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

crystal structure: monoclinic, space group C_{2h}^6 – C2/c, $Z = 4$.

The structure can be described as hexagonal close packed with 2/5 of the octahedral holes filled in such a way as to lead to hexagonal layers parallel to $(2\,\bar{1}\,0)$ with the *a*-axis in (001) (Fig. 1).

lattice parameters

a	12.73 Å	RT		64L,
b	4.88 Å			70W
c	5.56 Å			
β	105.1°			

density

d	5.29 g cm^{-3}	X-ray density	64L, 70W

atomic position parameters

	– *x*	– *y*	– *z*	
8 Nb in (f) sites	0.140,	0.249,	0.238	64L,
4 O(1) in (c) sites	0,	0.25,	0.099	70W
8 O(2) in (f) sites	0.389,	0.031,	0.054	
8 O(3) in (f) sites	0.295,	0.375,	0.426	

Nb–O distances in each of the octahedra

d(Nb–0)	1.91 Å	RT	64L
	1.81 Å		
	2.06 Å		
	2.12 Å		
	2.19 Å		
	1.94 Å		

References:

64L Laves, F., Petter, W., Wulf, H.: Naturwiss. 51 (1964) 633.
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.

B–Nb_2O_5. Idealized structure and its relationship to rutile and PdF_3 [70W].