

ZnO	<i>hP4</i>	(186) $P6_3mc - b^2$
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ZnO [2], zincite, Strukturbericht notation B4; ZnS 2H [2], wurtzite; CuH [3]
 Structural features: Close-packed O layers in h stacking; Zn in tetrahedral voids (stacking sequence BbCc). ZnO₄ tetrahedra share vertices to form a 3D-framework. See Fig. IV.16.

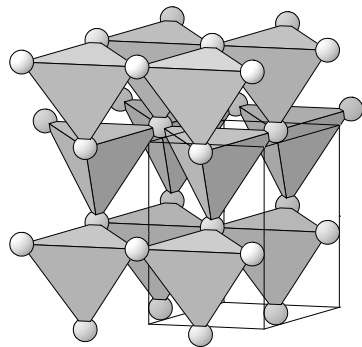


Fig. IV.16. **ZnO**
 Arrangement of ZnO₄ tetrahedra.

Sawada H. et al. (1996) [1]
 OZn
 $a = 0.32488$, $c = 0.52054$ nm, $c/a = 1.602$, $V = 0.0476$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0		tetrahedron Zn ₄
Zn2	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.381		tetrahedron O ₄

Transformation from published data: origin shift 0 0 0.119
 Experimental: single crystal, diffractometer, X-rays, wR = 0.015, T = 296 K
 Remarks: Electron density study. Strukturbericht notation B4 was defined on ZnS wurtzite.

References: [1] Sawada H., Wang R., Sleight A.W. (1996), J. Solid State Chem. 122, 148-150. [2] Bragg W.L. (1921), Z. Kristallogr. 56, 116. [3] Mueller H., Bradley A.J. (1926), Proc. K. Ned. Akad. Wet. 25, 27.