

[H<sub>2</sub>O]*hP36*(185) *P6<sub>3</sub>cm* – dc<sup>4</sup>**H<sub>2</sub>O form I hexagonal** [1], ice I<sub>h</sub>Structural features: H<sub>2</sub>O molecules are interconnected via H bonding to form a tridymite-type framework.

Bernal J.D., Fowler R.H. (1933) [1]

H<sub>2</sub>O $a = 0.782$ ,  $c = 0.736$  nm,  $c/a = 0.941$ ,  $V = 0.3898$  nm<sup>3</sup>,  $Z = 12$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	12 <i>d</i>	1	0.105	0.333	0.449		single atom O
O2	6 <i>c</i>	.. <i>m</i>	0.33333	0	0.037		non-colinear H <sub>2</sub>
H3	6 <i>c</i>	.. <i>m</i>	0.33333	0	0.148		single atom O
O4	6 <i>c</i>	.. <i>m</i>	0.33333	0	0.412		non-colinear H <sub>2</sub>
H5	6 <i>c</i>	.. <i>m</i>	0.405	0	0.0		single atom O

Transformation from published data: origin shift 0 0 0.0255

Remarks: Structure proposal based on crystal chemical considerations. The structure of hexagonal ice was redetermined in space group (194) *P6<sub>3</sub>/mmc* in [2], where the authors supersede an alternative model in space group (186) *P6<sub>3</sub>mc* from [3].

References: [1] Bernal J.D., Fowler R.H. (1933), J. Chem. Phys. 1, 515-548. [2] Peterson S.W., Levy H.A. (1957), Acta Crystallogr. 10, 70-76. [3] Rundle R.E. (1953), J. Chem. Phys. 21, 1311.