substance: MoO_3
property: phase diagram, crystal structure, lattice parameters, interatomic distances

phase diagram: Fig. 1

crystal structure

Layer structure, ideally the layers can be envisaged as octahedra fused together as shown in Fig. 2 [63K]. Space group: D_{2h}^{16} – Pbnm, Z = 4. Projection of the structure on the (100), (010) and (001) planes: Fig. 3. The coordination about the Mo atoms is better thought of a distorted tetrahedron (Fig. 4 [63K]) and the fourfold coordination is built up into layers involving two further more distant neighbours about each Mo (Fig. 5 [63K]). Crystals of MoO_3 can be grown by a variety of techniques [68D, 79F].

lattice parameters

a	3.9628 Å	RT	63K
b	13.855 Å		
c	3.6964 Å		

interatomic distances and angles at RT

(distances in Å)

Mo – Mo	1 – 1'	3.4379	σ = 0.0006 Å	angle O – Mo – O, $\sigma \approx 0.30^o$		63K
	1 – 1	3.9628	‖ [100]	2– 1 – 2'	735º	
	1 – 1	3.6964	‖ [001]	2 – 1 – 3	91.5º	
Mo – O	1 – 2	2.332	$\sigma \approx$ 0.00 Å	2 – 1 – 3'	76.3º	
	1 – 2'	2·1.948		2 – 1 – 4	164.9º	
	1 – 3	1.734		2' – 1 – 2	143.1º	
	1 – 3'	2.251		2' – 1 – 3	2·98.3º	
	1 – 4	1.671		2' – 1 – 3'	2·78.4º	
O – O	2 – 2'	2·2.578	$\sigma \approx$ 0.011 Å	2' – 1 – 4	2·103.8º	
	2 – 3	2.831		3 – 1 – 3'	167.8º	
	2 – 3'	2.942		3 – 1 – 4	103.6º	
	2 – 3"	2·2.664		3' – 1 – 4	88.6º	
	2 – 3"'	2 2.790		structurally the O-ions can be		
	2 – 4	2·2.853		divided into three categories		
	3 – 2	2.942		O [1]: singly coordinated O at		
	3 – 2'	2.831		1.67 Å from Mo atom (position 4)		
	3 – 2"	2·2.664		O [2]: doubly coordinated O at		
	3 – 2"'	2·2.790		1.73 Å and 2.25 Å		
	3 – 3'	2·3.033		(positions 3, 3')		
	3 – 4	2.677		O [3]: triply coordinated O at		
	3 – 4'	2.770		1.95 Å and 2.33 Å		
	3 – 4"	2·3.240		(positions 2, 2')		
	4 – 2	2·2.853				
	4 – 3	2.677				
	4 – 3'	2.770				
	4 – 3"	2·3.240				
	4 – 4'	4·2.823				

References:

63K Kihlborg, L.: Ark. Kemi 21 (1963) 357.
68D Deb, S. K.: Proc. Roy. Soc. A304 (1968) 211.
69C Chang, L. L. Y., Phillips, B.: J. Am. Ceram. Soc. 52 (1969) 530.
79F Fourcandot, G., Gourmada, M., Mercier, J.: J. Cryst. Growth 46 (1979) 132.

Fig. 1.

Mo – O. Equilibrium phase diagram [69C].

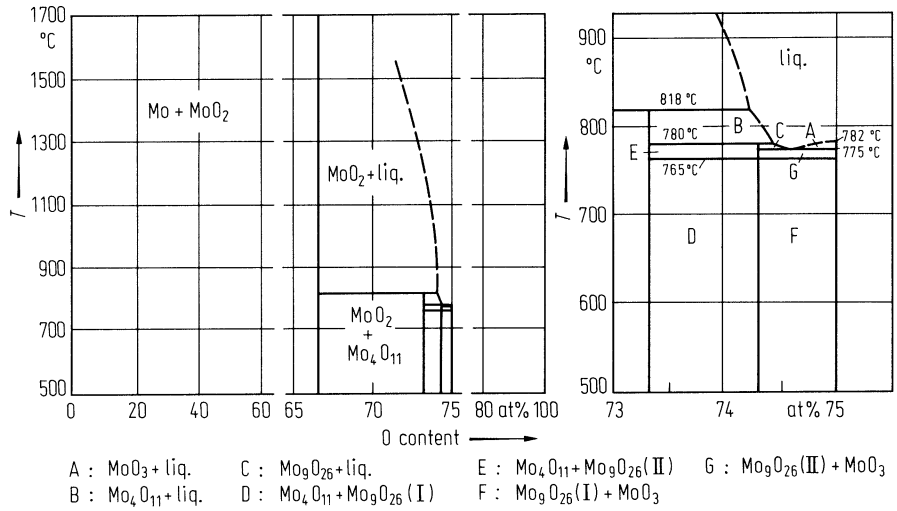

Fig. 2.

MoO_3. Part of a single layer idealized as regular octahedra fused together [63K].

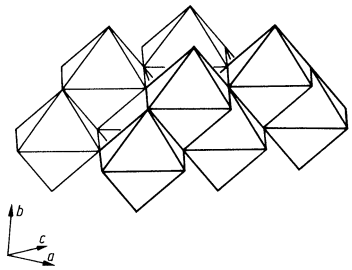

Fig. 3.

MoO_3. Projections of the crystal structure along (a) the [100]-, (b) the [010]- and (c) the [001]-directions [63K]. Unit cell is indicated.

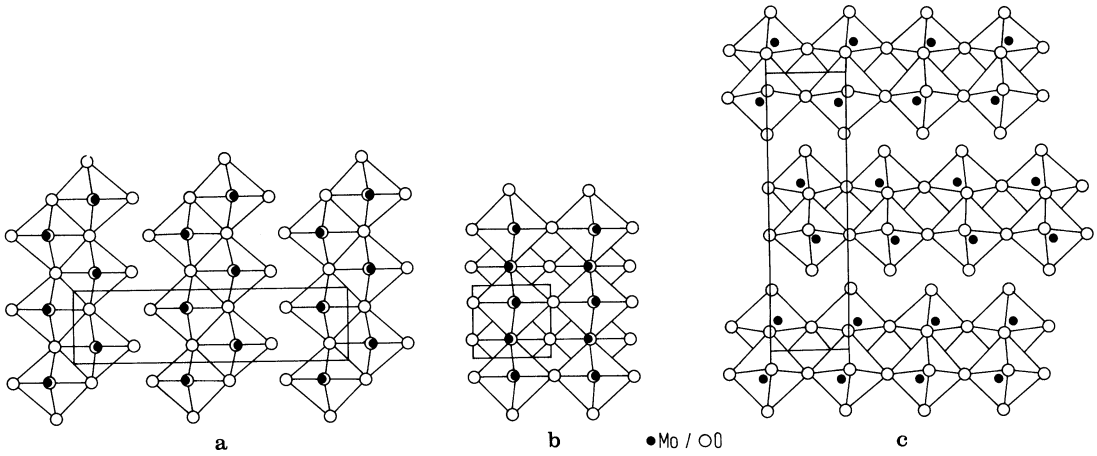

Fig. 4.

MoO_3. Coordination about each molybdenum ion [63K].

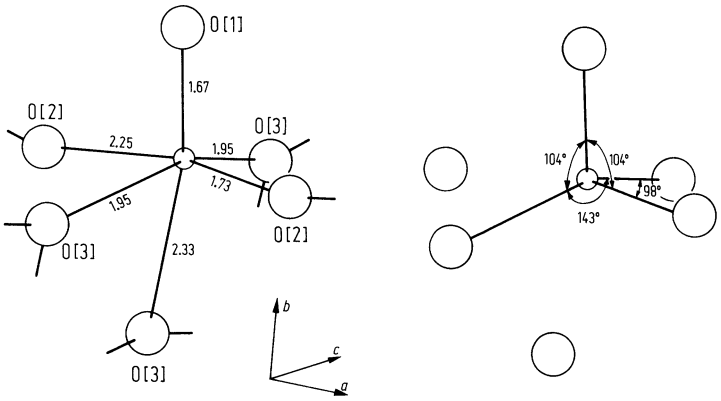

Fig. 5.

MoO_3. Structure visualized as built up of 4 coordinated Mo atoms (small spheres) [63K].