

Closo-carboranes as dual CH- π and BH- π donors: Theoretical study and biological significance.

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Electronic Supplementary Information

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PDB codes: 3VJT, 3VJS, 4MDG, 4Q78, 4MDL, 4MDM, 2C2S, 2C2T, 1ZTZ, 3I8W, 5E7V, 4Z0L, 5B5J

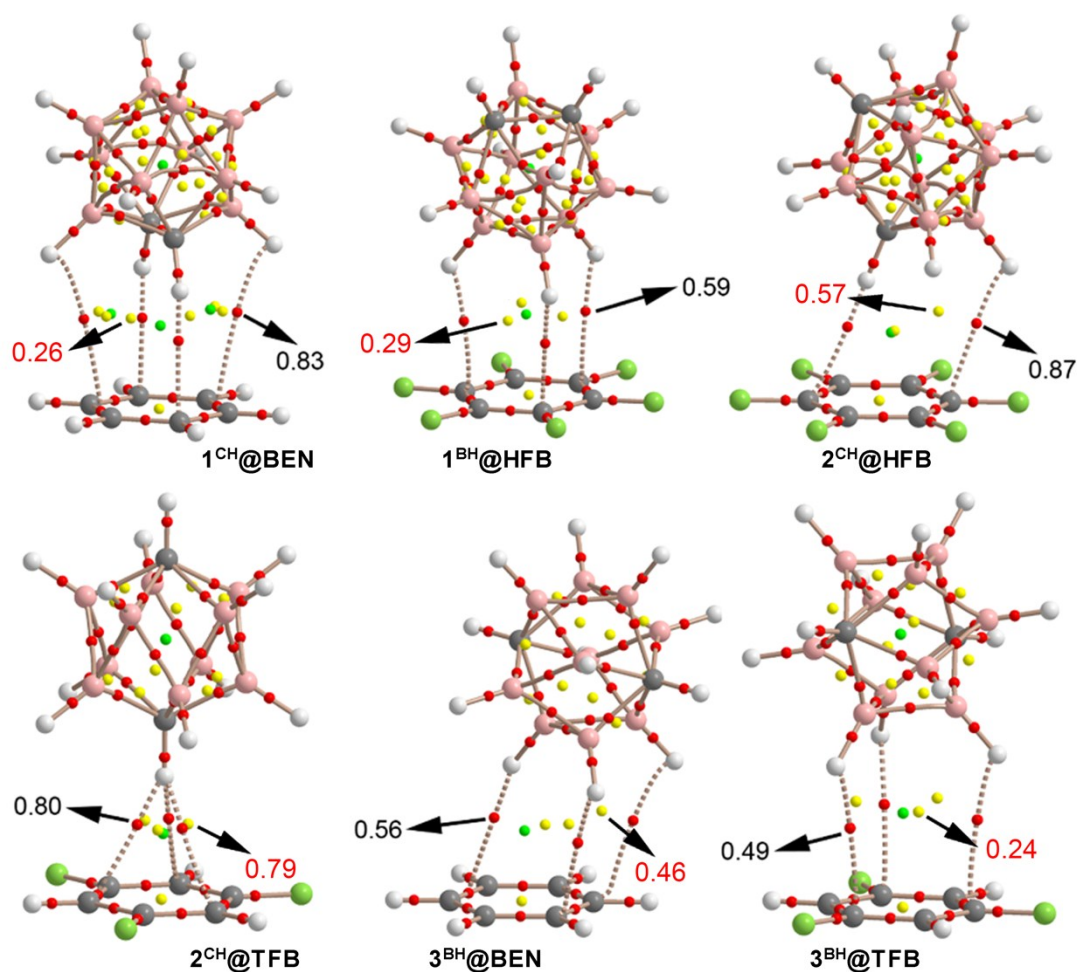
TableS1. SAPT interaction energies (E_{total} , kcal/mol) and their partitioning into the electrostatic, exchange, induction, dispersion and contributions (E_{ee} , E_{ex} , E_{ind} and E_{disp} , respectively, kcal/mol) using the DF-DFT-SAPT approach.

Complex	E_{ee}	E_{ex}	E_{ind}	E_{disp}	E_{total}
1^{CH}BEN	-5.0 (48%) ^a	6.8	-0.7 (7%) ^a	-4.8 (45%) ^a	-3.6
1^{CH}HFB	0.5 (9%) ^a	4.6	-0.5 (10%) ^a	-4.3 (81%) ^a	0.2
1^{BH}TFB	-1.4 (25%) ^a	4.3	-0.1 (2%) ^a	-4.0 (73%) ^a	-1.1
2^{CH}TFB	-1.5 (27%) ^a	4.4	-0.1 (3%) ^a	-4.0 (70%) ^a	-1.2
2^{BH}HFB	-2.6 (35%) ^a	5.8	-0.2 (3%) ^a	-4.7 (62%) ^a	-1.6
3^{CH}BEN	-3.8 (41%) ^a	6.2	-0.5 (10%) ^a	-4.9 (49%) ^a	-2.9

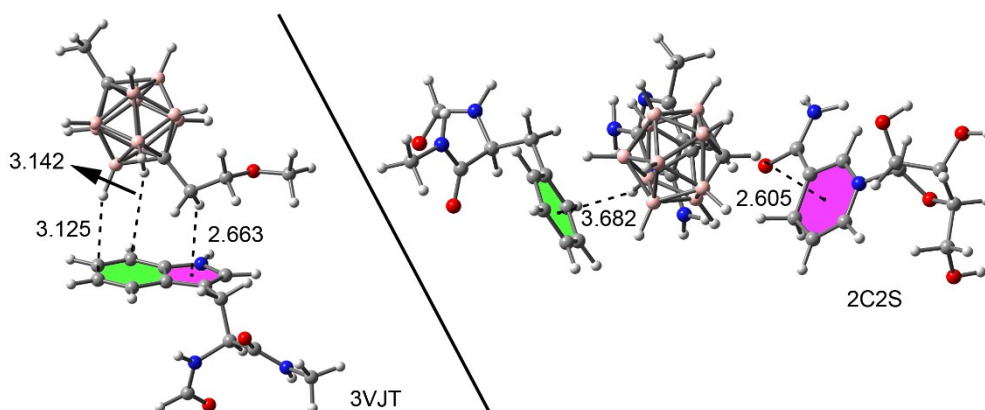
^a The percentatges were calculated taking into account only the favorable contributions (E_{ee} , E_{ind} and E_{disp}) which are discussed in the main text.

Additional AIM analyses:

Figure S1 gathers additional AIM analyses regarding the $\text{CH}\cdots\pi$ and $\text{BH}\cdots\pi$ complexes described in the main text. As noted, in case of complex **1^{CH}@BEN**, both $\text{CH}\cdots\pi$ and $\text{BH}\cdots\pi$ interactions are characterized by the presence of two bond CPs connecting the CH and BH bonds of the o-carborane with the C atoms and the C-C bond CPs of the arene moiety, respectively. In complex **1^{BH}@HFB**, three symmetrically distributed bond CPs connect the BH bonds of the o-carborane with the C atoms of hexafluorobenzene, thus characterizing the $\text{BH}\cdots\pi$ interactions. For complex **2^{CH}@HFB** concurrent $\text{CH}\cdots\pi$ and $\text{BH}\cdots\pi$ interactions are observed, owing to the presence of two bond CPs connecting both CH and BH bonds of the m-carborane to the C atoms of the arene. In complex **2^{CH}@TFB**, the $\text{CH}\cdots\pi$ interaction is characterized by the presence of three symmetrically distributed bond CPs connecting a CH bond of the p-carborane unit with three C atoms of the arene. Finally, in complexes **3^{BH}@BEN** and **3^{BH}@TFB** the $\text{BH}\cdots\pi$ interactions are characterized by the presence of three bond CPs connecting the B-H bonds of the p-carborane with the aromatic moieties of benzene and trifluorobenzene, respectively. It is also important to note that in all cases several ring CPs emerge owing to the formation of some supramolecular rings and a cage critical point (with the exception of complex 7, where three of them are observed), which further characterizes the interaction.



FigS1. Distribution of critical points and bond paths in some representative complexes. Bond, ring and cage critical points are denoted by red, yellow and green dots, respectively. The bond paths connecting bond critical points are also represented. The value of the density at the bond and ring (in red) critical points ($\rho \cdot 10^2$) is also indicated.



FigS2. Theoretical models used to evaluate the $\text{CH} \cdots \pi$ and $\text{BH} \cdots \pi$ interactions present in the PDB structures 3VJT and 2C2S. Distances in Å.

Cartesian coordinates

7.

B	0.0000000	1.4424865	-0.7645591
B	-1.4322433	0.8862414	-1.6398253
B	-1.4322433	-0.8862414	-1.6398253
B	0.0000000	-1.4424865	-0.7645591
B	1.4322433	0.8862414	-1.6398253
B	0.0000000	1.4455892	-2.5248609
B	-0.8880322	0.0000000	-3.0743422
B	0.0000000	-1.4455892	-2.5248609
B	1.4322433	-0.8862414	-1.6398253
C	-0.8061790	0.0000000	-0.3482151
H	-1.2680623	0.0000000	0.6286772
B	0.8880322	0.0000000	-3.0743422
C	0.8061790	0.0000000	-0.3482151
H	1.2680623	0.0000000	0.6286772
H	-1.5345235	0.0000000	-4.0701890
H	-2.4460285	1.4766843	-1.4715604
H	-2.4460285	-1.4766843	-1.4715604
H	0.0000000	-2.3215831	0.0270487
H	0.0000000	-2.4763605	-3.1131308
H	2.4460285	-1.4766843	-1.4715604
H	1.5345235	0.0000000	-4.0701890
H	2.4460285	1.4766843	-1.4715604
H	0.0000000	2.4763605	-3.1131308
H	0.0000000	2.3215831	0.0270487
C	0.6942016	1.2032141	3.2410118
C	-0.6942016	1.2032141	3.2410118
C	-1.3881642	0.0000000	3.2474361

C	-0.6942016	-1.2032141	3.2410118
C	0.6942016	-1.2032141	3.2410118
C	1.3881642	0.0000000	3.2474361
H	1.2360247	2.1420608	3.2384711
H	-1.2360247	2.1420608	3.2384711
H	-2.4724876	0.0000000	3.2559406
H	-1.2360247	-2.1420608	3.2384711
H	1.2360247	-2.1420608	3.2384711
H	2.4724876	0.0000000	3.2559406

8.

B	0.7773764	0.0050001	1.4436459
B	1.6462278	1.4418282	0.8868125
B	1.6462278	1.4418282	-0.8868125
B	0.7773764	0.0050001	-1.4436459
B	1.6598659	-1.4232240	0.8867309
B	2.5377458	0.0134757	1.4459097
B	3.0828731	0.9039904	0.0000000
B	2.5377458	0.0134757	-1.4459097
B	1.6598659	-1.4232240	-0.8867309
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H	1.4713210	2.4548374	-1.4760892
H	-0.0169150	0.0002113	-2.3208955

H	3.1255928	0.0162061	-2.4765804
H	1.4944281	-2.4376513	-1.4762511
H	4.0895573	-1.5139505	0.0000000
H	1.4944281	-2.4376513	1.4762511
H	3.1255928	0.0162061	2.4765804
H	-0.0169150	0.0002113	2.3208955
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C	-3.2760605	0.6835080	-1.2160504
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H	-3.2778095	1.2245417	-2.1521257
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F	-3.2498321	-1.3656926	2.3308023

9.

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B	-1.4329914	-0.8872152	-1.6579444
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B	0.0000000	1.4464975	-2.5418731
B	-0.8878605	0.0000000	-3.0914687
B	0.0000000	-1.4464975	-2.5418731
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H	-2.4461827	-1.4765892	-1.4861225
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H	1.5347889	0.0000000	-4.0864540
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C	-0.6933820	1.2022056	3.2834009
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C	-0.6933820	-1.2022056	3.2834009
C	0.6933820	-1.2022056	3.2834009
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F	1.3560137	2.3438404	3.2722833
F	-1.3560137	2.3438404	3.2722833
F	-2.7069546	0.0000000	3.2750204
F	-1.3560137	-2.3438404	3.2722833

10.

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B	2.0732233	-0.7865301	1.4320100
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C	-3.6706720	-0.8022155	1.2016953
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C	-3.4597018	1.2680133	0.0000000

C	-3.5300119	0.5781266	-1.2016776
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H	-3.3422501	2.3456744	0.0000000
H	-3.4670759	1.1168269	-2.1404409

11.

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H	-2.6114645	2.6814055	0.0000000
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H	-1.4358261	1.4236863	-2.4461250

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C	3.4373283	0.7582692	1.2143701
C	3.5071155	-0.6208007	1.1772518
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H	3.3962228	1.2973581	2.1502595
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F	3.5296437	-1.2883212	2.3320352
F	3.3204866	2.7474301	0.0000000

12.

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B	1.8373211	-1.0324271	1.4328718
B	1.0641832	-1.7383026	0.0000000
B	0.2719537	-0.4116785	-0.8874373
B	0.5569450	1.1080038	0.0000000
B	1.5249097	0.7140725	1.4331330
C	2.9519487	0.0678988	-0.8054056
H	3.9061558	0.2378264	-1.2828644

B	0.2719537	-0.4116785	0.8874373
C	2.9519487	0.0678988	0.8054056
H	3.9061558	0.2378264	1.2828644
H	-0.7032240	-0.5900810	-1.5396293
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H	1.5858489	1.3233230	2.4467647
H	-0.7032240	-0.5900810	1.5396293
H	2.1067336	-1.5818727	2.4470726
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H	3.7310864	-2.1536748	0.0000000
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C	-3.7196693	-1.0354312	0.0000000
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C	-3.2492875	0.9888293	1.1993720
C	-3.0949017	1.6642354	0.0000000
C	-3.2492875	0.9888293	-1.1993720
F	-4.0067773	-2.3267268	0.0000000
F	-3.0793828	1.6272347	-2.3454258
F	-3.0793828	1.6272347	2.3454258
F	-3.6951452	-1.0071246	2.3458395
F	-2.7864804	2.9504913	0.0000000
F	-3.6951452	-1.0071246	-2.3458395

13.

B	0.8868468	1.2282070	0.8858752
B	2.3877694	0.4932784	1.4368795

B	3.3159198	0.0310520	0.0000000
B	2.3877694	0.4932784	-1.4368795
B	0.8896391	-0.4410733	1.4353343
B	2.4010294	-1.1941616	0.8918695
B	2.4010294	-1.1941616	-0.8918695
B	0.8896391	-0.4410733	-1.4353343
C	2.3100146	1.4010654	0.0000000
H	2.7734450	2.3776380	0.0000000
B	0.8978744	-1.4766538	0.0000000
H	0.3278631	2.1227457	-1.4194983
H	2.9325254	-2.0422462	1.5295201
H	2.9270160	0.9480227	2.3887018
H	4.4917703	0.1792793	0.0000000
H	2.9270160	0.9480227	-2.3887018
H	2.9325254	-2.0422462	-1.5295201
H	0.2432733	-0.7244948	-2.3870085
H	0.2473561	-2.4672042	0.0000000
H	0.2432733	-0.7244948	2.3870085
H	0.3278631	2.1227457	1.4194983
C	0.1105010	0.0275720	0.0000000
H	-0.9695820	0.0404029	0.0000000
B	0.8868468	1.2282070	-0.8858752
C	-3.3379369	1.3123623	0.0000000
C	-3.3033970	0.6188003	-1.2027245
C	-3.2338621	-0.7681561	-1.2026010
C	-3.1988444	-1.4614758	0.0000000
C	-3.2338621	-0.7681561	1.2026010
C	-3.3033970	0.6188003	1.2027245
H	-3.3853084	2.3952552	0.0000000

H	-3.3229114	1.1602291	-2.1415972
H	-3.1967425	-1.3091996	-2.1410448
H	-3.1333084	-2.5431963	0.0000000
H	-3.1967425	-1.3091996	2.1410448
H	-3.3229114	1.1602291	2.1415972

14.

B	0.9332406	1.2276018	0.8865789
B	2.4116912	0.4490132	1.4371954
B	3.3256139	-0.0396938	0.0000000
B	2.4116912	0.4490132	-1.4371954
B	0.8876167	-0.4422453	1.4359543
B	2.3760401	-1.2386291	0.8919706
B	2.3760401	-1.2386291	-0.8919706
B	0.8876167	-0.4422453	-1.4359543
C	2.3595468	1.3592040	0.0000000
H	2.8508504	2.3220707	0.0000000
B	0.8655315	-1.4785800	0.0000000
H	0.3969840	2.1359961	-1.4200888
H	2.8825343	-2.1013844	1.5298515
H	2.9630651	0.8877863	2.3892717
H	4.5050067	0.0746035	0.0000000
H	2.9630651	0.8877863	-2.3892717
H	2.8825343	-2.1013844	-1.5298515
H	0.2312864	-0.7057555	-2.3865663
H	0.1837837	-2.4479583	0.0000000
H	0.2312864	-0.7057555	2.3865663
H	0.3969840	2.1359961	1.4200888
C	0.1245544	0.0490899	0.0000000

H	-0.9538225	0.0941168	0.0000000
B	0.9332406	1.2276018	-0.8865789
C	-3.3509950	1.3713565	0.0000000
C	-3.3207544	0.6496496	-1.1792126
C	-3.2605720	-0.7311215	-1.2154474
C	-3.2334339	-1.3905634	0.0000000
C	-3.2605720	-0.7311215	1.2154474
C	-3.3207544	0.6496496	1.1792126
H	-3.3900453	2.4515686	0.0000000
H	-3.2252650	-1.2712197	-2.1512194
H	-3.2252650	-1.2712197	2.1512194
F	-3.3357744	1.3173563	2.3313829
F	-3.1667762	-2.7193101	0.0000000
F	-3.3357744	1.3173563	-2.3313829

15.

B	1.0962121	1.3930906	0.8870041
B	2.4509750	0.4160257	1.4372424
B	3.2878554	-0.1947249	0.0000000
B	2.4509750	0.4160257	-1.4372424
B	0.8174770	-0.2544056	1.4363855
B	2.1806880	-1.2495130	0.8919530
B	2.1806880	-1.2495130	-0.8919530
B	0.8174770	-0.2544056	-1.4363855
C	2.5257726	1.3243552	0.0000000
H	3.1452748	2.2102600	0.0000000
B	0.6538685	-1.2770661	0.0000000
H	0.6909885	2.3673771	-1.4195100
H	2.5600433	-2.1749744	1.5298422

H	3.0574916	0.7733659	2.3896052
H	4.4714216	-0.2463483	0.0000000
H	3.0574916	0.7733659	-2.3896052
H	2.5600433	-2.1749744	-1.5298422
H	0.1292900	-0.4251800	-2.3856252
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H	0.1292900	-0.4251800	2.3856252
H	0.6909885	2.3673771	1.4195100
C	0.1311462	0.3387928	0.0000000
H	-0.9301033	0.5377019	0.0000000
B	1.0962121	1.3930906	-0.8870041
C	-3.5062717	1.1779911	0.0000000
C	-3.3823479	0.4953338	-1.2012391
C	-3.1397395	-0.8701305	-1.2010412
C	-3.0227751	-1.5535836	0.0000000
C	-3.1397395	-0.8701305	1.2010412
C	-3.3823479	0.4953338	1.2012391
F	-3.4878260	1.1477833	2.3455413
F	-2.7939425	-2.8530122	0.0000000
F	-3.4878260	1.1477833	-2.3455413
F	-3.0137187	-1.5172182	-2.3448463
F	-3.7315271	2.4806707	0.0000000
F	-3.0137187	-1.5172182	2.3448463

16.

B	-2.8606993	0.6320680	-0.8872280
B	-2.2397056	-0.9189436	-1.4368818
B	-1.8486927	-1.8787866	0.0000000
B	-2.2397056	-0.9189436	1.4368818

B	-1.1935105	0.5035876	-1.4360310
B	-0.5578543	-1.0586513	-0.8912998
B	-0.5578543	-1.0586513	0.8912998
B	-1.1935105	0.5035876	1.4360310
C	-3.1397722	-0.7719257	0.0000000
H	-4.1487314	-1.1597715	0.0000000
B	-0.1585788	0.4190570	0.0000000
H	-3.7111790	1.2559772	1.4210324
H	0.2465581	-1.6525116	-1.5299520
H	-2.7341933	-1.4216995	-2.3887088
H	-2.0859979	-3.0399816	0.0000000
H	-2.7341933	-1.4216995	2.3887088
H	0.2465581	-1.6525116	1.5299520
H	-0.8625586	1.1252367	2.3886163
H	0.8739069	0.9951834	0.0000000
H	-0.8625586	1.1252367	-2.3886163
H	-3.7111790	1.2559772	-1.4210324
C	-1.6036221	1.3168828	0.0000000
H	-1.5340503	2.3955331	0.0000000
B	-2.8606993	0.6320680	0.8872280
C	3.7301666	1.7601711	0.0000000
C	3.5949720	1.0793582	1.2020752
C	3.3249118	-0.2818928	1.2016824
C	3.1899345	-0.9621247	0.0000000
C	3.3249118	-0.2818928	-1.2016824
C	3.5949720	1.0793582	-1.2020752
H	3.9378274	2.8243036	0.0000000
H	3.6954365	1.6118039	2.1411361
H	3.2092443	-0.8124528	2.1399398

H	2.9647655	-2.0223008	0.0000000
H	3.2092443	-0.8124528	-2.1399398
H	3.6954365	1.6118039	-2.1411361

17.

B	-2.9881509	0.5922656	-0.8869947
B	-2.1034241	-0.8249084	-1.4365423
B	-1.5490767	-1.7005347	0.0000000
B	-2.1034241	-0.8249084	1.4365423
B	-1.3250940	0.7599176	-1.4365386
B	-0.4235501	-0.6660836	-0.8918574
B	-0.4235501	-0.6660836	0.8918574
B	-1.3250940	0.7599176	1.4365386
C	-3.0147475	-0.8390920	0.0000000
H	-3.9397706	-1.3983855	0.0000000
B	-0.2930925	0.8574008	0.0000000
H	-3.9345517	1.0574066	1.4209222
H	0.4697201	-1.1083592	-1.5340029
H	-2.4998165	-1.4065434	-2.3891524
H	-1.5757611	-2.8851090	0.0000000
H	-2.4998165	-1.4065434	2.3891524
H	0.4697201	-1.1083592	1.5340029
H	-1.1086659	1.4298200	2.3889993
H	0.6246173	1.6058414	0.0000000
H	-1.1086659	1.4298200	-2.3889993
H	-3.9345517	1.0574066	-1.4209222
C	-1.8714750	1.4886341	0.0000000
H	-1.9950200	2.5626317	0.0000000
B	-2.9881509	0.5922656	0.8869947

C	3.5915994	1.4057431	0.0000000
C	3.5280072	0.7506968	1.2145090
C	3.3919350	-0.6237670	1.1774051
C	3.3222948	-1.3423371	0.0000000
C	3.3919350	-0.6237670	-1.1774051
C	3.5280072	0.7506968	-1.2145090
H	3.5709890	1.2892863	2.1506331
H	3.2008631	-2.4162045	0.0000000
H	3.5709890	1.2892863	-2.1506331
F	3.7106448	2.7351498	0.0000000
F	3.3170637	-1.2866003	-2.3322165
F	3.3170637	-1.2866003	2.3322165

18.

B	-2.9144876	0.7356493	-0.8873182
B	-2.1050613	-0.7262668	-1.4369568
B	-1.5972595	-1.6301620	0.0000000
B	-2.1050613	-0.7262668	1.4369568
B	-1.2452415	0.8160795	-1.4375861
B	-0.4197754	-0.6551260	-0.8914860
B	-0.4197754	-0.6551260	0.8914860
B	-1.2452415	0.8160795	1.4375861
C	-3.0153929	-0.6926455	0.0000000
H	-3.9681631	-1.2033499	0.0000000
B	-0.2122607	0.8597729	0.0000000
H	-3.8347990	1.2497593	1.4214558
H	0.4481955	-1.1455072	-1.5341918
H	-2.5304785	-1.2862574	-2.3896596
H	-1.6845334	-2.8114319	0.0000000

H	-2.5304785	-1.2862574	2.3896596
H	0.4481955	-1.1455072	1.5341918
H	-0.9917121	1.4736524	2.3892386
H	0.7409036	1.5623812	0.0000000
H	-0.9917121	1.4736524	-2.3892386
H	-3.8347990	1.2497593	-1.4214558
C	-1.7529704	1.5725409	0.0000000
H	-1.8188726	2.6515715	0.0000000
B	-2.9144876	0.7356493	0.8873182
C	3.5575357	1.2695727	0.0000000
C	3.4701328	0.5831018	1.1998811
C	3.2971574	-0.7913500	1.1998362
C	3.2096541	-1.4782788	0.0000000
C	3.2971574	-0.7913500	-1.1998362
C	3.4701328	0.5831018	-1.1998811
F	3.7012045	2.5851964	0.0000000
F	3.2001121	-1.4456198	-2.3449018
F	3.2001121	-1.4456198	2.3449018
F	3.5333826	1.2429582	-2.3449299
F	3.5333826	1.2429582	2.3449299
F	3.0253047	-2.7873139	0.0000000

19.

B	2.3695365	-1.2251071	-0.8872032
B	2.3695365	-1.2251071	0.8872032
B	2.3838217	0.4624390	1.4354800
B	2.3925657	1.5055427	0.0000000
B	0.8803630	-0.4572444	-1.4339139
B	0.8716232	-1.4992454	0.0000000

B	0.8803630	-0.4572444	1.4339139
B	0.8946023	1.2285662	0.8863138
B	0.8946023	1.2285662	-0.8863138
C	3.1532256	-0.0104391	0.0000000
H	4.2343902	-0.0195872	0.0000000
H	3.0161278	0.7667212	-2.3895313
H	0.2482101	-0.7616078	2.3881187
H	2.9923409	-2.0415758	1.4769510
H	3.0161278	0.7667212	2.3895313
H	3.0305854	2.5030602	0.0000000
H	0.2722345	2.0451469	1.4760989
H	0.2722345	2.0451469	-1.4760989
H	0.2482101	-0.7616078	-2.3881187
H	0.2338824	-2.4968616	0.0000000
H	2.9923409	-2.0415758	-1.4769510
C	0.1131705	0.0151002	0.0000000
H	-0.9670085	0.0237844	0.0000000
B	2.3838217	0.4624390	-1.4354800
C	-3.2585258	-1.3932616	0.0000000
C	-3.2643158	-0.6990212	-1.2025904
C	-3.2753138	0.6895898	-1.2026324
C	-3.2805862	1.3838447	0.0000000
C	-3.2753138	0.6895898	1.2026324
C	-3.2643158	-0.6990212	1.2025904
H	-3.2394925	-2.4768909	0.0000000
H	-3.2501953	-1.2409477	-2.1412232
H	-3.2698359	1.2316783	-2.1412437
H	-3.2789819	2.4676786	0.0000000
H	-3.2698359	1.2316783	2.1412437

H	-3.2501953	-1.2409477	2.1412232
20.			
B	2.3796671	-1.2267302	-0.8873925
B	2.3796671	-1.2267302	0.8873925
B	2.3943142	0.4614357	1.4357033
B	2.4032066	1.5050182	0.0000000
B	0.8912832	-0.4583441	-1.4345713
B	0.8820251	-1.5013428	0.0000000
B	0.8912832	-0.4583441	1.4345713
B	0.9057525	1.2286806	0.8868870
B	0.9057525	1.2286806	-0.8868870
C	3.1629533	-0.0117700	0.0000000
H	4.2441415	-0.0210863	0.0000000
H	3.0259334	0.7654501	-2.3899948
H	0.2570362	-0.7619086	2.3876675
H	3.0020365	-2.0430683	1.4772343
H	3.0259334	0.7654501	2.3899948
H	3.0411563	2.5022973	0.0000000
H	0.2807231	2.0434473	1.4764120
H	0.2807231	2.0434473	-1.4764120
H	0.2570362	-0.7619086	-2.3876675
H	0.2409841	-2.4968423	0.0000000
H	3.0020365	-2.0430683	-1.4772343
C	0.1263895	0.0145597	0.0000000
H	-0.9529176	0.0235928	0.0000000
B	2.3943142	0.4614357	-1.4357033
C	-3.2744452	-1.3641453	0.0000000
C	-3.2810038	-0.7044203	-1.2153191

C	-3.2984654	0.6778077	-1.1790636
C	-3.3060264	1.3999690	0.0000000
C	-3.2984654	0.6778077	1.1790636
C	-3.2810038	-0.7044203	1.2153191
H	-3.2643607	-1.2450957	-2.1512560
H	-3.3091299	2.4808776	0.0000000
H	-3.2643607	-1.2450957	2.1512560
F	-3.2970393	1.3447925	-2.3313862
F	-3.2500911	-2.6952214	0.0000000
F	-3.2970393	1.3447925	2.3313862

21.

B	2.3751600	-1.2260633	-0.8877203
B	2.3751600	-1.2260633	0.8877203
B	2.3940719	0.4623587	1.4363392
B	2.4056211	1.5059552	0.0000000
B	0.8890967	-0.4540245	-1.4356208
B	0.8774188	-1.4972423	0.0000000
B	0.8890967	-0.4540245	1.4356208
B	0.9079477	1.2337347	0.8873582
B	0.9079477	1.2337347	-0.8873582
C	3.1608916	-0.0128248	0.0000000
H	4.2420730	-0.0249658	0.0000000
H	3.0263479	0.7650435	-2.3903214
H	0.2507707	-0.7557267	2.3866904
H	2.9948471	-2.0443374	1.4772779
H	3.0263479	0.7650435	2.3903214
H	3.0454246	2.5017613	0.0000000
H	0.2826621	2.0494239	1.4753818

H	0.2826621	2.0494239	-1.4753818
H	0.2507707	-0.7557267	-2.3866904
H	0.2317288	-2.4899020	0.0000000
H	2.9948471	-2.0443374	-1.4772779
C	0.1278578	0.0209810	0.0000000
H	-0.9506514	0.0328148	0.0000000
B	2.3940719	0.4623587	-1.4363392
C	-3.2719663	-1.3948313	0.0000000
C	-3.2799221	-0.7017012	-1.2013301
C	-3.2953369	0.6853160	-1.2013441
C	-3.3029435	1.3784663	0.0000000
C	-3.2953369	0.6853160	1.2013441
C	-3.2799221	-0.7017012	1.2013301
F	-3.2909582	1.3472140	-2.3442213
F	-3.2462326	-2.7152205	0.0000000
F	-3.2909582	1.3472140	2.3442213
F	-3.2616187	-1.3633034	-2.3442546
F	-3.3053581	2.6991397	0.0000000
F	-3.2616187	-1.3633034	2.3442546

22.

B	2.2443817	0.8761282	-1.4352320
B	3.2863194	0.8097336	0.0000000
B	2.2443817	0.8761282	1.4352320
B	0.5597963	0.9825289	0.8863717
B	1.2178989	-0.5561824	-1.4347106
B	2.9030711	-0.6632384	-0.8874838
B	2.9030711	-0.6632384	0.8874838
B	1.2178989	-0.5561824	1.4347106

B	0.1748522	-0.4916997	0.0000000
C	1.8285115	1.6770154	0.0000000
H	1.8973681	2.7560100	0.0000000
H	-0.2085964	1.6618888	-1.4771816
H	3.6743664	-1.3412776	1.4769472
H	4.3277006	1.3730782	0.0000000
H	2.5936769	1.4840159	2.3896375
H	-0.2085964	1.6618888	1.4771816
H	0.8686431	-1.1634421	2.3894991
H	-0.8631976	-1.0563651	0.0000000
H	0.8686431	-1.1634421	-2.3894991
H	3.6743664	-1.3412776	-1.4769472
H	2.5936769	1.4840159	-2.3896375
C	1.6352092	-1.3567326	0.0000000
H	1.5659290	-2.4357064	0.0000000
B	0.5597963	0.9825289	-0.8863717
C	-3.2419180	0.8613033	-0.6937562
C	-3.2419180	0.8613033	0.6937562
C	-3.4656068	-0.3190454	1.3879204
C	-3.6894222	-1.5000934	0.6939893
C	-3.6894222	-1.5000934	-0.6939893
C	-3.4656068	-0.3190454	-1.3879204
H	-3.0608309	1.7824629	-1.2354768
H	-3.0608309	1.7824629	1.2354768
H	-3.4605996	-0.3196321	2.4719433
H	-3.8612066	-2.4230833	1.2363241
H	-3.8612066	-2.4230833	-1.2363241
H	-3.4605996	-0.3196321	-2.4719433

23.

B	-2.0617609	0.7806940	1.4348640
B	-3.0924799	0.9410370	0.0000000
B	-2.0617609	0.7806940	-1.4348640
B	-0.3945149	0.5211108	-0.8868885
B	-1.3696961	-0.8395648	1.4348208
B	-3.0372338	-0.5799108	0.8869750
B	-3.0372338	-0.5799108	-0.8869750
B	-1.3696961	-0.8395648	-1.4348208
B	-0.3400798	-1.0005476	0.0000000
C	-1.4822964	1.4725001	0.0000000
H	-1.3151193	2.5408051	0.0000000
H	0.5003948	1.0188340	1.4793691
H	-3.9358369	-1.0757906	-1.4770328
H	-3.9879776	1.7158488	0.0000000
H	-2.2703576	1.4484788	-2.3898770
H	0.5003948	1.0188340	-1.4793691
H	-1.1596571	-1.5072431	-2.3896946
H	0.5499331	-1.7802791	0.0000000
H	-1.1596571	-1.5072431	2.3896946
H	-3.9358369	-1.0757906	1.4770328
H	-2.2703576	1.4484788	2.3898770
C	-1.9497501	-1.5315136	0.0000000
H	-2.1158556	-2.5999785	0.0000000
B	-0.3945149	0.5211108	0.8868885
C	3.4416002	0.7385958	1.1775892
C	3.4473096	1.4606754	0.0000000
C	3.4416002	0.7385958	-1.1775892
C	3.4344889	-0.6422507	-1.2147576

C	3.4302317	-1.3002652	0.0000000
C	3.4344889	-0.6422507	1.2147576
H	3.4460925	2.5414550	0.0000000
H	3.4197783	-1.1830621	-2.1505245
H	3.4197783	-1.1830621	2.1505245
F	3.4101844	-2.6338574	0.0000000
F	3.4326989	1.4071686	2.3316868
F	3.4326989	1.4071686	-2.3316868

24.

B	-2.0551629	0.7672101	1.4353550
B	-3.0900855	0.8953722	0.0000000
B	-2.0551629	0.7672101	-1.4353550
B	-0.3816237	0.5592901	-0.8869026
B	-1.3130046	-0.8312341	1.4357844
B	-2.9875491	-0.6235428	0.8872082
B	-2.9875491	-0.6235428	-0.8872082
B	-1.3130046	-0.8312341	-1.4357844
B	-0.2804928	-0.9597207	0.0000000
C	-1.4971337	1.4769882	0.0000000
H	-1.3622746	2.5499071	0.0000000
H	0.4958886	1.0858455	1.4813433
H	-3.8699160	-1.1473939	-1.4771496
H	-4.0089348	1.6418427	0.0000000
H	-2.2832026	1.4282678	-2.3903365
H	0.4958886	1.0858455	-1.4813433
H	-1.0801289	-1.4917541	-2.3900201
H	0.6326745	-1.7126666	0.0000000
H	-1.0801289	-1.4917541	2.3900201

H	-3.8699160	-1.1473939	1.4771496
H	-2.2832026	1.4282678	2.3903365
C	-1.8710612	-1.5408123	0.0000000
H	-2.0031075	-2.6140614	0.0000000
B	-0.3816237	0.5592901	0.8869026
C	3.3509012	0.7565389	1.1999343
C	3.3213898	1.4478005	0.0000000
C	3.3509012	0.7565389	-1.1999343
C	3.4082374	-0.6275906	-1.2002185
C	3.4375581	-1.3186164	0.0000000
C	3.4082374	-0.6275906	1.2002185
F	3.4709464	-2.6407919	0.0000000
F	3.3045971	1.4183663	2.3440912
F	3.3045971	1.4183663	-2.3440912
F	3.2432732	2.7685391	0.0000000
F	3.4145875	-1.2908934	2.3442504
F	3.4145875	-1.2908934	-2.3442504