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Icosahedral metallacarborane/carborane species derived from 1,1′-bis(*o*-carborane)

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Supplementary Information

Table S1 ^{11}B NMR chemical shifts (ppm) for key reference compounds recorded from $CDCl_3$ solutions at room temperature.

Compound	Chemical shifts (integrals)	$<\delta(^{11}B)>$
1,1′-bis(*o*-carborane)	-1.7 (2B), -2.4 (2B), -9.2 (4B), -10.4 (8B), -12.5 (4B)	-8.9
1,2-*closo*-$C_2B_{10}H_{12}$	-2.3 (2B), -9.2 (2B), -13.6 (4B), -14.8 (2B)	-10.7
3-(*p*-cymene)-3,1,2-*closo*-$RuC_2B_9H_{11}$	1.9 (1B), 0.3 (1B), -7.7 (2B), -9.2 (2B), -19.5 (2B), -24.2 (1B)	-10.5
3-Cp-3,1,2-*closo*-$CoC_2B_9H_{11}$	6.8 (1B), 3.6 (1B), -4.9 (2B), -6.0 (2B), -16.2 (2B), -22.5 (1B)	-7.3
2-Cp-2,1,8-*closo*-$CoC_2B_9H_{11}$	0.9 (2B), -1.5 (1B), -3.1 (1B), -8.2 (1B), -9.1 (1B), -12.0 (1B), -17.9 (1B), -19.3 (1B)	-7.7

Tables S2-S5 Computational Models

S2-S5 correspond to the models of 1,2-*closo*-$C_2B_{10}H_{12}$, 1,1′-bis(*o*-carborane) (C2–C1–C1′–C2′ = 180°), 1,1′-bis(*o*-carborane) (C2–C2–C1′–C2′ = 108°) and 1,1′-bis(*o*-carborane) (180-108 TS), respectively.

S2

BP86 Energy = -332.070551
Enthalpy 0K = -331.898064
Enthalpy 298K = -331.889094
Free Energy 298K = -331.928965

C	0.00000	-0.81751	-1.28029
B	-1.46144	-0.00006	-0.85692
B	-1.45739	0.00007	0.91589
B	-0.89565	1.44519	0.02608
C	0.00000	0.81731	-1.28042
B	0.89565	1.44519	0.02608
B	-0.00000	0.89495	1.46911
B	0.00000	-0.89473	1.46925
B	0.89566	-1.44519	0.02629
B	-0.89565	-1.44519	0.02629
B	1.46144	-0.00006	-0.85692
B	1.45739	0.00007	0.91589
H	-2.34529	-0.00013	-1.65542
H	-1.48905	2.46631	-0.14342
H	0.00000	1.29804	-2.26041
H	-2.49431	0.00012	1.50992
H	1.48904	2.46631	-0.14342
H	-1.48904	-2.46633	-0.14304
H	-0.00000	1.54602	2.47166
H	0.00000	-1.29838	-2.26022
H	0.00000	-1.54564	2.47190
H	1.48905	-2.46633	-0.14304
H	2.34529	-0.00012	-1.65542
H	2.49431	0.00012	1.50992

S3

BP86 Energy = -662.925395
Enthalpy 0K = -662.601303
Enthalpy 298K = -662.584499
Free Energy 298K = -662.641103

C	-0.76909	-0.00006	-0.05576
B	-1.60026	-1.46111	0.43286
B	-3.08687	-0.89388	1.22927
B	-3.12201	-1.45408	-0.46578
B	-1.62263	-0.89389	-1.25801
B	-3.14214	0.00047	-1.51362
B	-4.05326	0.00008	0.02403
B	-3.08679	0.89326	1.22976
B	-1.60011	1.46079	0.43366
C	-1.63549	-0.00039	1.35124
B	-1.62255	0.89448	-1.25753
B	-3.12185	1.45444	-0.46500
H	-0.93823	-2.35919	0.83888
H	-3.62352	-2.49438	-0.77083
H	-0.97763	-1.48900	-2.06592
H	-3.44856	-1.49306	2.19485
H	-3.66308	0.00079	-2.58927
H	-1.03371	-0.00064	2.26250
H	-5.24677	0.00010	0.07483
H	-3.44846	1.49195	2.19565
H	-0.93805	2.35857	0.84027
H	-0.97749	1.48999	-2.06512
H	-3.62327	2.49494	-0.76948
C	0.76911	-0.00009	0.05548
B	1.62238	0.89360	1.25799
B	3.14193	-0.00064	1.51372
B	3.12182	1.45407	0.46616
B	1.60020	1.46113	-0.43277
B	3.08701	0.89414	-1.22897
B	4.05327	0.00004	-0.02376
B	3.12188	-1.45444	0.46489
B	1.60019	-1.46078	-0.43403
B	1.62247	-0.89473	1.25730
C	1.63572	0.00056	-1.35139
B	3.08702	-0.89305	-1.22975
H	0.97729	1.48854	2.06597
H	3.62324	2.49433	0.77147
H	0.93810	2.35915	-0.83878
H	3.66278	-0.00106	2.58941
H	3.44883	1.49349	-2.19439
H	0.97745	-1.49030	2.06487
H	5.24678	0.00006	-0.07440
H	3.62326	-2.49498	0.76933
H	0.93801	-2.35840	-0.84080
H	1.03420	0.00098	-2.26288
H	3.44891	-1.49156	-2.19567

S4

BP86 Energy = -662.925695
Enthalpy 0K = -662.600456
Enthalpy 298K = -662.583851
Free Energy 298K = -662.639771

C	-0.76889	0.07328	-0.04638
B	-1.56583	-1.41189	-0.51362
B	-3.05030	-1.46731	0.46661
B	-3.09983	-0.91752	-1.23314
B	-1.62557	0.04108	-1.54390
B	-3.16807	0.87531	-1.22090
B	-4.05135	-0.05813	0.02289
B	-3.08177	-0.02814	1.52060
B	-1.61593	0.93893	1.21014
C	-1.61741	-0.78330	1.09007
B	-1.65934	1.48591	-0.48835
B	-3.15411	1.42690	0.48498
H	-0.88382	-2.36198	-0.72824
H	-3.58268	-1.59167	-2.09314
H	-0.98380	0.04486	-2.54921
H	-3.38498	-2.53087	0.88987
H	-3.70891	1.49562	-2.08714
H	-1.00301	-1.30559	1.82644
H	-5.24362	-0.11879	0.06710
H	-3.43993	-0.12298	2.65413
H	-0.96220	1.43710	2.06674
H	-1.03714	2.45734	-0.78344
H	-3.68115	2.43147	0.85884
C	0.76893	0.07321	0.04631
B	1.65932	1.48562	0.48919
B	3.16804	0.87459	1.22147
B	3.15416	1.42716	-0.48409
B	1.61600	0.93969	-1.20965
B	3.08183	-0.02724	-1.52061
B	4.05133	-0.05815	-0.02286
B	3.09975	-0.91826	1.23260
B	1.56580	-1.41220	0.51284
B	1.62552	0.04020	1.54392
C	1.61742	-0.78263	-1.09054
B	3.05027	-1.46703	-0.46745
H	1.03710	2.45688	0.78486
H	3.68122	2.43194	-0.85733
H	0.96227	1.43834	-2.06596
H	3.70887	1.49439	2.08808
H	3.44007	-0.12152	-2.65416
H	0.98360	0.04349	2.54913
H	5.24361	-0.11881	-0.06707
H	3.58262	-1.59292	2.09220
H	0.88374	-2.36241	0.72679
H	1.00309	-1.30455	-1.82723
H	3.38501	-2.53034	-0.89129

S5

BP86 Energy = -662.916997
Enthalpy 0K = -662.592201
Enthalpy 298K = -662.576305
Free Energy 298K = -662.630335
Negative frequency = -68.8 cm^{-1}

C	-0.77835	0.03730	0.05406
B	-1.64244	1.25707	-0.86384
B	-3.12325	0.45587	-1.44474
B	-3.17113	1.51389	-0.00944
B	-1.67200	1.25238	0.91777
B	-3.17852	0.46047	1.43992
B	-4.08635	-0.02609	-0.02096
B	-3.11081	-1.23662	-0.89105
B	-1.62244	-1.51323	0.03591
C	-1.66276	-0.41499	-1.28403
B	-1.64134	-0.44977	1.46792
B	-3.13886	-1.24367	0.89458
H	-1.01409	1.99890	-1.54059
H	-3.67916	2.59434	-0.04489
H	-1.07019	2.09162	1.50408
H	-3.48395	0.72619	-2.54881
H	-3.69879	0.78826	2.46455
H	-1.06803	-0.69257	-2.15562
H	-5.27962	-0.05574	-0.06919
H	-3.45808	-2.11457	-1.61971
H	-0.98976	-2.50698	-0.07459
H	-1.01575	-0.76843	2.43331
H	-3.62270	-2.14634	1.50952
C	0.77835	0.03730	-0.05406
B	1.64134	-0.44976	-1.46792
B	3.17851	0.46047	-1.43992
B	3.13886	-1.24367	-0.89458
B	1.62244	-1.51323	-0.03591
B	3.11081	-1.23662	0.89105
B	4.08635	-0.02609	0.02096
B	3.17113	1.51389	0.00944
B	1.64244	1.25707	0.86384
B	1.67200	1.25238	-0.91777
C	1.66276	-0.41499	1.28403
B	3.12325	0.45587	1.44474
H	1.01575	-0.76843	-2.43331
H	3.62270	-2.14634	-1.50952
H	0.98976	-2.50698	0.07459
H	3.69879	0.78826	-2.46455
H	3.45808	-2.11457	1.61971
H	1.07019	2.09162	-1.50408
H	5.27962	-0.05574	0.06919
H	3.67916	2.59434	0.04489
H	1.01409	1.99890	1.54059
H	1.06803	-0.69257	2.15562
H	3.48395	0.72619	2.54881