substance: MnO_2
property: phase diagram, crystal structure, lattice parameters

phase diagram: see Fig. 1.

crystal structure: rutile (β-MnO_2) (Fig. 2), tetragonal, space group D_{4h}^{14} – $P4_2/mnm$; Z = 2. In the rutile structure the metal ions occupy 2(a) points at (0, 0, 0); (1/2, 1/2, 1/2) and the oxygen ions are at 4(f) points ± (x, x, 0); (x+1/2, 1/2–x, 1/2), x = 0.30293(6) for MnO_2 [76B].

lattice parameters
at RT

a	4.3983 Å	see also Fig. 2	76B
c	2.8730 Å		
a	4.3980 Å		69R
c	2.8738 Å		
a	4.3977 Å		73C
c	2.8778 Å		
V	55.59 $Å^3$		76B
c/a	0.65321		
d(Mn–O)$_1$	1.8795 Å	equatorial/ axial,	76B
d(Mn–O)$_2$	1.8981 Å	mean value 1.8868 Å	
d(Mn–Mn)	2.86 Å	closest distance	69R
angle(O–Mn–O)	80.31°	angle on a shared edge	76B
dlog a/dT	$6.69 \cdot 10^{-6}$ K^{-1}		62B,
dlog c/dT	$6.92 \cdot 10^{-6}$ K^{-1}		69K,
			70H

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Fig. 1.

Phase diagram for the systems MnO_2/Mn_2O_3 and Mn_2O_3/Mn_3O_4 drawn from the data of [65O, 67S].

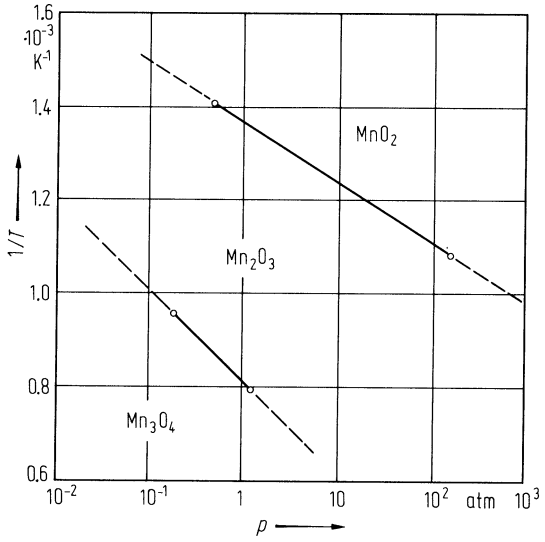

Fig. 2.

MnO_2. Crystal structure and dominant exchange interactions [71O].