

substance: Mn_2O_3

property: phase diagram, crystal structure, lattice parameters of high temperature phase

phase diagram: see Fig. 1.

high-temperature phase ($T \geq 302$ K):

crystal structure: undistorted cubic bixbyite structure, space group $T_h^7 - \text{Ia}3$. For this structure, at 302 K, $u = -0.035$, $x = 0.379$, $y = 0.147$, $z = 0.377$. The 8(a) sites are regular trigonal antiprisms and the 24(d) sites have three sets of two oxide ions.

Mn–O distances

$d(\text{Mn}-\text{O})$	2.003 \AA	Mn in 8(a) sites	71G
$d(\text{Mn}-\text{O})$	1.987 \AA	Mn in 24(d) sites	
	1.898 \AA		
	2.242 \AA		

lattice parameter

a	9.414 \AA	$T = 314 \text{ K}$	68G
	9.418 \AA	$T = 375 \text{ K}$	
	9.426 \AA	$T = 482 \text{ K}$	
	9.443 \AA	$T = 702 \text{ K}$	

References:

- 65O Otto, E. M.: J. Electrochem. Soc. 112 (1965) 367.
67S Shenouda, F., Aziz, S.: J. Appl. Chem. 17 (1967) 258.
68G Grant, R. W., Geller, S., Cape, J. A., Espinosa, G. P.: Phys. Rev. 175 (1968) 686.
71G Geller, S.: Acta Crystallogr. 27 (1971) 821.

Fig. 1.

Phase diagram for the systems $\text{MnO}_2/\text{Mn}_2\text{O}_3$ and $\text{Mn}_2\text{O}_3/\text{Mn}_3\text{O}_4$ drawn from the data of [65O, 67S].

