substance: V_2O_3
property: crystal structure, lattice parameters of pure material, room-temperature phase

Corundum structure, trigonal space group D_{3d}^6 – $R\bar{3}c$, Z = 6. This phase is normally V-deficient, phase diagram: Fig. 1. Detailed structure: Fig. 2.

lattice parameters

a	4.9717 Å	T = 298 K	lattice parameters as a function	78B1,
c	14.005 Å		of x in V_2O_{3+x} and as a	78B2
c/a	2.8283		function of pressure: Fig. 3	
a	$4.954 + 1.619\cdot10^{-4}\,T - 6.905\cdot10^{-8}\,T^2$	T = 298...1273 K	anomalous variation of lattice parameters above room temperature: Fig. 4	73E
c	$13.963 - 1.68\cdot10^{-4}\,T + 1.577\cdot10^{-7}\,T^2$			
a	4.9492 Å		variation of c/a ratio with	75R
c	13.998 Å		temperature: Fig. 5	
c/a	2.828			
V	296.94 Å^3			
a	4.951 Å			73P
c	14.007 Å			
a_{rh}	5.474 Å	T = 300 K	rhombohedral	78B1,
α_{rh}	53.80°		cell parameters	78B2

References:

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73E Eckert, L. J., Bradt, R. C.: J. Appl. Phys. 44 (1973) 3470.
73P Pouchard, M., Launay, J. C.: Mater. Res. Bull. 8 (1973) 95.
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78B1 Belbéoch, R., Kleinberger, R., Roulliay, M.: Solid State Commun. 25 (1978) 1043.
78B2 Belbéoch, R., Kleinberger, R., Roulliay, M.: J. Solid State Chem. 39 (1978) 1007.
80U Ueda, Y., Kosuge, K., Kachi, S.: J. Solid State Chem. 31 (1980) 171.
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Fig. 1.

V_2O_{3+x}. (Magnetic) phase diagram obtained from experimental results [80U]. PI: paramagnetic insulator, PM paramagnetic metal, AFI: antiferromagnetic insulator AFM: antiferromagnetic metal. Hatched area shows region where the upper transition is seen.

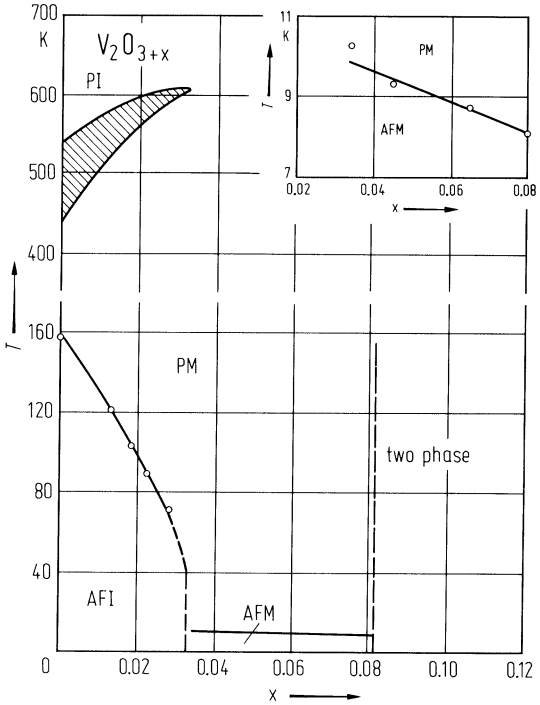

Fig. 2.

V_2O_3. Relationships between V-atoms in hexagonal, rhombohedral and monoclinic unit cells. The primitive rhombohedral axes are shown as bold lines in (a). The magnetic and crystallographic unit cells are shown in (b). Spins on the filled circles are opposite to those on the open circles. Assuming equivalent metal atoms, the magnetic monoclinic cell is half ($a'_m = 1/2\ a_m$) of the crystallographic cell. [81W]. $J_\alpha ... J_\varepsilon$ are magnetic coupling constants.

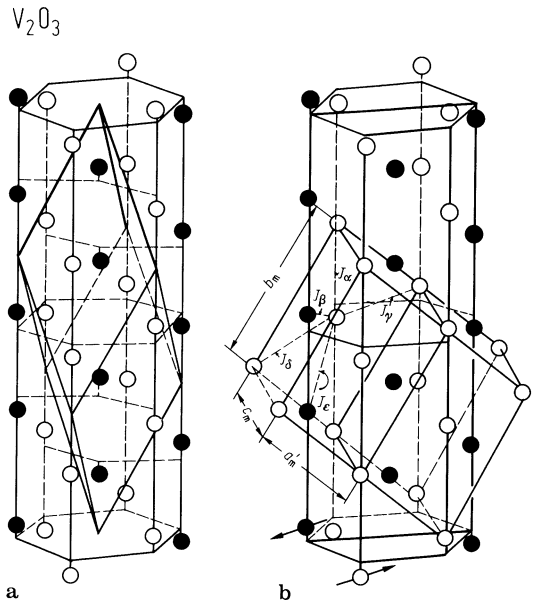

Fig. 3.

V_2O_{3+x}.Comparison of the lattice parameters vs. composition x for V_2O_{3+x}, $(V_{1-x}Ti_x)_2O_3$ and vs. pressure for V_2O_3 [70M].

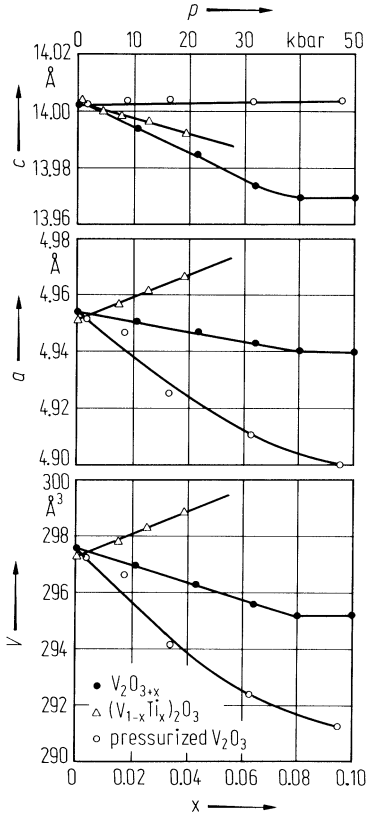

Fig. 4.

V_2O_3. Lattice constants a_{rh}, α_{rh} in the rhombohedral unit cell vs. temperature [78B1].

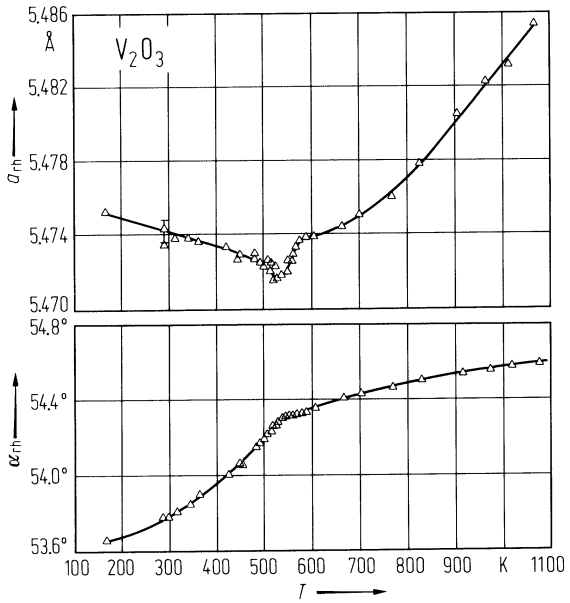

Fig. 5.

V_2O_3, $(V_{0.96}Cr_{0.04})_2O_3$. *c*/*a* ratios vs. temperature. Inset: *c*/*a* ratios for metal oxides of the corundum structure. Open circles: first heating cycle, triangles: second heating cycle, full circles: cooling cycle [69M].