

**Na<sub>2</sub>O<sub>2</sub> form I** [2]; EuAs [4]; K<sub>2</sub>S<sub>2</sub> [3]; Rb<sub>2</sub>C<sub>2</sub> [7]

Structural features: Distorted close-packed Na layers in h stacking; O in octahedral voids (displaced from the octahedron centers). O<sub>2</sub> dumbbells arranged in infinite linear chains parallel to [001]. See Fig. IV.5.

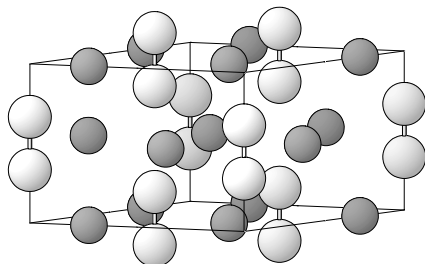


Fig. IV.5. **Na<sub>2</sub>O<sub>2</sub> form I**

Arrangement of Na atoms (dark) and O<sub>2</sub> dumbbells (light).

Tallman R.L. (1960) [1]

Na<sub>2</sub>O<sub>2</sub>

$a = 0.6207$ ,  $c = 0.4471$  nm,  $c/a = 0.720$ ,  $V = 0.1492$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	4 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.167		single atom O
Na2	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.634	0	$\frac{1}{2}$		trigonal prism O <sub>6</sub>
Na3	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.276	0	0		trigonal prism O <sub>6</sub>
O4	2 <i>e</i>	3. <i>m</i>	0	0	0.333		single atom O

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0  $\frac{1}{2}$

Experimental: powder, X-rays

Remarks: Phase stable at  $T < 785$  K. We deduced the space group from the coordinates of all the atoms in the unit cell. The same data are also reported in [8]. Preliminary data for [2] in [5]. Contrary to what is stated in [6], the data reported in [1] and [2] must be considered to be similar. The positions of Rb, part of the C atoms and the centers of the remaining C<sub>2</sub> dumbbells were determined in [7] (short interatomic distances:  $d(\text{C-C}) = 0.052$  nm).

References: [1] Tallman R.L. (1960), Diss. Abstr. 20, 4293. [2] Föppl H. (1957), Z. Anorg. Allg. Chem. 291, 12-50. [3] Föppl H., Busmann E., Frorath F.K. (1962), Z. Anorg. Allg. Chem. 314, 12-20. [4] Ono S., Hui F.L., Despault J.G., Calvert L.T., Taylor J.B. (1971), J. Less-Common Met. 25, 287-294. [5] Föppl H. (1954), Angew. Chem. 66, 335. [6] (1964), Structure Reports 21, 233. [7] Ruschewitz U., Müller P., Kockelmann W. (2001), Z. Anorg. Allg. Chem. 627, 513-522. [8] Tallman R.L., Margrave J.L., Bailey S.W. (1957), J. Am. Chem. Soc. 79, 2979-2980.