substance: WO_3
property: structural and related data of γ-WO_3

space group C_{2h}^5 – $P2_1/c$, $Z = 8$, distorted ReO_3-structure (Figs. 1).

lattice parameters

a	7.306(1) Å	RT	69L
b	7.540(1) Å		
c	7.692(1) Å		
β	90.88º		

interatomic distances (in Å) and fractional coordinates at RT

d(W(1)–O_{x1})	1.89(6)	d(W(2)–O_{x1})	1.92(7)	66L
d(W(1)–O_{x2})	1.91(6)	d(W(2)–O_{x2})	1.85(8)	
d(W(1)–O_{y1})	1.72(6)	d(W(2)–O_{y2})	1.85(7)	
d(W(1)–O_{y1})	2.16(6)	d(W(2)–O_{y2})	2.01(8)	
d(W(1)–O_{z1})	2.13(5)	d(W(2)–O_{z1})	1.75(5)	
d(W(1)–O_{z2})	1.79(5)	d(W(2)–O_{z2})	2.15(5)	

Atom	*x*	*y*	*z*	
W(1)	0.254(6)	0.037(5)	0.282(5)	69L
W(2)	0.250(9)	0.023(6)	0.784(5)	
O_{x1}	0.005(5)	0.042(5)	0.211(4)	
O_{x2}	0.993(6)	0.474(5)	0.218(5)	
O_{y1}	0.288(3)	0.262(6)	0.286(3)	
O_{y2}	0.211(3)	0.259(8)	0.730(3)	
O_{z1}	0.292(6)	0.043(5)	0.008(4)	
O_{z2}	0.279(7)	0.487(6)	0.993(3)	

density

d	7.21 g cm^{-3}	T = 22ºC	66L

In this temperature regime, substoichiometric $WO_{2.98}$ has been indexed on space group C_{2h}^2 – $P2_1/m$ ($Z = 4$) with

lattice parameters

a	7.354(5) Å	RT	66G
b	7.569(5) Å		
c	3.854(5) Å		
β	90.6º		

References:

66G Gebert, E., Ackermann, R. J.: Inorg. Chem. 5 (1966) 136.
66L Loopstra, H. O., Boldrini, P.: Acta Crystallogr. 21 (1966) 158.
69L Loopstra, H. O., Boldrini, P.: Acta Crystallogr. B25 (1969) 1420.
77S Salje, E.: Acta Crystallogr. B33 (1977) 574.

Fig. 1.

γ-WO_3 (monoclinic). Tilt structure at room temperature [77S]. Small circles W, large circles O.