substance: V_2O_3
property: interatomic distances and angles of pure material, room-temperature phase

interatomic distances and angles

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

(Two values for each distance correspond to the lower and upper limits.)

	T = 23ºC	115ºC	212ºC	300ºC	400ºC	600ºC
V(1)–V(2)	2.697(1)	2.705(1)	2.718(1)	2.728(1)	2.734(1)	2.738(1)
	2.705	2.714	2.730	2.741	2.748	2.755
V(1)–V(3)	2.880(1)	2.888(1)	2.900(1)	2.910(1)	2.916(1)	2.924(1)
	2.885	2.895	2.909	2.920	2.927	2.939
V(1)–O(1)	2.051(1)	2.053(1)	2.057(2)	2.061(1)	2.064(1)	2.066(1)
	2.061	2.065	2.072	2.078	2.083	2.090
V(1)–O(5)	1.968(1)	1.970(1)	1.973(1)	1.975(2)	1.977(2)	1.981(1)
	1.978	1.983	1.989	1.993	1.997	2.006
O(1)–O(2)	2.676(3)	2.675(3)	2.675(4)	2.676(3)	2.680(3)	2.681(3)
	2.685	2.685	2.687	2.690	2.696	2.701
O(1)–O(4)	2.804(1)	2.802(1)	2.800(1)	2.799(2)	2.799(2)	2.800(1)
	2.813	2.813	2.814	2.814	2.815	2.821
O(1)–O(5)	2.889(1)	2.891(2)	2.893(1)	2.895(2)	2.897(1)	2.901(1)
	2.894	2.898	2.903	2.906	2.909	2.916
O(4)–O(5)	2.952(1)	2.962(2)	2.978(1)	2.990(1)	2.997(2)	3.007(1)
	2.958	2.973	2.989	3.002	3.010	3.023
O(1)–V(1)–O(2)	81.45(7)	81.30(7)	81.11(7)	80.95(7)	80.93(7)	80.89(7)
O(1)–V(1)–O(4)	88.46(2)	88.27(2)	87.99(2)	87.77(2)	87.67(2)	87.52(2)
O(1)–V(1)–O(5)	91.90(5)	91.85(5)	91.74(5)	91.65(5)	91.55(5)	91.52(5)
O(1)–V(1)–O(6)	168.62(8)	168.26(8)	167.74(8)	167.33(8)	167.17(8)	167.00(7)
O(4)–V(1)–O(5)	97.17(3)	97.49(3)	97.98(3)	98.36(3)	98.56(3)	98.73(3)
V(1)–O(1)–O(2)	82.23(9)	82.44(9)	82.69(9)	82.90(9)	82.92(9)	82.98(9)
V(1)–O(2)–V(3)	91.54(3)	91.73(2)	92.01(2)	92.23(2)	92.35(2)	92.48(2)
V(2)–O(2)–V(3)	133.21(5)	133.18(4)	133.11(4)	133.04(4)	132.98(4)	132.98(4)

Only single-phase behaviour is seen in this temperature range [75M, 74C, 76R, 78B], and the anomalous variations in lattice parameters appear to correspond to a broad higher-order transition centred at 533 K.

References:

70D Dernier, P. D., Marezio, M.: Phys. Rev. B2 (1970) 3771.
74C Chandrashekhar, G. V., Sinha, A. P. B., Honig, J. M.: Phys. Lett. A47 (1974) 185.
75M McWhan, D. B., Jayaraman, A., Remeika, J. P., Rice, T. M.: Phys. Rev. Lett. 34(1975) 547.
75R Robinson, W. R.: Acta Crystallogr. B31 (1975) 1153.
76R Rice, C. E., Robinson, W. R.: Phys. Rev. B13 (1976) 3655.
78B Belbéoch, R., Kleinberger, R., Roulliay, M.: J. Solid State Chem. 39 (1978) 1007.

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), β-Cr– V_2O_3 (open circles), and ranges of thermal corrections for V_2O_3 (dot shaded) and β-Cr–V_2O_3 (line shaded) [75R].