substance: Nb_2O_5
property: crystal structure, lattice parameters, density of T-Nb_2O_5

crystal structure: orthorhombic, space group D_{2h}^9 – Pbam, Z = 8.4

The T-form exhibits a further type of structure containing 7-coordinate Nb [75K]. Unit cell projection: Fig. 1. There are 42 O ions in the unit cell and the Nb atoms occupy 16.8 positions. This structure is closely related to that of the phase 45 $Ta_2O_5 \cdot Al_2O_3 \cdot 4WO_3$, save that the missing O positions in the latter structure are filled in T-Nb_2O_5. The 16 Nb atoms lie in a sheet parallel to (001) and are surrounded by 6 or 7 O-atoms forming pentagonal bipyramids or distorted octahedra. These polyhedra are joined by edge or corner sharing within the (001) plane and exclusively by corner sharing along the [001] axis. The "spare" Nb occupy nine-coordinate additional sites at random between the sheets.

lattice parameters

a	6.170 Å	RT	72N
b	28.25 Å		
c	3.928 Å		
a	6.175 Å		75K
b	29.175 Å		
c	3.930 Å		

density

d_{calc}	5.236 g cm^{-3}	75K

interatomic distances
(in Å) [75K]

	Nb(1)		Nb(2)		Nb(3)		Nb(4)	
d(Nb–O)								
	O(11)	2.027(3)	O(5)	2.07(2)	O(6^{iii})	1.98(1)	O(9^{ii})	1.91(2)
	O(5)	2.04(2)	O(6)	2.07(1)	O(6)	1.99(1)	O(7)	1.96(2)
	O(8^{iv})	2.06(1)	O(9)	2.09(1)	O(10^{ii})	2.01(2)	O(8)	1.96(2)
	O(8^{iii})	2.09(1)	O(10)	2.09(2)	O(7)	2.08(2)	O(5^{iii})	2.02(2)
	O(9)	2.27(1)	O(7^{ii})	2.13(1)				
	O(1^{i})	1.792(5)	O(2^{i})	1.779(2)	O(3^{i})	1.782(5)	O(4^{i})	1.770(3)
	O(1)	2.142(5)	O(2)	2.154(3)	O(3)	2.151(6)	O(4)	2.193(3)
d(Nb–Nb)								
Min.	3.282(3)		3.286(3)		3.375(4)		3.282(3)	
Max.	4.039(6)		4.057(4)		4.057(4)		3.841(3)	
Av.	3.622		3.608		3.620		3.623	
d[O(5–11)–O(5–11)]								
Min.		2.32(3)		2.34(2)		2.34(2)		2.41(2)
Max.		2.59(2)		2.64(2)		3.55(1)		3.21(2)
Av.		2.45		2.45		2.77		2.74
d[O(1–4)–O(1–4)]								
Min.		2.78(1)		2.80(2)		2.76(2)		2.69(1)
Max.		2.93(1)		2.91(2)		2.82(2)		2.88(2)
Av.		2.87		2.87		2.80		2.79
	Nb(5)		Nb(6)		Nb(7)			
d(Nb–O)								
Mm	2.11(6)		2.11(1)		1.94			
Max.	2.66(4)		2.85(2)		3.00			
Av.	2.46		2.45		2.47			

symmetric code:

(i)	*x*	*y*	1+*z*	(iii)	1/2+*x*	1/2–*y*	*z*
(ii)	–1/2+*x*	1/2–*y*	*z*	(iv)	1/2–*x*	–1/2+*y*	*z*

References:

72N Nolander, B., Norm, R.: Acta Chem. Scand. 26 (1972) 3814.
75K Kato, K., Tamura, S.: Acta Crystallogr. B31 (1975) 673.

Fig. 1.

T-Nb_2O_5. Unit cell projection parallel [001]. The small open circles represent possible positions for the nine-coordinate "additional" Nb; full circles: Nb atoms; large open circles: oxygen. Upper part: space group Pbam, lower part: space group Pbmn [75K].