

**substance:** Nb<sub>2</sub>O<sub>5</sub>

**property:** crystal structure, lattice parameters of M-Nb<sub>2</sub>O<sub>5</sub>

**crystal structure:** tetragonal, space group D<sub>4h</sub><sup>17</sup> – I4/mmm; Z = 16. The idealized M-form is given in Fig. 1 and a projection of the unit cell in Fig. 2. M-Nb<sub>2</sub>O<sub>5</sub> can be grown by chemical vapour transport provided a SnO<sub>2</sub> catalyst is present [68E].

**lattice parameters**

<i>a</i>	20.01 Å	RT	70W
<i>c</i>	3.84 Å		
<i>a</i>	20.44 Å	70M	
<i>c</i>	3.832 Å		

**density**

<i>d</i>	4.4 g cm <sup>-3</sup>	X-ray density	66S
	4.3...4.4 g cm <sup>-3</sup>	pycnometric density	66S

**atomic position parameters**

[70M]

Atom	Position	<i>x</i>	<i>y</i>	<i>z</i>
Nb(1)	8(i)	0.1294(6)	0	0
Nb(2)	8(i)	0.4047(9)	0	0
Nb(3)	16(l)	0.2738(5)	0.1344(5)	0
O(1)	8(j)	0.3479(74)	1/2	0
O(2)	8(j)	0.0731(64)	1/2	0
O(3)	16(l)	0.2095(55)	0.3402(55)	0
O(4)	8(h)	0.0678(42)	= <i>x</i>	0
O(5)	8(h)	0.2116(56)	= <i>x</i>	0
O(6)	16(l)	0.2095(34)	0.0727(33)	0
O(7)	16(l)	0.3555(45)	0.0630(44)	0

**Nb – O distances**

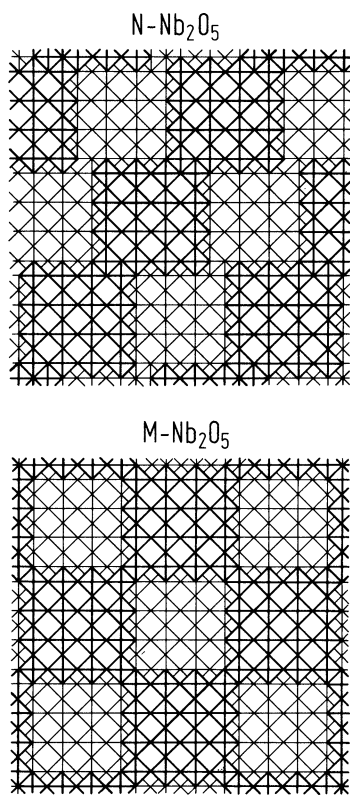
<i>d</i> (Nb(1)–O(1)) (2×)	1.971 Å	RT	70M
<i>d</i> (Nb(1)–O(4)) (2×)	1.874 Å		
<i>d</i> (Nb(1)–O(6)) (2×)	2.211 Å		
<i>d</i> (Nb(2)–O(2)) (2×)	2.455 Å		
<i>d</i> (Nb(2)–O(2)) (2×)	1.969 Å		
<i>d</i> (Nb(2)–O(7)) (2×)	1.636 Å		
<i>d</i> (Nb(3)–O(3))	2.048 Å		
<i>d</i> (Nb(3)–O(3)) (2×)	2.014 Å		
<i>d</i> (Nb(3)–O(5))	2.026 Å		
<i>d</i> (Nb(3)–O(6))	1.823 Å		
<i>d</i> (Nb(3)–O(7))	2.219 Å		

## References:

- 66S Schäfer, H., Gruehn, R., Schultz, F.: *Angew. Chem. Int. Ed. Engl.* 5 (1966) 40.
- 68E Emmenegger, F. P., Robinson, M. L. A.: *J. Phys. Chem. Solids* 29 (1968) 1673.
- 70M Mertin, W., Anderson, S., Gruehn, R.: *J. Solid State Chem.* 1 (1970) 419.
- 70W Wadsley, A. D., Anderson, S.: *Perspectives in Structural Chemistry*, Dunitz, J. D., Ibers, J. A. (eds.)  
New York: Academic Press 3 (1970) 1.

**Fig. 1.**

N- and M-Nb<sub>2</sub>O<sub>5</sub>. Idealized structure [70M].



**Fig. 2.**

M-Nb<sub>2</sub>O<sub>5</sub>. Projection of the unit cell in the *ab* plane [70M].

