substance: Ti_2O_3
property: crystal structure, lattice parameters, density

crystal structure: same as α-Al_2O_3, trigonal space group D_{3d}^6 – $R\bar{3}c$, $Z = 2$ (rhombohedral system), $Z = 6$ (hexagonal system). Projection of the structure on the (110) plane: Fig. 1. If the temperature is raised, the unit cell dimensions alter in a very anomalous manner so as to increase the *c*/*a* ratio dramatically [77R, 76R]. This change is reflected in the considerable expansion in the Ti – Ti separation across a shared face (Fig. 2).

lattice parameters, interatomic distances and angles

(distances in Å, angles in °, from [77R])

Parameter	T = 23°C	117°C	177°C	217°C	292°C	348°C	440°C	595°C
a_{hex}	5.1570(4)	5.1571(4)	5.1417(3)	5.1348(5)	5.1286(3)	5.1260(4)	5.1257(4)	5.1251(4)
c_{hex}	13.610(1)	13.631(1)	13.731(1)	13.783(2)	13.839(2)	13.878(2)	13.914(2)	13.957(2)
V(Å^3)	313.46	313.95	314.38	314.71	315.24	315.81	316.59	317.48
c/*a*	2.639	2.643	2.670	2.684	2.698	2.707	2.715	2.723
d(Ti(1)–Ti(2))	2.582(2)	2.590(2)	2.622(2)	2.645(1)	2.670(2)	2.685(1)	2.699(1)	2.722(2)
	2.592	2.601	2.636	2.659	2.686	2.701	2.717	2.743
d(Ti(1)–Ti(3))	2.994(1)	2.994(1)	2.987(1)	2.984(1)	2.983(1)	2.983(1)	2.984(1)	2.985(1)
	3.002	3.003	2.997	2.996	2.995	2.995	2.998	3.003
d(Ti(1)–O(1))	2.068(2)	2.070(2)	2.074(2)	2.077(2)	2.081(2)	2.083 (2)	2.088(2)	2.093(2)
	2.081	2.086	2.093	2.096	2.102	2.104	2.113	2.123
d(Ti(1)-O(5))	2.024(1)	2.024(1)	2.021(1)	2.020(1)	2.018(1)	2.018(1)	2.017(2)	2.017(2)
	2.037	2.040	2.040	2.040	2.040	2.040	2.042	2.048
d(O(1)–O(2))	2.798(4)	2.798(4)	2.784(4)	2.773(4)	2.764(4)	2.759(4)	2.762(4)	2.753(5)
	2.808	2.811	2.801	2.790	2.781	2.777	2.782	2.778
d(O(1)–O(4))	2.791(1)	2.793(1)	2.803(1)	2.807(1)	2.812(1)	2.816(1)	2.821(1)	2.824(1)
	2.802	2.807	2.819	2.825	2.830	2.834	2.842	2.850
d(O(1)–O(5))	2.879(1)	2.882(1)	2.893(1)	2.900(1)	2.907(1)	2.912(1)	2.916(1)	2.923(1)
	2.889	2.894	2.908	2.916	2.923	2.928	2.934	2.946
d(O(4)–O(5))	3.071(2)	3.071(2)	3.065(2)	3.065(2)	3.064(2)	3.065(2)	3.063(2)	3.067(2)
	3.080	3.082	3.079	3.080	3.080	3.080	3.080	3.090
angles								
O(1)–Ti(1)–O(2)	85.16(7)	85.03(7)	84.30(7)	83.77(6)	83.23(7)	82.93(7)	82.80(8)	82.34(8)
O(1)–Ti(1)–O(4)	85.98(2)	86.02(2)	86.35(2)	86.46(2)	86.60(3)	86.69(2)	86.81(3)	86.85(3)
O(1)–Ti(1)–O(5)	89.41(5)	89.45(5)	89.86(5)	90.12(5)	90.33(6)	90.47(6)	90.48(6)	90.64(6)
O(1)–Ti(1)–O(6)	169.96(8)	169.42(8)	169.42(8)	168.98(7)	168.54(8)	168.32(8)	168.24(9)	167.78(9)
O(4)–Ti(1)–O(5)	98.64(3)	98.66(3)	98.59(3)	98.68(3)	98.78(4)	98.80(3)	98.80(4)	98.98(4)
Ti(1)–O(1)–Ti(2)	77.24(9)	77.42(9)	78.41(9)	79.13(9)	79.85(10)	80.25(10)	80.44(10)	81.06(11)
Ti(1)–O(2)–Ti(3)	94.02(2)	93.98(2)	93.65(2)	93.54(2)	93.40(3)	93.30(3)	93.19(3)	93.15(3)
Ti(2)–O(2)–Ti(3)	132.29(5)	132.30 (5)	132.45(5)	132.56(4)	132.61(5)	132.65(5)	132.59(5)	132.76(5)

density

d	4.590(1) g cm^{-3}	RT	77R

Earlier workers [73E, 68R] reported similar data, [75B] presents thermal expansion data below room temperature.

References:

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73E Eckert, L. J., Bradt, R. C.: J. Appl. Phys. 44 (1973) 3470.
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Fig. 1.

Ti_2O_3. Projection of the structure on (110) [77R].

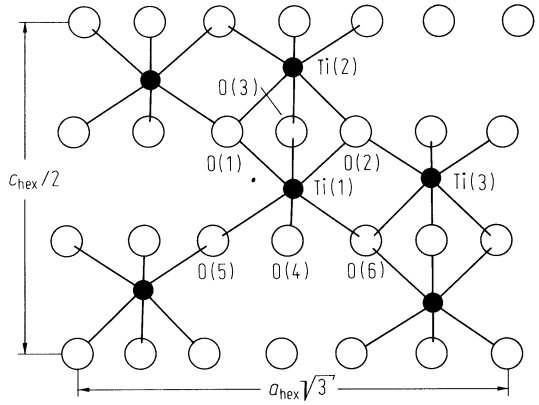

Fig. 2.

Ti_2O_3. Interatomic distances vs. temperature [77R].