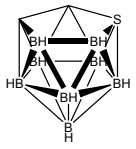
319 **$C_2H_{10}B_8S$** **7,8-Dicarba-10-thia-*nido*-undecaborane(10)** **C_s** assumed

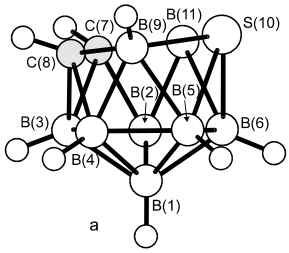
ED, *ab initio* calculations



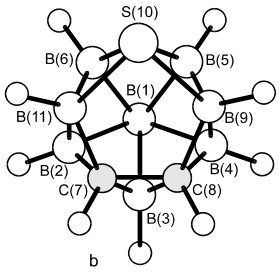
r_a	Å [a])	θ [b])	deg [a])
C(7)–C(8)	1.518(6)	C(7)–C(8)–B(9)	113.8(2)
S(10)–B(5)	2.032(4)	B(2)–B(6)–B(5)	105.9(10)
S(10)–B(9)	1.918(4)	B(9)–S(10)–B(11)	93.1(6) [c])
C(7)–B(2)	1.740(14)	φ_1 [d])	4.3(2)
C(7)–B(3)	1.686(6)	φ_2 [e])	178.3 [f])
C(7)–B(11)	1.573(6)		
B(5)–B(6)	1.898(13)		
B(5)–B(9)	1.873(5)		
B(4)–B(9)	1.755(8)		
B(2)–B(6)	1.762(13)		
B(3)–B(4)	1.753(22)		
B(1)–B(2)	1.788(3)		
B(1)–B(3)	1.790(14)		
B(1)–B(5)	1.782(13)		
C–H	1.140(3)		
B–H(mean)	1.240(3)		

The coplanarity of the B(2), B(3), B(4), B(5) and B(6) atoms was assumed. The differences for some structural parameters were assumed at the values from MP2(fc)/6-31G* calculations.
The nozzle was at 339 K.

[a]) Estimated standard errors.
[b]) Unidentified, possibly θ_a.
[c]) Dependent parameter.
[d]) Angle between the C(7)C(8)B(9)B(11) and B(2)B(3)B(4)B(5)B(6) planes; positive values when B(9) and B(11) are more elevated than C(7) and C(8).
[e]) Angle between the B(9)S(10)B(11) and C(7)C(8)B(9)B(11) planes; $\varphi_2 < 180°$ when the B(9)S(10)B(11) plane is bent upward.
[f]) Refined and then fixed.



a



b

a) Perspective view.
b) View showing the molecular C_s symmetry.

Hnyk, D., Hofmann, M., Schleyer, P.v.R., Bühl, M., Rankin, D.W.H.: J. Phys. Chem. **100** (1996) 3435.