Electronic Supplementary Material (ESI) for Dalton Transactions

Untethered 4,1,2-MC_2B_{10} supraicosahedral metallacarboranes, their C,C'-dimethyl 4,1,6-, 4,1,8- and 4,1,12-MC_2B_{10} analogues, and DFT study of the (4,)1,2- to (4,)1,6- isomerisations of C_2B_{11} carboranes and MC_2B_{10} metallacarboranes

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Supplementary information

Table S1
Computational model for 1,2-*closo*-$C_2B_{11}H_{13}$

SCF (BP86) Energy =	-357.477135		
Enthalpy 0K =	-357.293739		
Enthalpy 298K =	-357.283857		
Free Energy 298K =	-357.326308		
C	1.67400	0.72129	0.05551
C	1.67400	-0.72129	0.05551
B	0.49223	1.70208	-0.36832
B	0.83432	-0.00000	-1.37451
B	0.41069	0.99716	1.31409
B	0.49223	-1.70208	-0.36832
B	-0.81747	0.87235	-1.29721
B	-1.06761	1.47150	0.36720
B	0.41069	-0.99716	1.31409
B	-0.81747	-0.87235	-1.29721
B	-1.02918	0.00000	1.40849
B	-1.06762	-1.47150	0.36720
B	-1.89463	0.00000	-0.17740
H	2.65505	1.20617	0.06704
H	2.65505	-1.20617	0.06704
H	0.90439	2.79569	-0.61890
H	1.51212	-0.00000	-2.35526
H	0.90410	1.53931	2.25848
H	0.90439	-2.79569	-0.61890
H	-1.12920	1.46698	-2.28878
H	-1.68035	2.46924	0.61114
H	0.90409	-1.53931	2.25848
H	-1.12920	-1.46698	-2.28878
H	-1.55475	0.00000	2.48505
H	-1.68035	-2.46924	0.61114
H	-3.08417	0.00000	-0.29436

Table S2
Computational model for TS1 in $C_2B_{11}H_{13}$ isomerisation

SCF (BP86) Energy =	-357.461680		
Enthalpy 0K =	-357.279138		
Enthalpy 298K =	-357.269757		
Free Energy 298K =	-357.311268		
Negative frequency =	-174.5 cm^{-1}		
C	0.22465	-1.28361	-0.87840
C	1.55287	-0.93749	-0.03497
B	-1.26558	-1.32795	-0.08331
B	0.22660	-1.50815	0.84379
B	-0.91973	-0.18335	-1.45086
B	2.00164	0.51991	0.02498
B	-0.98121	-0.36783	1.41934
B	-1.86713	0.33210	0.00214
B	0.71160	0.55618	-1.36105
B	0.70118	0.27108	1.41496
B	-0.75524	1.45712	-0.79233
B	0.76543	1.65196	0.11711
B	-0.76985	1.32626	0.96972
H	0.43417	-2.12366	-1.54659
H	2.29176	-1.74839	-0.08340
H	-1.95908	-2.28766	-0.23054
H	0.46929	-2.58014	1.31094
H	-1.35971	-0.44374	-2.53020
H	3.14695	0.85088	0.07966
H	-1.50637	-0.67837	2.44823
H	-3.04930	0.50544	-0.01332
H	1.33111	0.56196	-2.38276
H	1.33611	0.27227	2.42855
H	-1.13566	2.40162	-1.42077
H	1.22273	2.75526	0.19775
H	-1.12560	2.20448	1.70033

Table S3
Computational model for INT in $C_2B_{11}H_{13}$ isomerisation

SCF (BP86) Energy =	-357.462202		
Enthalpy 0K =	-357.279251		
Enthalpy 298K =	-357.269312		
Free Energy 298K =	-357.311827		
C	0.13560	-1.11519	-1.06316
C	1.44258	-1.04787	-0.08940
B	-1.37726	-1.18880	-0.26407
B	0.07049	-1.68464	0.58938
B	-0.94449	0.12461	-1.43254
B	2.03233	0.36511	0.00504
B	-1.00252	-0.51957	1.36174
B	-1.82892	0.47815	0.10512
B	0.71144	0.77127	-1.30348
B	0.78276	-0.08021	1.37135
B	-0.65632	1.64033	-0.52873
B	0.90483	1.57188	0.29839
B	-0.60246	1.17791	1.18402
H	0.31118	-1.82276	-1.87831
H	2.12485	-1.90318	-0.16661
H	-2.14866	-2.05289	-0.55075
H	0.19928	-2.84122	0.85511
H	-1.41193	0.05395	-2.52981
H	3.20619	0.57602	0.04790
H	-1.53807	-0.92110	2.35302
H	-2.99051	0.75360	0.15696
H	1.30823	0.86450	-2.33553
H	1.40448	-0.24866	2.37857
H	-1.01462	2.69981	-0.95352
H	1.45859	2.61048	0.51921
H	-0.82743	1.92950	2.08801

Table S4
Computational model for TS2 in $C_2B_{11}H_{13}$ isomerisation

SCF (BP86) Energy =	-357.439640
Enthalpy 0K =	-357.258393
Enthalpy 298K =	-357.248861
Free Energy 298K =	-357.290659

Negative frequency = -235.9 cm^{-1}

C	0.13647	-0.49345	-1.42610
C	1.94299	-0.63452	-0.11174
B	-1.06844	-1.31593	-0.67062
B	0.62533	-1.54718	-0.09829
B	-1.29834	0.36741	-1.25188
B	1.88918	0.86769	-0.29031
B	-0.68187	-1.22639	1.09941
B	-1.87503	-0.12283	0.39238
B	0.24481	1.23652	-1.03244
B	0.92027	-0.33877	1.28802
B	-1.12545	1.48621	0.10715
B	0.52586	1.46740	0.70716
B	-0.66474	0.50284	1.55001
H	0.52812	-0.78016	-2.40448
H	2.85533	-1.24484	-0.06348
H	-1.54186	-2.29256	-1.16646
H	0.91760	-2.70235	-0.23058
H	-1.90920	0.60229	-2.25194
H	2.82704	1.59826	-0.42679
H	-1.01035	-2.12086	1.82016
H	-3.04149	-0.24081	0.62530
H	0.53843	1.96971	-1.93637
H	1.59004	-0.64458	2.23618
H	-1.78135	2.48414	0.15195
H	1.01637	2.44825	1.19267
H	-0.92326	0.80642	2.67797

Table S5
Computational model for 1,6-*closo*-$C_2B_{11}H_{13}$

SCF (BP86) Energy = -357.501126
Enthalpy 0K = -357.317197
Enthalpy 298K = -357.307366
Free Energy 298K = -357.349670

C	0.42784	-1.38101	-0.73337
C	-1.88753	-0.20012	0.00934
B	0.96448	0.06271	-1.42423
B	-0.85264	-0.10302	-1.34863
B	1.75037	-0.68279	0.02381
B	-1.07367	-1.50814	0.01039
B	0.08770	1.50153	-0.93441
B	1.54985	1.08417	-0.05235
B	0.45877	-1.41204	0.95485
B	-1.42771	1.27170	0.01854
B	0.99861	0.17887	1.42519
B	-0.81766	-0.03852	1.38049
B	0.12302	1.58332	0.83063
H	0.61565	-2.29094	-1.31005
H	-2.96660	-0.37079	0.03183
H	1.44770	-0.02974	-2.51242
H	-1.36555	-0.32189	-2.40384
H	2.80560	-1.23413	-0.05262
H	-1.63121	-2.56304	-0.02088
H	0.00242	2.43502	-1.67953
H	2.53949	1.75295	-0.09516
H	0.60661	-2.44329	1.53869
H	-2.27206	2.11810	0.03059
H	1.50270	0.25359	2.50783
H	-1.39124	-0.10590	2.42592
H	0.05907	2.59800	1.46256

Table S6
Computational model for 4-Cp-4,1,2-*closo*-$CoC_2B_{10}H_{12}$

SCF (BP86) Energy = -671.573707
Enthalpy 0K = -671.320179
Enthalpy 298K = -671.305690
Free Energy 298K = -671.358506

C	-0.40364	-1.54071	0.72954
C	-0.40357	-1.54857	-0.71393
B	-0.67243	-0.26253	1.69185
Co	0.75897	-0.03749	-0.00049
B	-2.13325	-1.11861	0.99545
B	-0.67318	-0.28099	-1.68925
B	-0.65256	1.38247	0.88714
B	-2.16083	0.61548	1.47025
B	-2.13397	-1.12924	-0.98290
B	-0.65280	1.37221	-0.90168
B	-3.00950	0.02936	0.00029
B	-2.16149	0.59978	-1.47629
B	-2.16931	1.60967	-0.00848
H	0.01329	-2.41470	1.24161
H	0.01315	-2.42806	-1.21667
H	-0.26878	-0.47323	2.80357
H	-2.65788	-2.03285	1.56508
H	-0.26999	-0.50242	-2.79906
H	-0.11706	2.26221	1.50643
H	-2.71414	1.00614	2.45892
H	-2.65893	-2.04990	-1.54178
H	-0.11796	2.24523	-1.53106
H	-4.20057	-0.10934	0.00165
H	-2.71535	0.97986	-2.46875
H	-2.72771	2.67008	-0.01393
C	2.22156	1.38646	-0.00802
C	2.36229	0.55844	1.16196
C	2.60450	-0.78703	0.72165
C	2.60548	-0.79576	-0.71063
C	2.36398	0.54435	-1.16761
H	1.99562	2.45127	-0.01461
H	2.25470	0.88901	2.19428
H	2.70618	-1.65910	1.36826
H	2.70824	-1.67560	-1.34645
H	2.25797	0.86243	-2.20401

Table S7
Computational model for TS in $CpCoC_2B_{10}H_{12}$ isomerisation

SCF (BP86) Energy = -671.500012
Enthalpy 0K = -671.249855

Enthalpy 298K =		-671.235247	
Free Energy 298K =		-671.288241	
Negative frequency =		-321.1 cm^{-1}	
C	-0.64462	-0.11560	-1.40446
C	-0.16710	1.61466	-0.26251
B	-0.39358	-1.51680	-0.52749
Co	0.83744	0.05422	-0.02107
B	-1.97269	-1.10255	-1.26443
B	-1.60536	2.06331	-0.21357
B	-0.50319	-0.94626	1.21731
B	-1.87705	-1.76676	0.41799
B	-2.32483	0.64071	-1.14369
B	-0.85646	0.93474	1.23585
B	-3.10594	-0.56494	-0.00608
B	-2.70486	1.03149	0.56796
B	-2.14631	-0.36867	1.48872
H	-0.26315	0.06155	-2.41424
H	0.60409	2.37870	-0.44904
H	0.22580	-2.44447	-0.96675
H	-2.32345	-1.63149	-2.28063
H	-1.89343	3.22520	-0.30384
H	0.07700	-1.49377	2.11391
H	-2.18612	-2.88944	0.69768
H	-2.79734	1.10935	-2.14210
H	-0.47878	1.52773	2.21045
H	-4.25645	-0.89068	-0.05422
H	-3.61530	1.70761	0.95754
H	-2.59809	-0.48115	2.59353
C	2.47645	-0.17890	1.26523
C	2.43862	-1.25985	0.33236
C	2.54143	-0.70234	-0.99184
C	2.69195	0.71686	-0.87391
C	2.63181	1.04204	0.51839
H	2.35823	-0.25701	2.34511
H	2.27819	-2.30956	0.57271
H	2.48378	-1.26791	-1.92206
H	2.76527	1.42464	-1.70013
H	2.64895	2.04416	0.94856

Table S8
Computational model for 4-Cp-4,1,6-*closo*-$CoC_2B_{10}H_{12}$

SCF (BP86) Energy =		-671.585878	
Enthalpy 0K =		-671.332316	
Enthalpy 298K =		-671.317736	
Free Energy 298K =		-671.370832	
C	-0.78763	-0.90123	-1.23408
C	-0.26838	1.70592	-0.40754
B	-0.64507	-1.54671	0.32751
Co	0.76487	0.01832	-0.01432
B	-2.21160	-1.47543	-0.55265
B	-0.56366	0.76414	-1.59195
B	-0.64904	-0.29255	1.63206
B	-2.15172	-1.09288	1.18164
B	-2.19601	-0.01225	-1.50343
B	-0.56481	1.45171	1.09581
B	-3.01669	0.01733	0.04661
B	-1.99537	1.46409	-0.30311
B	-2.13176	0.65557	1.42152
H	-0.40061	-1.49918	-2.06562
H	0.16968	2.67449	-0.66556
H	-0.12465	-2.62110	0.44683
H	-2.69758	-2.47369	-0.99566
H	-0.23761	1.04675	-2.71119
H	-0.13423	-0.49165	2.69969
H	-2.69574	-1.83040	1.95323
H	-2.69910	0.01454	-2.58806
H	-0.20772	2.28742	1.88290
H	-4.20498	0.16407	0.01922
H	-2.56715	2.48610	-0.55633
H	-2.70661	1.17305	2.33824
C	2.42995	0.44156	1.11051
C	2.27273	-0.97806	0.95766
C	2.32058	-1.27530	-0.45003
C	2.53386	-0.04765	-1.16668
C	2.59600	1.00927	-0.20533
H	2.38675	0.99569	2.04731
H	2.08472	-1.69277	1.75719
H	2.16899	-2.25950	-0.89327
H	2.57260	0.06726	-2.24967
H	2.68773	2.07208	-0.42957

Table S9
Computational model for 4-(C_6H_6)-4,1,2-*closo*-$RuC_2B_{10}H_{12}$

SCF (BP86) Energy =		-659.377165	
Enthalpy 0K =		-659.106832	
Enthalpy 298K =		-659.091388	
Free Energy 298K =		-659.147544	
C	0.72241	-1.55187	-0.76688
C	0.72232	-1.58867	0.68351
B	0.96622	-0.23504	-1.70153
B	0.92390	1.40363	-0.86216
B	0.92513	1.35760	0.93393
B	2.44252	-1.13056	0.95826
B	2.44389	-1.07926	-1.01682
B	2.44551	0.66024	-1.45483
B	2.44260	1.62224	0.04239
B	3.30428	0.05821	0.00130
B	2.44628	0.58333	1.48656
B	0.96507	-0.32105	1.68541
H	2.98260	-2.05353	1.49945
H	0.34672	-2.43458	-1.29704
H	0.34564	-2.49649	1.16867
H	0.58983	-0.43305	-2.82654
H	0.43130	2.31944	-1.46874
H	2.99906	1.07462	-2.43403
H	2.99611	2.68512	0.06868
H	4.49684	-0.07146	-0.00205
H	2.99935	0.94549	2.48648

H	0.58783	-0.57844	2.79808
H	0.43344	2.23909	1.59034
H	2.98487	-1.97255	-1.60480
Ru	-0.63262	-0.04147	-0.00201
C	-2.57980	-1.14383	-0.53216
C	-2.39582	-0.02370	-1.41187
C	-2.23990	1.28813	-0.86915
C	-2.18261	1.47251	0.54514
C	-2.31982	0.34690	1.42535
C	-2.55536	-0.95462	0.87857
H	-2.68600	-2.15028	-0.94717
H	-2.35378	-0.17506	-2.49336
H	-2.05709	2.13515	-1.53449
H	-1.95959	2.45956	0.95620
H	-2.22066	0.48297	2.50482
H	-2.63652	-1.81724	1.54653

Table S10
Computational model for TS in $(C_6H_6)RuC_2B_{10}H_{12}$ isomerisation

SCF (BP86) Energy =	-659.288565
Enthalpy 0K =	-659.022258
Enthalpy 298K =	-659.006338
Free Energy 298K =	-659.063471
Negative frequency =	-408.2 cm^{-1}

C	-0.96052	-0.09565	-1.47190
C	-0.35402	1.74180	-0.38315
B	-0.74247	-1.51698	-0.63462
B	-0.82817	-1.04251	1.16210
B	-1.13549	0.79121	1.34717
B	-2.54006	0.75481	-1.09332
B	-2.33462	-1.01037	-1.32103
B	-2.23503	-1.77137	0.31090
B	-2.47039	-0.47654	1.48644
B	-3.40309	-0.47875	-0.02160
B	-2.86822	1.04041	0.67568
B	-1.77547	2.11185	-0.05996
H	-3.04345	1.30287	-2.03437
H	-0.61620	0.07339	-2.49609
H	0.33769	2.53834	-0.73057
H	-0.17007	-2.45622	-1.11876
H	-0.27776	-1.69359	2.01227
H	-2.58328	-2.90182	0.50418
H	-2.96052	-0.65566	2.56636
H	-4.57730	-0.70098	-0.09172
H	-3.73101	1.73605	1.13342
H	-2.11213	3.26668	-0.04107
H	-0.72552	1.36109	2.32011
H	-2.74086	-1.47048	-2.35062
Ru	0.67139	0.06316	-0.03781
C	2.63157	0.18333	-1.30023
C	2.42020	-1.16666	-0.87104
C	2.31718	-1.47301	0.51775
C	2.28369	-0.42276	1.48029
C	2.46038	0.93417	1.05680
C	2.67758	1.21697	-0.32770
H	2.73756	0.41629	-2.36309
H	2.33215	-1.96817	-1.60887
H	2.11441	-2.50014	0.83183
H	2.09280	-0.64877	2.53178
H	2.41975	1.74584	1.78734
H	2.77147	2.25848	-0.65212

Table S11
Computational model for 4-(C_6H_6)-4,1,6-*closo*-$RuC_2B_{10}H_{12}$

SCF (BP86) Energy =	-659.389488
Enthalpy 0K =	-659.119077
Enthalpy 298K =	-659.103603
Free Energy 298K =	-659.159136

C	1.08021	0.76509	-1.33881
C	0.58409	-1.76469	-0.22964
B	0.92516	1.58832	0.15267
B	0.92663	0.47386	1.59117
B	0.86063	-1.32334	1.24430
B	2.49604	-0.14667	-1.48781
B	2.49738	1.41382	-0.70757
B	2.43371	1.22412	1.05615
B	2.42357	-0.48198	1.48767
B	3.31114	0.00559	0.05461
B	2.30499	-1.47720	-0.13211
B	0.86501	-0.93778	-1.51054
H	3.00646	-0.29284	-2.55972
H	0.72261	1.27076	-2.24168
H	0.18680	-2.77289	-0.38356
H	0.44832	2.69122	0.14504
H	0.46020	0.80340	2.65084
H	2.97758	2.04422	1.73974
H	3.00367	-0.88965	2.45507
H	4.50066	-0.13657	0.04155
H	2.88851	-2.51475	-0.27054
H	0.55963	-1.35043	-2.59571
H	0.52195	-2.08537	2.11212
H	2.98347	2.35786	-1.25735
Ru	-0.64228	-0.02523	-0.01005
C	-2.48515	-0.22965	-1.35022
C	-2.28346	1.14610	-0.98613
C	-2.23370	1.52775	0.39360
C	-2.27427	0.53151	1.41081
C	-2.39880	-0.85242	1.04877
C	-2.55317	-1.21936	-0.33233
H	-2.51763	-0.52071	-2.40331
H	-2.16159	1.90578	-1.76289
H	-2.04707	2.57051	0.66160
H	-2.12632	0.81012	2.45673
H	-2.36128	-1.62402	1.82133
H	-2.62168	-2.27619	-0.60604

Table S12
Computational model for [7,8-*nido*-$C_2B_{10}H_{12}]^{2-}$

SCF (BP86) Energy =	-331.989197		
Enthalpy 0K =	-331.825567		
Enthalpy 298K =	-331.816391		
Free Energy 298K =	-331.857459		
C	-1.68595	-0.72588	-0.50554
C	-1.68596	0.72707	-0.50520
B	-0.46809	-1.66706	-0.66931
B	-0.77471	-0.98413	1.02184
B	-0.46809	1.66823	-0.66764
B	1.08238	-0.85813	-1.21826
B	0.90068	-1.46365	0.44595
B	-0.77541	0.98182	1.02247
B	1.08321	0.86016	-1.21702
B	0.60802	-0.00116	1.46961
B	0.90044	1.46291	0.44785
B	1.85132	-0.00011	0.16198
H	-2.68849	-1.19402	-0.48984
H	-2.68854	1.19511	-0.48944
H	-0.77187	-2.84415	-0.83249
H	-1.40043	-1.54430	1.90000
H	-0.77135	2.84558	-0.82972
H	1.75843	-1.53295	-1.98830
H	1.41673	-2.46998	0.89870
H	-1.40149	1.54002	1.90166
H	1.75904	1.53587	-1.98635
H	0.86391	-0.00113	2.65749
H	1.41643	2.46822	0.90296
H	3.04037	0.00026	0.43238

Table S13
Computational model for TS1 in $[C_2B_{10}H_{12}]^{2-}$ isomerisation

SCF (BP86) Energy =	-331.953022		
Enthalpy 0K =	-331.791567		
Enthalpy 298K =	-331.782440		
Free Energy 298K =	-331.823514		
Negative frequency =	-394.6406 cm^{-1}		
C	0.14069	1.75175	-0.09755
C	1.40708	1.12977	-0.60271
B	-1.26619	1.27688	-0.59650
B	-0.67212	0.91948	1.14737
B	1.92700	-0.21023	-0.22448
B	-1.10033	-0.30966	-1.43160
B	-1.77429	-0.23447	0.22371
B	0.96098	0.05589	1.36706
B	0.54086	-0.88448	-1.32736
B	-0.51767	-0.85406	1.34543
B	0.89027	-1.45064	0.40250
B	-0.76685	-1.59846	-0.26256
H	0.28230	2.81903	0.16175
H	2.06655	1.84375	-1.15685
H	-2.17456	2.09774	-0.68537
H	-1.08220	1.57383	2.08936
H	3.09131	-0.51648	-0.41724
H	-1.83315	-0.59409	-2.37188
H	-2.94668	-0.39106	0.51669
H	1.63471	0.36775	2.32505
H	1.08752	-1.49055	-2.23516
H	-0.85947	-1.35161	2.39969
H	1.50493	-2.45218	0.71736
H	-1.16614	-2.74646	-0.35973

Table S14
Computational model for INT in $[C_2B_{10}H_{12}]^{2-}$ isomerisation

SCF (BP86) Energy =	-331.979297		
Enthalpy 0K =	-331.816259		
Enthalpy 298K =	-331.806983		
Free Energy 298K =	-331.848263		
C	0.61175	-1.52706	0.45376
C	-0.61078	-1.52705	-0.45431
B	1.82775	-0.74625	-0.11139
B	0.86096	-0.09386	1.34658
B	-1.82739	-0.74727	0.11091
B	0.97109	0.11119	-1.48124
B	1.47826	0.98753	-0.02236
B	-0.97153	0.11019	1.48134
B	-0.86064	-0.09337	-1.34675
B	-0.00292	1.43469	0.90590
B	-1.47905	0.98688	0.02304
B	0.00226	1.43573	-0.90540
H	0.66625	-2.40778	1.12484
H	-0.66484	-2.40726	-1.12615
H	3.00445	-1.02889	0.06295
H	1.47088	-0.16882	2.39873
H	-3.00368	-1.03129	-0.06386
H	1.45630	0.13198	-2.59942
H	2.44372	1.72756	0.02018
H	-1.45641	0.13036	2.59964
H	-1.47046	-0.16873	-2.39893
H	0.12575	2.44615	1.57009
H	-2.44479	1.72654	-0.01912
H	-0.12698	2.44762	-1.56873

Table S15
Computational model for TS2 in $[C_2B_{10}H_{12}]^{2-}$ isomerisation

SCF (BP86) Energy =	-331.921718		
Enthalpy 0K =	-331.761328		
Enthalpy 298K =	-331.752130		
Free Energy 298K =	-331.793222		
Negative frequency =	-484.6 cm^{-1}		
C	-0.77888	-0.72169	-1.07495
C	-1.53290	1.13979	-0.49550
B	0.70203	-0.11011	-1.56718
B	0.63768	-1.54231	-0.47160
B	-1.96728	-0.14587	0.12323

B	1.23789	1.30887	-0.67532
B	1.81099	-0.26437	-0.13234
B	-0.78659	-1.34384	0.59786
B	-0.23031	1.76535	0.13896
B	0.79961	-0.95302	1.20421
B	-0.55418	0.17388	1.52291
B	1.03153	0.83670	1.05348
H	-1.35497	-1.28416	-1.82217
H	-2.15101	1.70428	-1.23510
H	1.01756	-0.41687	-2.71002
H	0.83165	-2.69247	-0.81397
H	-3.08963	-0.63725	0.07942
H	2.14691	2.07848	-0.96355
H	2.99412	-0.55314	-0.16625
H	-1.38194	-2.35639	0.89860
H	-0.43912	2.90832	0.56303
H	1.28075	-1.66528	2.06325
H	-1.03070	0.35731	2.62534
H	1.64016	1.42224	1.93303

Table S16
Computational model for [7,9-*nido*-$C_2B_{10}H_{12}]^{2-}$

SCF (BP86) Energy = -332.009355
Enthalpy 0K = -331.845583
Enthalpy 298K = -331.836339
Free Energy 298K = -331.877622

C	0.50339	-1.35017	-0.85794
C	-1.96463	-0.19885	-0.47288
B	1.08578	0.12498	-1.36460
B	1.66944	-0.69199	0.16862
B	-1.09450	-1.45517	-0.48254
B	0.22852	1.57945	-0.95055
B	1.49152	1.06371	0.16573
B	0.22617	-1.46772	0.80525
B	-1.45412	1.23599	-0.42906
B	0.66269	0.09023	1.45878
B	-1.09669	-0.13962	1.05437
B	-0.08873	1.52928	0.77264
H	0.88835	-2.26751	-1.33120
H	-3.05263	-0.36614	-0.36065
H	1.88288	0.06721	-2.29453
H	2.72869	-1.26521	0.32947
H	-1.61746	-2.56493	-0.50122
H	0.37501	2.66960	-1.49178
H	2.49100	1.72031	0.40286
H	0.32063	-2.51196	1.41450
H	-2.29281	2.13379	-0.35500
H	0.96917	0.10238	2.63372
H	-1.80316	-0.25158	2.03691
H	-0.27262	2.48243	1.50857