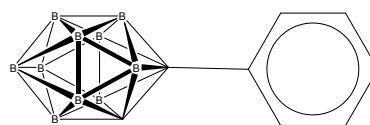
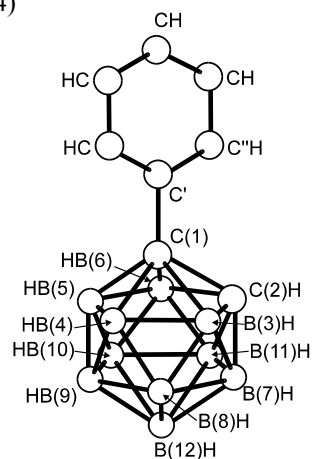


852 $C_8H_{16}B_{10}$ ED, *ab initio*
calculations1-Phenyl-1,2-dicarba-*closo*-dodecaborane(12) C_1 

r_a	\AA^a	θ^b	deg^a
C(1)–C(2)	1.627(8)	C(2)–C(1)–C'	119.6(17)
C(1)–B(3)	1.718(8)	C(2)–C(1)–B(4)	110.6(4)
C(1)–B(4)	1.722(7)	C(1)–C(2)–B(7)	110.6(4)
B(3)–B(4)	1.771(6)	θ'^c	54 ^d
B(4)–B(5)	1.770(9)		
B(8)–B(12)	1.816(5)		
B(4)–B(8)	1.772(9)		
B(9)–B(12)	1.779(12)		
B(7)–B(12)	1.806(14)		
B(3)–B(8)	1.788(18)		
C(1)–C'	1.500(8)		
C–C (ring)	1.394(2)		
B–H	1.176(13)		
C–H	1.120(12)		



Local C_{2v} symmetry for the C_2B_{10} cage and D_{6h} for the phenyl ring were assumed. The ED data were consistent equally with conformations in which $\theta' = 90^\circ$ (C_s symmetry, refinement A) or $\theta' = 54^\circ$ (C_1 symmetry, refinement B). Both conformations exhibit geometrical parameters similar to those found in the *ab initio* (RHF/6-31G*) optimization in C_1 symmetry except for the C(2)C(1)C' bond angle, which is considerably larger in refinement A [$126.3(7)^\circ$] than in B [$119.6(17)^\circ$], *cf.* HF/6-31G* 118.3° . *Ab initio* energies were computed lower for refinement B than for A by 0.3 kJ mol^{-1} . Thus, considered in conjunction with the *ab initio* study, ED refinement B, with $\theta' = 54^\circ$, was favored over refinement A. The parameters taken from the refinement B are listed. The nozzle was at *ca.* 488 K.

^a) Estimated standard errors.^b) Unidentified, possibly θ_a .^c) $\theta' = 90^\circ - \angle[C(2)–C(1)–C'–C'']$; $\tau = 0^\circ$ for the *syn* position.^d) Refined, then fixed.

Brain, P.T., Cowie, J., Donohoe, D.J., Hnyk, D., Rankin, D.W.H., Reed, D., Reid, B.D., Robertson, H.E., Welch, A.J., Hofmann, M., Schleyer, P.v.R.: *Inorg. Chem.* **35** (1996) 1701.