

substance: WO₃

property: structural and related data of orthorhombic WO₃:

space group D_{2h}¹⁶ – Pmnb, Z = 8, see Figs. 1 and 2.

lattice parameters

<i>a</i>	7.341(4) Å	<i>T</i> = 480°C	77S
<i>b</i>	7.570(4) Å		
<i>c</i>	7.754(4) Å		

linear thermal expansion

α_a	$1.7 \cdot 10^{-5} \text{ K}^{-1}$	<i>T</i> = 480	77S
α_b	$-1.3 \cdot 10^{-6} \text{ K}^{-1}$...680°C	
α_b	$1.8 \cdot 10^{-5} \text{ K}^{-1}$		

interatomic distances (in Å) and fractional coordinates

Atom	<i>x</i>	<i>y</i>	<i>z</i>	
W(1)	0.25	0.029	0.031	77S
W(2)	0.25	0.030	0.532	
O(1)	0	0	0	
O(1')	0.5	0	0	
O(2)	0	0	0.5	77S
O(2')	0.5	0.5	0	
O(3)	0.25	0.269	0.027	
O(4)	0.25	0.278	0.471	
O(5)	0.25	0.004	0.262	
O(6)	0.25	0.015	0.776	
<i>d</i> (W(1)–O(1))	1.86	<i>d</i> (W(2)–O(2))	1.87	
<i>d</i> (W(1)–O(1'))	1.86	<i>d</i> (W(2)–O(2'))	1.87	
<i>d</i> (W(1)–O(3))	1.81	<i>d</i> (W(2)–O(3))	2.03	
<i>d</i> (W(1)–O(4))	1.91	<i>d</i> (W(2)–O(4))	1.94	
<i>d</i> (W(1)–O(5))	1.81	<i>d</i> (W(2)–O(5))	2.10	
<i>d</i> (W(1)–O(6))	1.98	<i>d</i> (W(2)–O(6))	1.89	

References:

77S Salje, E.: Acta Crystallogr. B33 (1977) 574.

Fig. 1.

WO_3 (orthorhombic). Projection of the structure on ac -plane (a) and bc -plane (b) [77S]. Small circles W, large circles O.

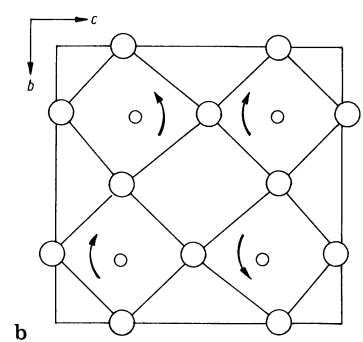
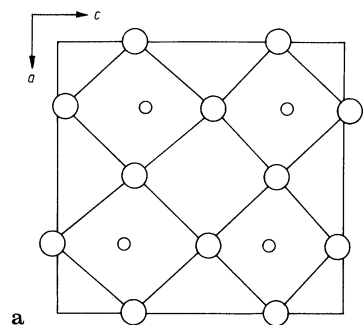


Fig. 2.

WO₃ (orthorhombic). Structure [77S]. (a), (b) and (c) show three different projections indicated by the axes *a*, *b*, *c*.

