

substance: V₂O₃

property: interatomic distances in pure material, low-temperature phase

changes in interatomic distances

(in Å) (from [70D]) (see also Fig. 1)

	Monoclinic V ₂ O ₃ (<i>T</i> = 148 K)	Corundum *) (trigonal) V ₂ O ₃ (<i>T</i> = 148 K)
V(1) – V(2)	2.745(2)	2.700(1)
V(1) – V(3)	2.987(4)	2.872(1)
(<i>a-c</i> plane)		
V(1)–V(3)	2.861(9)	2.872(1)
(adjacent layer)		
V(1)–V(3)	2.876(9)	2.872(1)
(adjacent layer)		
V(1)–O(1)	2.028(8)	2.046(1)
V(1)–O(5)	2.065(14)	2.046(1)
V(1)–O(3)	2.108(12)	2.046(1)
V(1)–O(2)	1.989(10)	1.967(1)
V(1)–O(4)	1.954(11)	1.967(1)
V(1)–O(6)	1.963(11)	1.967(1)
O(1)–O(2)	2.84(1)	2.803(1)
O(1)–O(3)	2.67(3)	2.664(2)
O(1)–O(5)	2.68(2)	2.664(2)
O(3)–O(5)	2.68(2)	2.664(2)
O(1)–O(6)	2.83(1)	2.890(1)
O(2)–O(6)	2.99(3)	2.947(1)
O(2)–O(4)	2.99(3)	2.947(1)
O(4)–O(6)	2.97(1)	2.947(1)

*) Corundum data obtained from low-temperature lattice parameters and RT positional parameters

References:

- 70D Dernier, P. D., Marezio, M.: Phys. Rev. B2 (1970) 3771.
75R Robinson, W. R.: Acta Crystallogr. B31 (1975) 1153.

Fig. 1

V_2O_3 . (a) Projection of the structure onto a plane perpendicular to $[\bar{1}\bar{1}0]$. The V-atoms are at zero height and the O are above and below the plane. The arrows indicate the direction of translation of V in the M - AF transition [70D], (b) variation of V-V and V-O distances for V_2O_3 (full circles), $\beta\text{-Cr-V}_2\text{O}_3$ (open circles), and ranges of thermal corrections for V_2O_3 (dot shaded) and $\beta\text{-Cr-V}_2\text{O}_3$ (line shaded) [75R].

