substance: Nb_2O_5
property: crystal structure, lattice parameters of R-Nb_2O_5

crystal structure: monoclinic, space group C_{2h}^3 – C2/m, Z = 2.

The structure is essentially identical to that of idealized V_2O_5 [66G] (Fig. 1). The unit cell contains 4 Nb and 4 O at the 4(i) positions x, 0, z; $–x$, 0, $–z$; x, 1/2, 1/2+z; –x, 1/2, 1/2–z, where, for Nb, x = 0.07(1), z = 0.146(2), for O, x = 0.00(4), z = 0.68(1). There are two further O at the 2(a) positions 0, 0, 0; 0, 1/2, 1/2. The R-form is metastable and converts to the P-form on slow heating and to the N-form on rapid heating [75P].

lattice parameters

a	12.79 Å	RT	66G,
b	3.826 Å		70W
c	3.983 Å		
β	90.75°		

References:

66G Gruehn, R.: J. Less-Common Met. 11 (1966) 119.

70W Wadsley, A. D., Anderson, S.: Perspectives in Structural Chemistry, Dunitz, J. D., Ibers, J. A. (eds.) New York: Academic Press 3 (1970) 1.

75P Plies, Y., Gruehn, R.: J. Less-Common Met. 42 (1975) 77.

Fig. 1.

R–Nb_2O_5. Idealized structure [66G]. Dashed lines indicate unit cell.