

substance: chromium sesquioxide (Cr₂O₃)

property: crystal structure, lattice parameters

crystal structure: corundum, space group $D_{3d}^6 - R\bar{3}c$, $Z = 6$. Rhombohedral unit cell: Fig. 1. Connection with hexagonal unit cell: $a_{\text{hex}} = 2 a_{\text{rh}} \sin(\alpha_{\text{rh}}/2)$, $c_{\text{hex}} = 3 a_{\text{rh}} \cos \gamma$, where $\sin \gamma = (2/3^{1/2}) \sin(\alpha_{\text{rh}}/2)$. In corundum, Cr atoms occupy the 12(c) sites at $\pm (0\ 0\ z, 0\ 0\ z+1/2)$ and O atoms occupy the 18(e) sites at $\pm (x\ 0\ 1/4; 0\ x\ 1/4; -x, -x\ 1/4)$, where $z = 0.3475(3)$, $x = 0.306(4)$ [62N]. There is a lattice anomaly near the Néel temperature ($T_N \approx 33^\circ\text{C}$) (Fig. 2).

lattice parameters

(hexagonal unit cell)

a	4.9607 Å	RT	62N
c	13.599 Å		
a	4.95762(8) Å	RT	67S
c	13.5874(10) Å		
a	4.9590 Å	$T = 25^\circ\text{C}$	72K
c	13.589 Å		
a	4.9999 Å	$T = 1070^\circ\text{C}$	
c	13.680 Å		
a	5.0191 Å	$T = 1470^\circ\text{C}$	
c	13.731 Å		
a	5.0324 Å	$T = 1670^\circ\text{C}$	
c	13.765 Å		
$d(\text{Cr-Cr})$	2.65 Å	across a shared face	66L
	2.89 Å	across a shared edge	
$d(\text{Cr-O}_1)$	2.016 Å	$p \approx 1$ bar	66L
	1.965 Å	$p \approx 28.6$ kbar	
$d(\text{Cr-O}_2)$	1.965 Å	$p \approx 1$ bar	66L
	1.906 Å	$p \approx 28.6$ kbar	

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

From [66L]:

a_{hex} [Å]	c_{hex} [Å]	a_{rh} [Å]	α_{rh} [deg]	V/V_0	p [kbar]
4.961	13.600	5.362	55.11	1.000	10^{-3}
4.940	13.579	5.350	54.99	0.990	20
4.918	13.558	5.338	54.87	0.980	50
4.897	13.537	5.325	54.74	0.970	85
4.876	13.516	5.312	54.62	0.960	122
4.854	13.496	5.299	54.49	0.950	161
4.832	13.475	5.286	54.36	0.940	203
4.811	13.454	5.273	54.23	0.930	244
4.790	13.433	5.260	54.10	0.920	286
4.779	13.422	5.253	54.04	0.915	308

From [80F] at RT

a_{hex} [Å]	c_{hex} [Å]	c/a	p [kbar]
4.9511	13.5656	2.740	0.001
4.9371	13.530	2.740	18.6
4.9233	13.4953	2.741	40.6
4.9128	13.4689	2.742	56.8

References:

- 62N Newnham, R. E., de Haan, Y. M.: Z. Kristallogr. 117 (1962) 235.
66L Lewis, G. K., Drickamer, H. G.,: J. Chem. Phys. 45 (1966) 224.
67S von Steinwehr, H. E.: Z. Kristallogr. 125 (1967) 377.
70S Samuelson, E. J., Hutchings, M. I., Shirane, G.: Physica 48 (1970) 13.
72K Kudielka, H.: Monatsh. Chem. 103 (1972) 72.
76A Alberts, H. L., Boeyens, J. C. A.: J. Mag. Magn. Mater. 2 (1976) 327.
80F Finger, L. W., Hazen, R. M.: J. Appl. Phys. 51 (1980) 5362.

Fig. 1.

Cr_2O_3 . Rhombohedral cell of the corundum structure [70S]. Small spheres are metal ions.

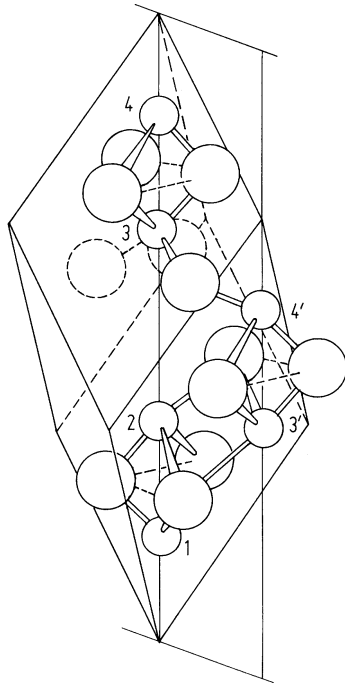


Fig. 2.

Cr_2O_3 . Reciprocal lattice parameters a^* and α^* of the rhombohedral setting vs. temperature [76A].

