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

crystal structure: monoclinic, space group C_{2h}^3 – C2/m. Closely related to M-Nb_2O_5.

Unit cell: Fig. 1. N-Nb_2O_5 is made by chemical vapour transport and favourable growth conditions are discussed in [66S].

lattice parameters

a	28.51 Å	RT	67A
b	3.830 Å		
c	17.48 Å		
β	120.8º		

atomic position parameters

[67A]

Atom	Position	*x*	*y*	*z*
Nb(1)	4(i)	0.0615(3)	0	0.0990(5)
Nb(2)	4(i)	0.1577(3)	1/2	0.0995(5)
Nb(3)	4(i)	0.2903(3)	1/2	0.0958(5)
Nb(4)	4(i)	0.4265(3)	1/2	0.0968(5)
Nb(5)	4(i)	0.0194(3)	0	0.3716(5)
Nb(6)	4(i)	0.1553(3)	0	0.3694(5)
Nb(7)	4(i)	0.2511(3)	1/2	0.3653(5)
Nb(8)	4(i)	0.3885(3)	1/2	0.3670(5)
O(1)	4(i)	0.070	1/2	0.085
O(2)	4(i)	0.129	0	0.075
O(3)	4(i)	0.273	0	0.055
O(4)	4(i)	0.409	0	0.050
O(5)	4(i)	0.021	1/2	0.353
O(6)	4(i)	0.175	1/2	0.366
O(7)	4(i)	0.234	0	0.361
O(8)	4(i)	0.376	0	0.362
O(9)	4(i)	0.216	1/2	0.085
O(10)	4(i)	0.348	1/2	0.069
O(11)	4(i)	0.480	1/2	0.053
O(12)	4(i)	0.103	0	0.223
O(13)	4(i)	0.199	1/2	0.221
O(14)	4(i)	0.335	1/2	0.221
O(15)	4(i)	0.484	1/2	0.229
O(16)	4(i)	0.085	0	0.352
O(17)	4(i)	0.300	1/2	0.336
O(18)	4(i)	0.460	1/2	0.379
O(19)	4(i)	0.064	0	0.492
O(20)	4(i)	0.210	0	0.497

interatomic distances

[67A] (data in Å, RT values)

	Distance *d*		Mean value		Distance *d*		Mean value
2	Nb(1)–O(1)	1.96		2	Nb(5)–O(5)	1.95	
	Nb(1)–O(2)	2.19			Nb(5)–O(15)	2.09	
	Nb(1)–O(11)	1.98	2.01		Nb(5)–O(16)	2.08	1.93
	Nb(1)–O(12)	2.21			Nb(5)–O(18)	1.77	
	Nb(1)–O(12)	1.78			Nb(5)–O(19)	1.73	
2	Nb(2)–O(2)	2.03		2	Nb(6)–O(6)	2.01	
	Nb(2)–O(1)	2.36			Nb(6)–O(7)	2.33	
	Nb(2)–O(4)	2.18	2.03		Nb(6)–O(12)	2.10	2.03
	Nb(2)–O(9)	1.82			Nb(6)–O(16)	1.85	
	Nb(2)–O(13)	1.74			Nb(6)–O(20)	1.85	
2	Nb(3)–O(3)	2.00		2	Nb(7)–O(7)	1.97	
	Nb(3)–O(3)	2.18			Nb(7)–O(6)	2.18	
	Nb(3)–O(9)	2.02	1.99		Nb(7)–O(13)	2.07	1.99
	Nb(3)–O(10)	1.95			Nb(7)–O(17)	1.74	
	Nb(3)–O(14)	1.81			Nb(7)–O(20)	1.99	
2	Nb(4)–O(4)	2.03		2	Nb(8)–O(8)	1.94	
	Nb(4)–O(2)	2.47			Nb(8)–O(14)	2.08	
	Nb(4)–O(10)	2.00	2.08		Nb(8)–O(17)	2.26	2.03
	Nb(4)–O(11)	2.06			Nb(8)–O(18)	1.93	
	Nb(4)–O(15)	1.92			Nb(8)–O(19)	2.02	

References:

66S Schäfer, H., Gruehn, R., Schultz, F.: Angew. Chem. Int. Ed. Engl. 5 (1966) 40.
67A Anderson, S.: Z. Anorg. Allgem. Chem. 351 (4967) 106.

Fig. 1.

N–Nb_2O_5. Unit cell [67A]. Open and full circles: Nb atoms at $y = 0$ and $y = 1/2$.