substance: hematite (α-Fe_2O_3)
property: general characterization, crystal structure, lattice parameters

Fe_2O_3 is a line phase n-type semiconductor which, unusually, can also be doped p-type. Heating at 1 kbar oxygen and 500...700°C for long periods gave no evidence of higher oxide phases [71D, 72S].

crystal structure: rhombohedral (hexagonal), space group $D_{3d}^6 - R\bar{3}c$, $Z = 6$. See Figs. 1, 2.

lattice parameters

a_{rh}	5.427 Å	RT	temperature dependence: Fig. 3	62N
α_{rh}	55.271°		relationship between trigonal	
a_{hex}	5.0345 Å		and hexagonal unit cells: see	
c_{hex}	13.749 Å		[→6-5;1} (Cr_2O_3).	
a_{hex}	5.03490(9) Å	$T = 298$ K		67S
c_{hex}	13.7524(18) Å			
z(Fe)	0.355	RT		62N
x(O)	0.300			
d(Fe_1–O_1)	2.09 Å (2.116) Å	RT	for the Fe_i and O_i see Fig. 1;	62N
d(Fe_1–O_5)	1.96 Å (1.945) Å		values in parentheses: [69P]	
d(Fe_1–Fe_2)	2.89 Å (2.900) Å			
d(Fe_1–Fe_3)	2.97 Å (2.971) Å			
d(Fe_1–Fe_4)	3.37 Å (3.364) Å			
d(Fe_1–Fe_5)	3.70 Å (3.706) Å			
d(O_1–O_2)	2.62 Å (2.669) Å			
d(O_1–O_3)	3.06 Å (3.035) Å			
d(O_1–O_4)	2.76 Å (2.775) Å			
d(O_1–O_5)	2.89 Å (2.888) Å			
angles				
(Fe_1–O_1–Fe_2)	87.4° (86.6)°			
(O_1–O_2–Fe_3)	94.1° (94.0) °			
(Fe_1–O_5-Fe_4)	118.2° (119.7)°			
(Fe_1–O_1–Fe_5)	132.1° (131.7)°			
(O_1–Fe_1–O_2)	77.5° (78.2)°			
(O_1–Fe_1–O_5)	85.9° (86.1)°			
(O_5–Fe_1–O_6)	102.7° (102.6)°			
(O_1–Fe_1–O_6)	161.5° (162.4)°			

The cell constants show an anomaly in the region of the Néel temperature (≈ 690°C) (Fig. 3). Dilatometry also shows anomalies at 684 and 726°C [62R], at 687°C only [64I]. Anomalies in differential thermal analysis: 675 and 725°C [62A].

pressure dependence of a_{hex}, c_{hex}, a_{rh}, α_{rh}, V/V_0

From [66L]:

a_{hex} [Å]	c_{hex} [Å]	a_{rh} [Å]	α_{rh} [°]	V/V_0	p [kbar]
5.035	13.749	5.427	55.27	1.000	0.001
5.017	13.705	5.409	55.26	0.990	48
5.000	13.661	5.392	55.24	0.980	79
4.982	13.617	5.374	55.22	0.970	106
4.964	13.574	5.356	55.20	0.960	130
4.946	13.530	5.338	55.18	0.950	154
4.928	13.487	5.320	55.17	0.940	176
4.910	13.444	5.302	55.15	0.930	198
4.893	13.400	5.284	55.14	0.920	220
4.884	13.375	5.275	55.13	0.915	230

From [80F] at RT

a_{hex} [Å]	c_{hex} [Å]	c/a	p [kbar]
5.0346	13.7473	2.731	0.001
5.0250	13.7163	2.729	15.4
5.0143	13.6733	2.727	31.4
5.0080	13.6467	2.725	41.6
5.0067	13.6111	2.725	43.9
5.0020	13.6202	2.723	52.4

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Fig. 1.

Fe_2O_3. Projection of the corundum structure on $(2\,\bar{1}\,0)$. The figures refer to the vertical distances (in Å) from the oxygens to the plane of projection for the isostructural Al_2O_3. The metal ions lie at height zero [62N].

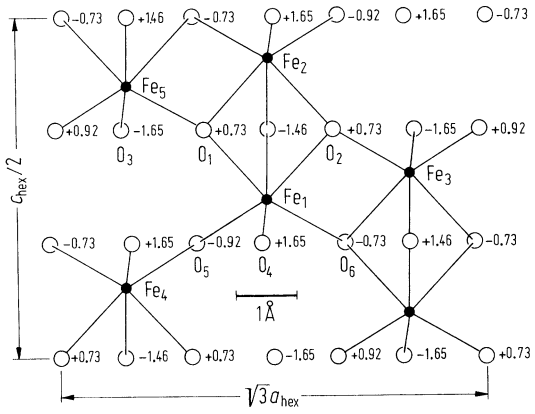

Fig. 2.

Fe_2O_3. The rhombohedral unit cell of the corundum structure [70S].

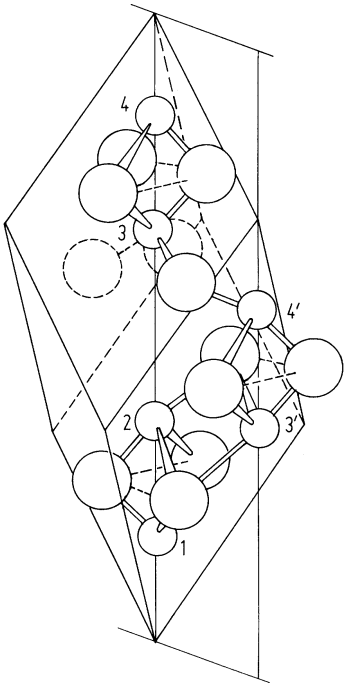

Fig. 3.

Fe_2O_3. Lattice parameters a_{hex} (a), c_{hex} (b) and the ratio c_{hex}/a_{hex} (c) vs. temperature. Anomaly found near the Néel temperature ($T_N \approx 682^oC$) [77N].