

Supporting information

(1) Atomic coordinates (Å) as obtained from RMP2(fc)/6-31G* optimizations and (2) the GIAO-SCF/H//RMP2(fc)/6-31G* results (ppm) for (a) 2,1-PCB₈H₉ (b) 6,1-PCB₈H₉.

1).

(a)

	x	y	z
C(1)	1.526822	0.529186	0.000000
P(2)	0.000000	1.589058	0.000000
B(3,5)	0.680776	0.072902	+/-1.317588
B(4)	1.245760	-1.056827	0.000000
B(6,9)	-1.137723	0.197080	+/-0.945233
B(7,8)	-0.250045	-1.395990	+/-0.914373
B(10)	-1.665252	-1.120061	0.000000
H(1)	2.506424	0.993554	0.000000
H(3,5)	1.100678	0.332186	+/-2.397464
H(4)	2.202866	-1.760957	0.000000
H(6,9)	-1.862107	0.717020	+/-1.734457
H(7,8)	-0.230958	-2.265955	+/-1.727110
H(10)	-2.718066	-1.665567	0.000000

(b)

	x	y	z
C(1)	1.084466	-1.441500	0.000000
B(2,3)	-0.128433	-1.119031	+/-0.978713
B(4,5)	1.409871	-0.158145	+/-0.910508
P(6)	-1.607536	-0.038379	0.000000
B(7,9)	-0.128433	0.669143	+/-1.318658
B(8)	0.950653	1.322112	0.000000
B(10)	-0.698489	1.668962	0.000000
H(1)	1.635690	-2.374285	0.000000
H(2,3)	-0.535483	-1.937537	+/-1.736849
H(4,5)	2.312881	-0.171984	+/-1.681692
H(7,9)	-0.387347	0.996156	+/-2.432785
H(8)	1.690766	2.254617	0.000000
H(10)	-1.291178	2.696042	0.000000

2).

(a) δ = 55.7 B(10), 1.7 B(4), -12.0 B(3,5), -18.0 B(6,9), -20.2 B(7,8), 48.4 C(1)

(b) δ = 39.2 B(10), -5.6 B(8), -9.1 B(2,3), -16.9 B(4,5), -18.3 B(7,9), 58.7 C(1)