

| | | |
|---------------------------------|-----------|-------------|
| $d(\text{W}(2) - \text{O}(11))$ | 1.775(24) | |
| O(6) | 1.787(22) | |
| O(2) | 1.853(22) | |
| O(3) | 1.915(23) | |
| O(5) | 2.116(21) | |
| O(10) | 2.199(24) | |
| angle (O(2) – W(2) – O(5)) | 84.10(87) | |
| O(6) | 96.02(97) | |
| O(10) | 81.24(92) | |
| O(11) | 99.53(99) | |
| O(5) | O(10) | 78.41(85) |
| | O(3) | 79.57(89) |
| | O(11) | 93.70(94) |
| O(6) | O(10) | 84.96(96) |
| | O(3) | 95.66(99) |
| | O(11) | 102.85(104) |
| O(10) | O(3) | 81.96(93) |
| O(3) | O(11) | 95.30(101) |
| O(2) | O(3) | 158.57(99) |
| O(5) | O(6) | 163.17(95) |
| O(11) | O(10) | 170.97(95) |

W(3) O₆ octahedron

| | | |
|-------------------------|-----------|-------------|
| $d(W(3) - O(9))$ | 1.715(23) | |
| O(7) | 1.796(22) | |
| O(1) | 1.856(23) | |
| O(4) | 1.974(21) | |
| O(8) | 2.085(21) | |
| O(12) | 2.176(22) | |
| angle (O(7)–W(3)–O(12)) | | 86.24(92) |
| | O(9) | 101.08(102) |
| | O(1) | 99.89(100) |
| | O(4) | 91.83(94) |
| O(8) | O(12) | 77.41(81) |
| | O(9) | 94.85(93) |
| | O(1) | 82.73(92) |
| | O(4) | 81.27(86) |
| O(12) | O(1) | 83.40(93) |
| | O(4) | 80.46(85) |
| O(9) | O(1) | 100.16(104) |
| | O(4) | 94.11(97) |
| O(7) | O(8) | 163.08 (94) |
| O(12) | O(9) | 171.09(91) |
| O(1) | O(4) | 159.37(100) |

W(4) O₆ octahedron

| | | |
|-------------------------|------------|-------------|
| $d(W(4) - O(10))$ | 1.738(25) | |
| O(8) | 1.751(21) | |
| O(3) | 1.881(25) | |
| O(2) | 1.934(21) | |
| O(7) | 2.049(22) | |
| O(11) | 2.157(24) | |
| angle (O(7)–W(4)–O(10)) | 94.16(100) | |
| | O(11) | 78.48(88) |
| | O(2) | 79.50(88) |
| | O(3) | 84.53(93) |
| O(8) | O(10) | 99.03(104) |
| | O(11) | 88.01(93) |
| | O(2) | 95.13(93) |
| | O(3) | 97.49(98) |
| O(10) | O(2) | 93.06(101) |
| | O(3) | 100.55(106) |
| | O(7) | 81.43(88) |
| | O(8) | 83.18(93) |
| O(7) | O(8) | 166.03 (95) |
| O(10) | O(11) | 171.47(98) |
| O(2) | O(3) | 159.70(97) |

A second form has also been prepared differing from β -WO₃ in that there is no centre of symmetry (space group P1) [60T, 63C].

References:

- 60T Tanisaki, S.: J. Phys. Soc. Jpn. 15 (1960) 566.
- 63C Crowder, B. L., Sienko, M. J.: J. Chem. Phys. 38 (1963) 1576.
- 78D Diehl, R., Brandt, G., Salje, E.: Acta Crystallogr. BM (1978) 1105.

Fig. 1.

β -WO₃ (triclinic). Corner sharing O-octahedra around one unit cell (dotted line) [78D].

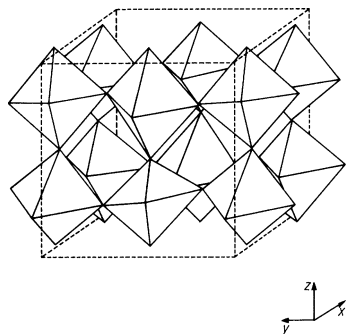


Fig. 2.

β - WO_3 (triclinic). Projection of the crystal structure onto (a) the a - b plane with W in $z \approx 3/4$, (b) the a - c plane with W in $y \approx 1/2$ and (c) the MC plane with W in $x \approx 1/4$ [78D].

