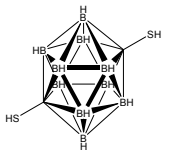
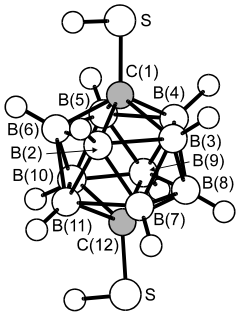
321 **$C_2H_{12}B_{10}S_2$** **1,12-Dicarbadodecaborane(12)-1,12-dithiol** **C_2** assumed

ED, ^{11}B NMR,
ab initio calculations



r_a	Å [a])	θ_a	deg [a])
B–B	1.770(4)	C–B–H	123.1(10)
Δ(B–B) [b])	0.01(9) [c])	C–S–H	92.8(30) [c])
B(2)–B(3) [d])	1.775(3)	τ_1 [e])	44.8(98) [c])
B(2)–B(7) [d])	1.765(9) [e])	τ_2 [d]) [f])	55.2(65)
S–H	1.319(33)		
C–B	1.706(4)		
C–S	1.785(10)		
B–H	1.180(6)		

Local D_{5d} symmetry was assumed for the $C_2B_{10}H_{10}$ core.
The nozzle temperature was 451 K.



[a]) Estimated standard errors.
[b]) [B(2)–B(3)] – [B(2)–B(7)].
[c]) Flexibly restrained to the value from MP2/6-31G* calculations.
[d]) Dependent parameter.
[e]) Torsional angle H–S–C(1)–B(5) from the *syn* position.
[f]) Torsional angle H–S…S–H from the *syn* position.

Hnyk, D., Holub, J., Hofmann, M., Schleyer, P.v.R., Robertson, H.E., Rankin, D.W.H.: J. Chem. Soc., Dalton Trans. (2000) 4617.