

substance: V₂O₃

property: properties of Cr and Al doped material: interatomic distances and angles

Doping with Cr has a marked effect on the lattice parameters [70D2]. Two forms of V₂O₃ Cr have been detected [74H, 75R] labelled α and β . The α -form converts smoothly into the β -form over a wide temperature range.

interatomic distances and angles

(distances in Å, angles in °, from [75R]): (see also Fig. 1)

(two values correspond to upper and lower limits on crystallographic distances)

	α Cr-V ₂ O ₃	β Cr-V ₂ O ₃		
	$T = 23^\circ\text{C}$	$T = 23^\circ\text{C}$	$T = 113^\circ\text{C}$	$T = 310^\circ\text{C}$
M(1)–M(2)	2.700(1) 2.706	2.747(1) 2.754	2.746(1) 2.754	2.739(1) 2.750
M(1)–M(3)	2.884(1) 2.889	2.917(1) 2.922	2.919(1) 2.925	2.920(1) 2.929
M(1)–O(1)	2.050(1) 2.060	2.061(1) 2.070	2.061(1) 2.072	2.062(2) 2.078
M(1)–O(5)	1.970(1) 1.981	1.976(1) 1.986	1.977(1) 1.989	1.979(1) 1.996
O(1)–O(2)	2.673(3) 2.682	2.661(2) 2.669	2.663(2) 2.673	2.670(2) 2.683
O(1)–O(4)	2.802(1) 2.813	2.792(1) 2.801	2.793(1) 2.803	2.796(1) 2.810
O(1)–O(5)	2.890(1) 2.899	2.897(1) 2.904	2.898(1) 2.905	2.899(1) 2.910
O(4)–O(5)	2.958(2) 2.966	3.004(1) 3.011	3.006(1) 3.015	3.006(1) 3.016
O(1)–M(1)–O(2)	81.36(5)	80.42(4)	80.47(4)	80.70(4)
O(1)–M(1)–O(4)	88.36(2)	87.51(1)	87.47(1)	87.51(1)
O(1)–M(1)–O(5)	91.91(4)	91.71(3)	91.68(3)	91.63(3)
O(1)–M(1)–O(6)	168.43(6)	166.50(5)	166.52(5)	166.81(5)
O(4)–M(1)–O(5)	97.32(2)	98.93(2)	98.95(2)	98.79(2)
M(1)–O(1)–M(2)	82.36(6)	83.60(5)	83.54(6)	83.24(6)
M(1)–O(2)–M(3)	91.64(2)	92.49(1)	92.53(2)	92.47(1)
M(2)–O(2)–M(3)	133.23(3)	133.05(2)	133.04(3)	133.04(3)

References:

- 70D1 Dernier, P. D., Marezio, M.: Phys. Rev. B2 (1970) 3771.
- 70D2 Dernier, P. D.: J. Phys. Chem. Solids 31 (1970) 2569.
- 74H Honig, J. M., Chandrashekhar, G. V., Sinha, A. P. B.: Phys. Rev. Lett. 32 (1974) 13.
- 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 [70D1], (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].

