

## Hambergite, Be<sub>2</sub>BO<sub>3</sub>(OH)

Hambergite

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Fluorine-hydroxyl variation in hambergite: A crystal-structure study

9.776 12.194 4.430 90 90 90 Pbc<sub>a</sub>

atom	x	y	z	Wyckoff
Be1	0.0030	0.1885	0.2632	8c
Be2	0.2376	0.0679	0.2767	8c
B	0.1063	0.1072	0.7729	8c
H	0.814	0.216	0.075	8c
O1	0.0372	0.1877	0.6192	8c
O2	0.1009	0.1026	0.0825	8c
O3	0.1871	0.0342	0.6175	8c
O4	0.3400	0.1731	0.2952	8c

(8 × 8c)

### Raman Active Modes

WP	A <sub>g</sub>	A <sub>u</sub>	B <sub>1g</sub>	B <sub>1u</sub>	B <sub>2g</sub>	B <sub>2u</sub>	B <sub>3g</sub>	B <sub>3u</sub>
8c	3	·	3	·	3	·	3	·

Total number of modes:

$$24A_g + 24 B_{1g} + 24 B_{2g} + 24B_{3g} = 96$$