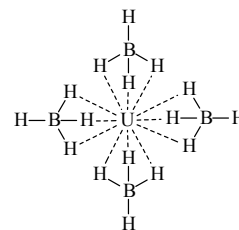


74 **B₄H₁₆U**ED, vibrational spectroscopy,
DFT calculations**Tetrakis(tetrahydroborato- $\kappa H, \kappa H'', \kappa H'''$)uranium(IV)**

Uranium(IV) tetrakis(tetrahydroborate)

T_d

r_a	Å ^{a)}	θ_a	deg ^{a)}
U...B	2.512(4)	U...B-H(b)	63.1(3)
U...H(b)	2.315(6)	H(b)-B-H(b)	101.1(4)
B-H(b)	1.316(5)	H(b)-B-H(t)	116.9(3)
B-H(t)	1.178(11)	B...U...B-H(b)	60 ^{b)}

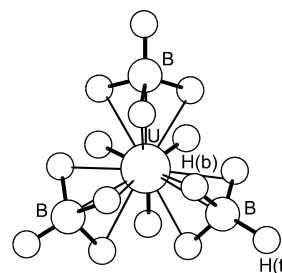


The best agreement between observed and calculated ED intensities was obtained for a model of T_d symmetry, but models of T symmetry with torsional angle $\tau(B...U...B-H(b)) > 42^\circ$ could not be ruled out.

The nozzle temperature was 62...65 °C.

The barrier to concerted rotation of the four BH₄ groups into eclipsed orientation was calculated to be 49 kJ mol⁻¹.

The calculations including spin-orbit interactions indicated that Jahn-Teller distortions from T_d symmetry are either absent or very small.



^{a)} 2.5 times the estimated standard errors including a systematic error.

^{b)} See comment.

Haaland, A., Shorokhov, D.J., Tutukin, A.V., Volden, H.V., Swang, O., McGrady, G.S., Kaltsoyannis, N., Downs, A.J., Tang, C.Y., Turner, J.F.C.: Inorg. Chem. **41** (2002) 6646.