substance: NbO_2
property: crystal structure, lattice parameters, density, low-temperature modification

low-temperature form ($T \leq 800^oC$):

crystal structure: tetragonal, space group $C_{4h}^6 - I4_1/a$, $Z = 32$.

A projection of the structure along the *c* axis is shown in Fig. 1, the essential structural element in Fig. 2. The structure is related closely to rutile with NbO_6 octahedra linked to form strings. Along the strings the Nb – Nb distances alternate (at RT) between 2.80 Å [62M], 2.74 Å [76C] and 3.20 Å [62M], 3.26 Å [76C], forming Nb – Nb doublets that further tilt along the <110> or <1 $\bar{1}$ 0> directions of the rutile subcell. The relationship between the tetragonal supercell and the rutile cell is $a_{tetr} = 2^{3/2}\, a_R$ and $c_{tetr} = 2\, c_R$.

lattice parameters (tetragonal supercell)

a	13.70 Å	RT	62M
c	5.987 Å		
a	13.699 Å		77G
c	5.982 Å		
a	13.696 Å		76C
c	5.981 Å		

density

d_{calc}	5.90 g cm^{-3}	62M

atomic position parameters

Atom	*x*	*y*	*z*		
Nb(1)	0.116(1)	0.123 (2)	0.488 (3)	all ions occupy 16(f) subsets of	76C
Nb(2)	0.133(1)	0.124(2)	0.031(2)	$I4_1/a$	
O(1)	0.987(1)	0.133(2)	– 0.005(3)		
O(2)	0.976(1)	0.126(2)	0.485(3)		
O(3)	0.274(1)	0.119(2)	0.987(3)		
O(4)	0.265(1)	0.126(2)	0.509(3)		

interatomic distances

d(Nb(1)–Nb(2))	2.74(2) Å	76C
d(Nb(1)–Nb(2'))	3.26(2) Å	
d(Nb(1)–O(1'))	2.10(2) Å	
d(Nb(1)–O(2))	1.93(2) Å	
d(Nb(1)–O(2'))	2.18(2) Å	
d(Nb(1)–O(3'))	2.02(2) Å	
d(Nb(1)–O(4))	2.04(2) Å	
d(Nb(1)–O(4'))	2.01(2) Å	
d(Nb(2)–O(1))	2.02(2) Å	
d(Nb(2)–O(1'))	2.06(2) Å	
d(Nb(2)–O(2'))	2.11(2) Å	
d(Nb(2)–O(3))	1.93(2) Å	
d(Nb(2)–O(3')	2.23(2) Å	
d(Nb(2)–O(4'))	2.03(2) Å	

References:

62M Marinder, B.-O.: Ark. Kemi 19 (1962) 435.
76C Cheetham, A. K., Rao, C. N. R.: Acta Crystallogr. B32 (1976) 1579.
77G Gannon, J. R., Tilley, R. J. D.: J. Solid State Chem. 20 (1977) 331.

Fig. 1.

NbO_2. Projection of the structure along the *c* axis [62M].

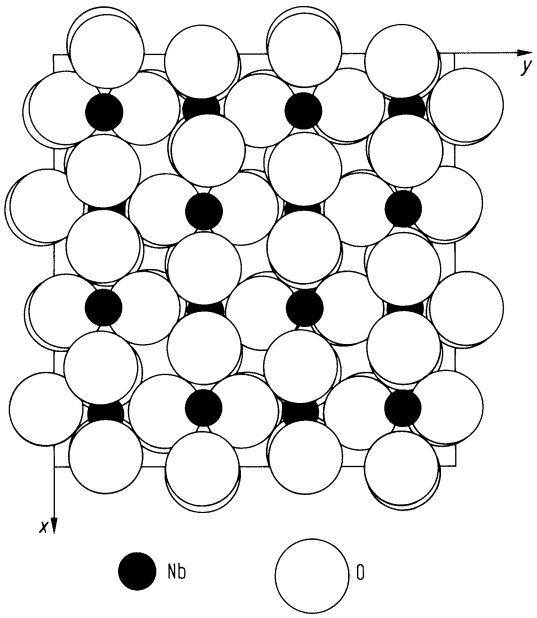

Fig. 2.

NbO_2. The essential structure unit [76C].