

Halogen···halogen interactions in decahalo-closo-carboranes: CSD analysis and theoretical study

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FigS1

The MEP (Molecular Electrostatic Potential) surfaces for compounds **7** to **9** are gathered in FigS1. As noted, the maximum values of electrostatic potential region are located along the C-H bonds, similarly to the *ortho* and *meta* series (**1** to **6**). However, all B-X bonds exhibit a nearly identical MEP value, due to the symmetry of the *para* series. Also in close agreement to the *ortho* and *meta* series (**1** to **6**), the σ -hole MEP values over the halogen atoms increase while the MEP values over the H atoms become less positive ongoing from compound **7** to **9**. Finally, the fact the halogen atoms show large green areas where the MEP value is close to zero, also supports the fact that these B-X bonds are well rounded to undergo type I halogen···halogen “like-like” interactions.

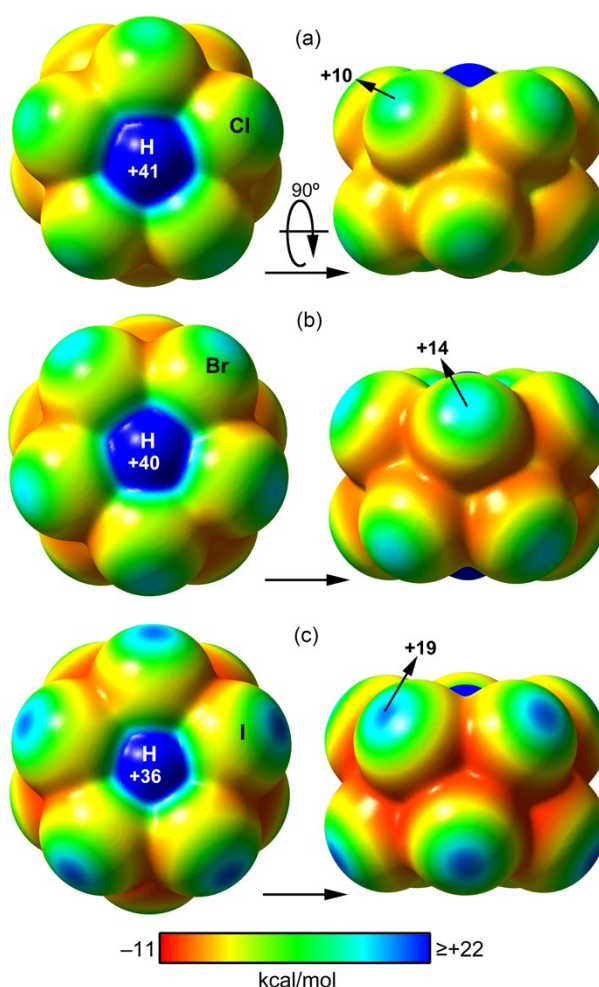


Fig.S1 Two views of the MEP surfaces for ortho compounds **7** (a), **8** (b) and **9** (c). Energy values at selected points of the surface (0.001 a.u.) are given in kcal/mol.

Table S1. SAPT interaction energies (E_{total} , kcal/mol) and their partitioning into the electrostatic, exchange, induction, dispersion and contributions (Elst, Exch, Ind and Disp, respectively, kcal/mol) using the DF-DFT-SAPT approach at the PBE0-D/def2-TZVP

Complex	Elst	Exch	Ind	Disp	Etotal
10	-0.78	1.51	-0.11	-3.16	-2.54
11	-1.12	2.18	-0.15	-3.52	-2.61
12	-1.63	2.67	-0.54	-3.86	-3.37
17	-1.01	1.23	-0.10	-2.84	-2.72
18	-1.85	2.65	-0.55	-3.92	-3.66
22	-1.03	1.99	-0.05	-2.59	-1.68
23	-1.39	1.63	-0.09	-3.00	-2.85
24	-1.70	1.28	-0.52	-3.00	-3.95

Cartesian Coordinates

10.

B	5.3536701	-0.4921201	1.4606930
B	4.0687527	-1.6020316	0.8987136
B	4.0687527	-1.6020316	-0.8987136
B	5.3536701	-0.4921201	-1.4606930
B	4.9464287	1.1565012	0.8989933
B	3.6610964	0.0463211	1.4688731
B	2.8569012	-0.6409998	0.0000000
B	3.6610964	0.0463211	-1.4688731
B	4.9464287	1.1565012	-0.8989933
C	5.4950042	-1.3835099	0.0000000
H	6.2680343	-2.1414918	0.0000000
B	3.4013350	1.0720842	0.0000000
C	5.9840736	0.1535489	0.0000000
H	7.0525638	0.3255136	0.0000000
Cl	6.4243467	-0.8337772	2.7970483
Cl	3.7881138	-3.0898621	1.7811466
Cl	2.8094717	0.3158480	2.9829505
Cl	1.1613407	-1.0965897	0.0000000
Cl	2.2796094	2.4250239	0.0000000
Cl	2.8094717	0.3158480	-2.9829505
Cl	6.4243467	-0.8337772	-2.7970483
Cl	3.7881138	-3.0898621	-1.7811466
Cl	5.5788555	2.5314094	-1.7819655
Cl	5.5788555	2.5314094	1.7819655
B	-4.9600026	-0.5572832	-1.4606086
B	-3.2599880	-0.5490673	-0.8995258
B	-3.2599880	-0.5490673	0.8995258
B	-4.9600026	-0.5572832	1.4606086
B	-5.7376786	0.9532336	-0.8991028
B	-4.0387639	0.9607789	-1.4690820
B	-2.9788290	0.9735104	0.0000000
B	-4.0387639	0.9607789	1.4690820
B	-5.7376786	0.9532336	0.8991028
C	-4.4796274	-1.3211285	0.0000000
H	-4.5641454	-2.3999221	0.0000000
B	-4.5174320	1.9042124	0.0000000
C	-5.8601932	-0.4843837	0.0000000
H	-6.7776139	-1.0577997	0.0000000

C1	-5.5430688	-1.5191692	-2.7962520
C1	-2.0753374	-1.4870173	-1.7854979
C1	-3.5773248	1.7227899	-2.9849327
C1	-1.4041770	1.7498534	0.0000000
C1	-4.5576319	3.6619808	0.0000000
C1	-3.5773248	1.7227899	2.9849327
C1	-5.5430688	-1.5191692	2.7962520
C1	-2.0753374	-1.4870173	1.7854979
C1	-7.1181778	1.5734947	1.7829517
C1	-7.1181778	1.5734947	-1.7829517

10. (B3LYP-D3/def2-TZVP)

B	5.3478133	-0.4898062	1.4700703
B	4.0603055	-1.6081369	0.9040698
B	4.0603055	-1.6081369	-0.9040698
B	5.3478133	-0.4898062	-1.4700703
B	4.9346151	1.1649123	0.9044256
B	3.6506384	0.0449973	1.4769080
B	2.8438865	-0.6471771	0.0000000
B	3.6506384	0.0449973	-1.4769080
B	4.9346151	1.1649123	-0.9044256
C	5.4909678	-1.3874902	0.0000000
H	6.2659294	-2.1407102	0.0000000
B	3.3863242	1.0746976	0.0000000
C	5.9801492	0.1630702	0.0000000
H	7.0465767	0.3352156	0.0000000
C1	6.4286618	-0.8316829	2.8123564
C1	3.7765577	-3.1053957	1.7931130
C1	2.7892074	0.3151418	2.9996378
C1	1.1376474	-1.1076759	0.0000000
C1	2.2530785	2.4336404	0.0000000
C1	2.7892074	0.3151418	-2.9996378
C1	6.4286618	-0.8316829	-2.8123564
C1	3.7765577	-3.1053957	-1.7931130
C1	5.5621204	2.5527597	-1.7939875
C1	5.5621204	2.5527597	1.7939875
B	-4.9547122	-0.5602708	-1.4697237
B	-3.2471855	-0.5590804	-0.9049710
B	-3.2471855	-0.5590804	0.9049710
B	-4.9547122	-0.5602708	1.4697237
B	-5.7298092	0.9599103	-0.9044367
B	-4.0256608	0.9567957	-1.4771073
B	-2.9601960	0.9661721	0.0000000
B	-4.0256608	0.9567957	1.4771073
B	-5.7298092	0.9599103	0.9044367
C	-4.4725070	-1.3310020	0.0000000
H	-4.5633098	-2.4073108	0.0000000
B	-4.5018737	1.9070327	0.0000000
C	-5.8612493	-0.4817601	0.0000000
H	-6.7781476	-1.0522655	0.0000000
C1	-5.5464369	-1.5279849	-2.8115579
C1	-2.0562281	-1.5038340	-1.7980984
C1	-3.5561925	1.7248517	-3.0017937
C1	-1.3725021	1.7423718	0.0000000

C1	-4.5332415	3.6772952	0.0000000
C1	-3.5561925	1.7248517	3.0017937
C1	-5.5464369	-1.5279849	2.8115579
C1	-2.0562281	-1.5038340	1.7980984
C1	-7.1144609	1.5947709	1.7948739
C1	-7.1144609	1.5947709	-1.7948739

10. BP86-D3/def2-TZVP

B	5.3422244	-0.4928462	1.4756067
B	4.0436759	-1.6040795	0.9066250
B	4.0436759	-1.6040795	-0.9066250
B	5.3422244	-0.4928462	-1.4756067
B	4.9412101	1.1686796	0.9069956
B	3.6427440	0.0569260	1.4795679
B	2.8301617	-0.6310578	0.0000000
B	3.6427440	0.0569260	-1.4795679
B	4.9412101	1.1686796	-0.9069956
C	5.4815067	-1.3960142	0.0000000
H	6.2552696	-2.1624392	0.0000000
B	3.3872945	1.0908400	0.0000000
C	5.9845351	0.1568674	0.0000000
H	7.0601406	0.3240169	0.0000000
C1	6.4167179	-0.8420449	2.8231587
C1	3.7462154	-3.0997909	1.7960427
C1	2.7831181	0.3336667	3.0026740
C1	1.1196979	-1.0790375	0.0000000
C1	2.2663112	2.4608993	0.0000000
C1	2.7831181	0.3336667	-3.0026740
C1	6.4167179	-0.8420449	-2.8231587
C1	3.7462154	-3.0997909	-1.7960427
C1	5.5782138	2.5533573	-1.7971578
C1	5.5782138	2.5533573	1.7971578
B	-4.9504310	-0.5663042	-1.4755691
B	-3.2386901	-0.5658083	-0.9076692
B	-3.2386901	-0.5658083	0.9076692
B	-4.9504310	-0.5663042	1.4755691
B	-5.7277649	0.9572776	-0.9071767
B	-4.0176732	0.9564104	-1.4799102
B	-2.9500435	0.9641286	0.0000000
B	-4.0176732	0.9564104	1.4799102
B	-5.7277649	0.9572776	0.9071767
C	-4.4675064	-1.3421880	0.0000000
H	-4.5573992	-2.4268501	0.0000000
B	-4.4960782	1.9079342	0.0000000
C	-5.8619858	-0.4895094	0.0000000
H	-6.7867667	-1.0628674	0.0000000
C1	-5.5398654	-1.5312311	-2.8224236
C1	-2.0472147	-1.5103011	-1.8026878
C1	-3.5477063	1.7247781	-3.0049219
C1	-1.3616667	1.7408467	0.0000000
C1	-4.5280058	3.6788747	0.0000000
C1	-3.5477063	1.7247781	3.0049219
C1	-5.5398654	-1.5312311	2.8224236
C1	-2.0472147	-1.5103011	1.8026878
C1	-7.1125063	1.5940885	1.7984479

C1 -7.1125063 1.5940885 -1.7984479

11.

B	5.9078227	-0.1261265	1.4606280
B	5.0020052	-1.5629094	0.8992014
B	5.0020052	-1.5629094	-0.8992014
B	5.9078227	-0.1261265	-1.4606280
B	5.0368534	1.3322557	0.8991987
B	4.1313247	-0.1046360	1.4664609
B	3.5629873	-0.9962438	0.0000000
B	4.1313247	-0.1046360	-1.4664609
B	5.0368534	1.3322557	-0.8991987
C	6.3026920	-0.9399082	0.0000000
H	7.2632795	-1.4376923	0.0000000
B	3.5838932	0.8010581	0.0000000
C	6.3221929	0.6777375	0.0000000
H	7.2946085	1.1521257	0.0000000
B	-5.7874801	-0.3379856	-1.4596516
B	-4.2969705	-1.1525125	-0.8983174
B	-4.2969705	-1.1525125	0.8983174
B	-5.7874801	-0.3379856	1.4596516
B	-5.7351964	1.3601707	-0.8989220
B	-4.2461635	0.5443352	-1.4659353
B	-3.3142644	0.0425703	0.0000000
B	-4.2461635	0.5443352	1.4659353
B	-5.7351964	1.3601707	0.8989220
C	-5.7368251	-1.2402749	0.0000000
H	-6.3344111	-2.1419700	0.0000000
B	-4.2071095	1.6009006	0.0000000
C	-6.5395648	0.1632514	0.0000000
H	-7.6199281	0.1054961	0.0000000
Br	-6.8637028	-0.9533965	2.9096946
Br	-6.7195943	2.6826644	1.8705778
Br	-6.7195943	2.6826644	-1.8705778
Br	-3.3203463	3.3029696	0.0000000
Br	-3.4102189	1.0209976	-3.1257538
Br	-3.4102189	1.0209976	3.1257538
Br	-1.4003441	-0.0576588	0.0000000
Br	-3.6517104	-2.6692369	-1.8698669
Br	-3.6517104	-2.6692369	1.8698669
Br	1.9387873	-2.0183662	0.0000000
Br	3.1659238	-0.0933011	3.1244301
Br	3.1659238	-0.0933011	-3.1244301
Br	1.9842261	1.8597568	0.0000000
Br	5.2524769	2.9661680	-1.8708330
Br	5.2524769	2.9661680	1.8708330
Br	7.1468097	-0.1413616	-2.9108940
Br	7.1468097	-0.1413616	2.9108940
Br	5.1778838	-3.2020013	1.8706931
Br	5.1778838	-3.2020013	-1.8706931
Br	-6.8637028	-0.9533965	-2.9096946

12.

B 5.9045082 -0.4508700 1.4633857

B	4.6474356	-1.5953579	0.9000893
B	4.6474356	-1.5953579	-0.9000893
B	5.9045082	-0.4508700	-1.4633857
B	5.4537920	1.1880555	0.9003861
B	4.1945142	0.0437770	1.4669280
B	3.4075065	-0.6659201	0.0000000
B	4.1945142	0.0437770	-1.4669280
B	5.4537920	1.1880555	-0.9003861
C	6.0656163	-1.3392831	0.0000000
H	6.8609207	-2.0735015	0.0000000
B	3.9089697	1.0618026	0.0000000
C	6.5157094	0.2140102	0.0000000
H	7.5797143	0.4100221	0.0000000
B	-5.5074090	-0.5847555	-1.4627778
B	-3.8061192	-0.5937077	-0.9001651
B	-3.8061192	-0.5937077	0.9001651
B	-5.5074090	-0.5847555	1.4627778
B	-6.2695786	0.9360991	-0.9003909
B	-4.5682567	0.9268698	-1.4666670
B	-3.5085874	0.9290283	0.0000000
B	-4.5682567	0.9268698	1.4666670
B	-6.2695786	0.9360991	0.9003909
C	-5.0315277	-1.3525852	0.0000000
H	-5.1316939	-2.4297837	0.0000000
B	-5.0371755	1.8762118	0.0000000
C	-6.4069574	-0.4983855	0.0000000
H	-7.3282202	-1.0649273	0.0000000
I	-6.2526340	-1.7848652	3.0549936
I	-7.9336139	1.7098307	1.9896579
I	-5.0803534	4.0145513	0.0000000
I	-4.0096568	1.8212816	3.3261400
I	-1.5690420	1.8241281	0.0000000
I	-2.3722964	-1.7388107	1.9901677
I	1.3615609	-1.2797501	0.0000000
I	3.1715236	0.3387272	3.3205748
I	2.5201389	2.6901346	0.0000000
I	4.3508296	-3.4061118	1.9895187
I	7.2601704	-0.8447272	3.0561147
I	6.1735014	2.8766888	1.9882965
I	6.1735014	2.8766888	-1.9882965
I	7.2601704	-0.8447272	-3.0561147
I	3.1715236	0.3387272	-3.3205748
I	4.3508296	-3.4061118	-1.9895187
I	-4.0096568	1.8212816	-3.3261400
I	-2.3722964	-1.7388107	-1.9901677
I	-7.9336139	1.7098307	-1.9896579
I	-6.2526340	-1.7848652	-3.0549936

13.

B	5.4623854	-0.4377666	1.4610473
B	4.1921617	-1.5642876	0.8987459
B	4.1921617	-1.5642876	-0.8987459
B	5.4623854	-0.4377666	-1.4610473
B	5.0341453	1.2050614	0.8990881
B	3.7627791	0.0784477	1.4688166

B	2.9673780	-0.6194155	0.0000000
B	3.7627791	0.0784477	-1.4688166
B	5.0341453	1.2050614	-0.8990881
C	5.6154493	-1.3271626	0.0000000
H	6.3982280	-2.0750736	0.0000000
B	3.4906660	1.1003372	0.0000000
C	6.0846080	0.2158293	0.0000000
H	7.1507705	0.4015791	0.0000000
Cl	6.5373687	-0.7654231	2.7973176
Cl	3.9307383	-3.0557522	1.7809565
Cl	2.9068892	0.3374028	2.9823652
Cl	1.2778212	-1.0969666	0.0000000
Cl	2.3564648	2.4435725	0.0000000
Cl	2.9068892	0.3374028	-2.9823652
Cl	6.5373687	-0.7654231	-2.7973176
Cl	3.9307383	-3.0557522	-1.7809565
Cl	5.6478083	2.5885136	-1.7817824
Cl	5.6478083	2.5885136	1.7817824
B	-5.0637521	-0.6082367	-1.4592751
B	-3.3645701	-0.5886970	-0.8988021
B	-3.3645701	-0.5886970	0.8988021
B	-5.0637521	-0.6082367	1.4592751
B	-5.8498635	0.8974402	-0.8985572
B	-4.1519165	0.9155685	-1.4657699
B	-3.0932222	0.9354973	0.0000000
B	-4.1519165	0.9155685	1.4657699
B	-5.8498635	0.8974402	0.8985572
C	-4.5774226	-1.3696870	0.0000000
H	-4.6564910	-2.4487221	0.0000000
B	-4.6355907	1.8555330	0.0000000
C	-5.9655275	-0.5398079	0.0000000
H	-6.8788827	-1.1193431	0.0000000
Br	-1.3730039	1.7801776	0.0000000
Br	-3.6587120	1.7401366	3.1266352
Br	-4.6996929	3.7735523	0.0000000
Br	-3.6587120	1.7401366	-3.1266352
Br	-7.3550446	1.5699034	1.8703988
Br	-7.3550446	1.5699034	-1.8703988
Br	-5.7003402	-1.6717523	-2.9095916
Br	-5.7003402	-1.6717523	2.9095916
Br	-2.0608529	-1.5955086	1.8713367
Br	-2.0608529	-1.5955086	-1.8713367

14.

B	5.6144281	-0.3980684	1.4611860
B	4.3459469	-1.5265645	0.8987450
B	4.3459469	-1.5265645	-0.8987450
B	5.6144281	-0.3980684	-1.4611860
B	5.1836700	1.2439232	0.8991893
B	3.9137934	0.1154363	1.4688369
B	3.1194366	-0.5839957	0.0000000
B	3.9137934	0.1154363	-1.4688369
B	5.1836700	1.2439232	-0.8991893
C	5.7689458	-1.2871242	0.0000000
H	6.5529561	-2.0337814	0.0000000

B	3.6408659	1.1362978	0.0000000
C	6.2356762	0.2565367	0.0000000
H	7.3015516	0.4440631	0.0000000
Cl	6.6896577	-0.7238317	2.7975715
Cl	4.0865526	-3.0182809	1.7809421
Cl	3.0566800	0.3734081	2.9818495
Cl	1.4311324	-1.0659311	0.0000000
Cl	2.5080837	2.4819357	0.0000000
Cl	3.0566800	0.3734081	-2.9818495
Cl	6.6896577	-0.7238317	-2.7975715
Cl	4.0865526	-3.0182809	-1.7809421
Cl	5.7943743	2.6287372	-1.7816646
Cl	5.7943743	2.6287372	1.7816646
B	-5.2095678	-0.6578094	-1.4625801
B	-3.5081267	-0.6179453	-0.9005011
B	-3.5081267	-0.6179453	0.9005011
B	-5.2095678	-0.6578094	1.4625801
B	-6.0151240	0.8407785	-0.9003340
B	-4.3141840	0.8802492	-1.4668206
B	-3.2544525	0.9128242	0.0000000
B	-4.3141840	0.8802492	1.4668206
B	-6.0151240	0.8407785	0.9003340
C	-4.7116950	-1.4112854	0.0000000
H	-4.7807319	-2.4908755	0.0000000
B	-4.8100261	1.8159074	0.0000000
C	-6.1113943	-0.5970829	0.0000000
H	-7.0159773	-1.1898906	0.0000000
I	-5.9216084	-1.8789551	3.0542181
I	-5.9216084	-1.8789551	-3.0542181
I	-7.7005242	1.5680144	-1.9891098
I	-7.7005242	1.5680144	1.9891098
I	-4.9152234	3.9522019	0.0000000
I	-3.7826045	1.7899772	-3.3268118
I	-3.7826045	1.7899772	3.3268118
I	-1.3427459	1.8644901	0.0000000
I	-2.0415641	-1.7212139	-1.9887010
I	-2.0415641	-1.7212139	1.9887010

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B	5.6317998	-0.4018573	1.4706604
B	4.3538600	-1.5306939	0.9041111
B	4.3538600	-1.5306939	-0.9041111
B	5.6317998	-0.4018573	-1.4706604
B	5.2054647	1.2488859	0.9046881
B	3.9298050	0.1188504	1.4768105
B	3.1289327	-0.5804883	0.0000000
B	3.9298050	0.1188504	-1.4768105
B	5.2054647	1.2488859	-0.9046881
C	5.7827006	-1.2980847	0.0000000
H	6.5639496	-2.0448120	0.0000000
B	3.6587852	1.1452655	0.0000000
C	6.2590167	0.2561107	0.0000000
H	7.3239867	0.4371334	0.0000000
Cl	6.7149011	-0.7344627	2.8131553
Cl	4.0814826	-3.0300558	1.7929581

C1	3.0638368	0.3826013	2.9981006
C1	1.4279365	-1.0593283	0.0000000
C1	2.5220131	2.5034487	0.0000000
C1	3.0638368	0.3826013	-2.9981006
C1	6.7149011	-0.7344627	-2.8131553
C1	4.0814826	-3.0300558	-1.7929581
C1	5.8201174	2.6426660	-1.7937488
C1	5.8201174	2.6426660	1.7937488
B	-5.2245544	-0.6622556	-1.4704326
B	-3.5133347	-0.6187553	-0.9070225
B	-3.5133347	-0.6187553	0.9070225
B	-5.2245544	-0.6622556	1.4704326
B	-6.0360006	0.8443296	-0.9067870
B	-4.3289210	0.8809936	-1.4776934
B	-3.2618449	0.9179088	0.0000000
B	-4.3289210	0.8809936	1.4776934
B	-6.0360006	0.8443296	0.9067870
C	-4.7170748	-1.4159319	0.0000000
H	-4.7876674	-2.4930704	0.0000000
B	-4.8274419	1.8233867	0.0000000
C	-6.1317914	-0.5958185	0.0000000
H	-7.0316436	-1.1914994	0.0000000
I	-5.9539811	-1.9183336	3.0596691
I	-5.9539811	-1.9183336	-3.0596691
I	-7.7452340	1.5752742	-2.0085694
I	-7.7452340	1.5752742	2.0085694
I	-4.9349381	3.9872150	0.0000000
I	-3.7926946	1.8016189	-3.3622616
I	-3.7926946	1.8016189	3.3622616
I	-1.3292451	1.8868814	0.0000000
I	-2.0293840	-1.7379641	-2.0076264
I	-2.0293840	-1.7379641	2.0076264

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B	5.6040546	-0.4002679	1.4765196
B	4.3188352	-1.5260252	0.9067280
B	4.3188352	-1.5260252	-0.9067280
B	5.6040546	-0.4002679	-1.4765196
B	5.1849918	1.2558647	0.9073161
B	3.8978947	0.1301788	1.4794225
B	3.0938298	-0.5680145	0.0000000
B	3.8978947	0.1301788	-1.4794225
B	5.1849918	1.2558647	-0.9073161
C	5.7542260	-1.3014276	0.0000000
H	6.5367716	-2.0589149	0.0000000
B	3.6328536	1.1597753	0.0000000
C	6.2394469	0.2564479	0.0000000
H	7.3130573	0.4359909	0.0000000
C1	6.6820181	-0.7369552	2.8241035
C1	4.0371532	-3.0249194	1.7956099
C1	3.0316682	0.3981804	3.0002979
C1	1.3908904	-1.0428670	0.0000000
C1	2.5060000	2.5273413	0.0000000
C1	3.0316682	0.3981804	-3.0002979
C1	6.6820181	-0.7369552	-2.8241035

C1	4.0371532	-3.0249194	-1.7956099
C1	5.8047304	2.6486574	-1.7967684
C1	5.8047304	2.6486574	1.7967684
B	-5.2015630	-0.6673715	-1.4755730
B	-3.4875582	-0.6339274	-0.9087900
B	-3.4875582	-0.6339274	0.9087900
B	-5.2015630	-0.6673715	1.4755730
B	-6.0064187	0.8454712	-0.9085001
B	-4.2948376	0.8752200	-1.4783584
B	-3.2270049	0.9046478	0.0000000
B	-4.2948376	0.8752200	1.4783584
B	-6.0064187	0.8454712	0.9085001
C	-4.6976563	-1.4314924	0.0000000
H	-4.7727686	-2.5171193	0.0000000
B	-4.7899874	1.8202241	0.0000000
C	-6.1150737	-0.5995522	0.0000000
H	-7.0265568	-1.1933729	0.0000000
I	-5.9299916	-1.9053450	3.0738610
I	-5.9299916	-1.9053450	-3.0738610
I	-7.7050269	1.5883997	-2.0083155
I	-7.7050269	1.5883997	2.0083155
I	-4.8857926	3.9784886	0.0000000
I	-3.7540654	1.7912146	-3.3571179
I	-3.7540654	1.7912146	3.3571179
I	-1.2943405	1.8603146	0.0000000
I	-2.0108321	-1.7536102	-2.0082872
I	-2.0108321	-1.7536102	2.0082872

15.

B	-0.8975699	-6.3182331	0.8981463
B	-1.0530296	-4.6168914	-1.4532249
B	0.5330388	-5.4205676	-1.4532004
B	0.5330388	-5.4205676	1.4532004
B	-1.0530296	-4.6168914	1.4532249
B	-1.1492327	-3.5660487	0.0000000
B	0.3774023	-3.7197927	-0.8979424
B	0.3774023	-3.7197927	0.8979424
B	0.6898742	5.7999438	-1.4543763
B	-0.1694961	4.2377874	-1.4537215
B	-1.0028838	5.7306411	0.8987643
B	1.5230183	4.3075837	-0.8982559
B	0.3461677	3.3148202	0.0000000
B	-0.1694961	4.2377874	1.4537215
B	0.6898742	5.7999438	1.4543763
B	1.5230183	4.3075837	0.8982559
C	1.5957146	5.7650685	0.0000000
B	0.1747626	6.7228948	0.0000000
H	2.5411714	6.2935998	0.0000000
C	1.2578335	-4.8805780	0.0000000
H	2.3371016	-4.7808941	0.0000000
B	0.6291773	-6.4725237	0.0000000
C	-1.7778456	-5.1571822	0.0000000
H	-2.8571236	-5.2566560	0.0000000
B	-0.8975699	-6.3182331	-0.8981463
C	-1.0746226	4.2738939	0.0000000

H	-2.0200157	3.7453207	0.0000000
B	-1.0028838	5.7306411	-0.8987643
I	0.3175723	1.1844228	0.0000000
I	3.1798471	3.5175322	-1.9856861
I	3.1798471	3.5175322	1.9856861
I	1.3407354	6.8161534	3.2132749
I	1.3407354	6.8161534	-3.2132749
I	-0.8205578	3.2162388	3.2096477
I	-0.8205578	3.2162388	-3.2096477
I	-2.6607605	6.5174446	1.9863704
I	-2.6607605	6.5174446	-1.9863704
I	0.2013517	8.8558646	0.0000000
Br	1.2146316	-2.3000482	1.8693836
Br	-2.2582590	-2.0071076	0.0000000
Br	-2.0577406	-4.1939478	3.0246356
Br	-1.7363102	-7.7363507	1.8695532
Br	1.5385120	-5.8397179	3.0251767
Br	1.5385120	-5.8397179	-3.0251767
Br	1.7388242	-8.0304462	0.0000000
Br	-2.0577406	-4.1939478	-3.0246356
Br	-1.7363102	-7.7363507	-1.8695532
Br	1.2146316	-2.3000482	-1.8693836

16.

B	-5.9460923	-0.7413201	0.8899748
B	-4.2578212	-1.0129511	1.4339925
B	-3.2568051	0.3730905	0.8901787
B	-4.3189691	1.4808819	0.0000000
B	-5.9460923	-0.7413201	-0.8899748
B	-4.8789388	-1.8780714	0.0000000
B	-3.2062324	-1.1860689	0.0000000
B	-3.2568051	0.3730905	-0.8901787
C	-4.9145101	0.5699754	1.2994331
H	-5.1336460	1.1000205	2.2184307
B	-4.2578212	-1.0129511	-1.4339925
B	5.2987264	1.7467560	0.0000000
B	3.8000289	1.4148622	0.8901639
B	3.8615767	-0.2940878	1.4344451
B	5.4164951	-1.0067511	0.8904356
B	3.8000289	1.4148622	-0.8901639
B	2.8922210	0.1477717	0.0000000
B	3.8971138	-1.3589626	0.0000000
B	5.4164951	-1.0067511	-0.8904356
C	5.2873058	0.6577562	1.2997443
H	5.7650798	0.9764152	2.2181564
B	3.8615767	-0.2940878	-1.4344451
C	5.2873058	0.6577562	-1.2997443
B	6.2975839	0.2502403	0.0000000
H	5.7650798	0.9764152	-2.2181564
C	-4.9145101	0.5699754	-1.2994331
H	-5.1336460	1.1000205	-2.2184307
B	-5.9802119	0.7925849	0.0000000
Cl	-5.1794916	-3.6103424	0.0000000
Cl	-3.9587287	-1.7359458	3.0021122
Cl	-3.9587287	-1.7359458	-3.0021122

C1	-1.7711608	-2.1999993	0.0000000
C1	-1.9763318	1.0213950	1.8941090
C1	-1.9763318	1.0213950	-1.8941090
C1	-4.1345136	3.2180482	0.0000000
C1	-7.3397048	1.8897498	0.0000000
C1	-7.3106354	-1.1898777	-1.8939055
C1	-7.3106354	-1.1898777	1.8939055
C1	3.2080062	-0.7280646	3.0013613
C1	3.2080062	-0.7280646	-3.0013613
C1	1.1377083	0.1053851	0.0000000
C1	3.0923921	2.6649531	1.8938815
C1	3.0923921	2.6649531	-1.8938815
C1	6.1114323	3.2932535	0.0000000
C1	8.0374156	0.4077989	0.0000000
C1	6.3019098	-2.1368624	-1.8949539
C1	6.3019098	-2.1368624	1.8949539
C1	3.1805742	-2.9642405	0.0000000

17.

B	-6.1664327	-0.7483740	0.8904802
B	-4.4795333	-1.0159031	1.4357955
B	-3.4857900	0.3725271	0.8905424
B	-4.5501039	1.4799069	0.0000000
B	-6.1664327	-0.7483740	-0.8904802
B	-5.0967289	-1.8794872	0.0000000
B	-3.4300687	-1.1834594	0.0000000
B	-3.4857900	0.3725271	-0.8905424
C	-5.1410704	0.5649100	1.3013631
H	-5.3625714	1.0957718	2.2190003
B	-4.4795333	-1.0159031	-1.4357955
B	5.5843432	1.7298832	0.0000000
B	4.0733476	1.4511126	0.8903312
B	4.0699462	-0.2564916	1.4360515
B	5.5957759	-1.0246088	0.8906667
B	4.0733476	1.4511126	-0.8903312
B	3.1210512	0.2204438	0.0000000
B	4.0668849	-1.3183904	0.0000000
B	5.5957759	-1.0246088	-0.8906667
C	5.5299393	0.6411493	1.3016493
H	6.0205588	0.9425208	2.2188574
B	4.0699462	-0.2564916	-1.4360515
Br	6.5183861	-2.3010964	1.9771325
Br	6.5183861	-2.3010964	-1.9771325
Br	3.3293248	-0.7091712	-3.1417359
Br	3.3469606	2.8500822	-1.9754492
Br	3.2234960	-3.0416107	0.0000000
Br	1.2055851	0.2481251	0.0000000
Br	3.3469606	2.8500822	1.9754492
Br	3.3293248	-0.7091712	3.1417359
Br	-1.8532098	-2.2752615	0.0000000
Br	-5.4226003	-3.7700191	0.0000000
Br	-2.0816045	1.0862997	-1.9762706
Br	-4.1451286	-1.8135400	-3.1432194
Br	-7.6612041	-1.2468326	-1.9767433
Br	-4.3407189	3.3770548	0.0000000

Br	-7.6612041	-1.2468326	1.9767433
Br	-4.1451286	-1.8135400	3.1432194
Br	-2.0816045	1.0862997	1.9762706
Br	6.5231777	3.3917814	0.0000000
C	5.5299393	0.6411493	-1.3016493
B	6.5260044	0.1985241	0.0000000
Br	8.4327893	0.2866883	0.0000000
H	6.0205588	0.9425208	-2.2188574
C	-5.1410704	0.5649100	-1.3013631
H	-5.3625714	1.0957718	-2.2190003
B	-6.2076516	0.7869320	0.0000000
Br	-7.7040587	1.9721772	0.0000000

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B	-6.1879867	-0.7546807	0.8923009
B	-4.4899823	-1.0200738	1.4399847
B	-3.4922690	0.3784717	0.8925326
B	-4.5633996	1.4891781	0.0000000
B	-6.1879867	-0.7546807	-0.8923009
B	-5.1099974	-1.8870517	0.0000000
B	-3.4354702	-1.1841379	0.0000000
B	-3.4922690	0.3784717	-0.8925326
C	-5.1587795	0.5692828	1.3046918
H	-5.3798889	1.0968791	2.2217956
B	-4.4899823	-1.0200738	-1.4399847
B	5.6043970	1.7388072	0.0000000
B	4.0859274	1.4617215	0.8920956
B	4.0792349	-0.2561936	1.4403870
B	5.6123368	-1.0332096	0.8925992
B	4.0859274	1.4617215	-0.8920956
B	3.1287697	0.2268320	0.0000000
B	4.0758562	-1.3225609	0.0000000
B	5.6123368	-1.0332096	-0.8925992
C	5.5503426	0.6436634	1.3051369
H	6.0391294	0.9424735	2.2216575
B	4.0792349	-0.2561936	-1.4403870
Br	6.5378851	-2.3227804	1.9910393
Br	6.5378851	-2.3227804	-1.9910393
Br	3.3303694	-0.7111128	-3.1611639
Br	3.3555678	2.8727819	-1.9889991
Br	3.2183872	-3.0586990	0.0000000
Br	1.1968790	0.2577319	0.0000000
Br	3.3555678	2.8727819	1.9889991
Br	3.3303694	-0.7111128	3.1611639
Br	-1.8443961	-2.2856215	0.0000000
Br	-5.4337906	-3.7960349	0.0000000
Br	-2.0797348	1.1005663	-1.9914287
Br	-4.1508945	-1.8246881	-3.1623806
Br	-7.6931593	-1.2611235	-1.9903439
Br	-4.3566205	3.4035898	0.0000000
Br	-7.6931593	-1.2611235	1.9903439
Br	-4.1508945	-1.8246881	3.1623806
Br	-2.0797348	1.1005663	1.9914287
Br	6.5559465	3.4128775	0.0000000
C	5.5503426	0.6436634	-1.3051369
B	6.5500119	0.1932489	0.0000000

Br	8.4737263	0.2788485	0.0000000
H	6.0391294	0.9424735	-2.2216575
C	-5.1587795	0.5692828	-1.3046918
H	-5.3798889	1.0968791	-2.2217956
B	-6.2327001	0.7876416	0.0000000
Br	-7.7437964	1.9813948	0.0000000

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B	-6.1493030	-0.7693514	0.8953253
B	-4.4453919	-1.0195670	1.4443802
B	-3.4586905	0.3907843	0.8952705
B	-4.5432915	1.4959887	0.0000000
B	-6.1493030	-0.7693514	-0.8953253
B	-5.0582931	-1.8936617	0.0000000
B	-3.3873957	-1.1740254	0.0000000
B	-3.4586905	0.3907843	-0.8952705
C	-5.1308612	0.5680472	1.3100109
H	-5.3585763	1.0985486	2.2337329
B	-4.4453919	-1.0195670	-1.4443802
B	5.5919907	1.7334967	0.0000000
B	4.0649599	1.4744584	0.8950038
B	4.0355341	-0.2466588	1.4448820
B	5.5611707	-1.0457333	0.8956209
B	4.0649599	1.4744584	-0.8950038
B	3.0906836	0.2498690	0.0000000
B	4.0177219	-1.3145787	0.0000000
B	5.5611707	-1.0457333	-0.8956209
C	5.5227005	0.6361439	1.3106415
H	6.0201707	0.9310028	2.2336978
B	4.0355341	-0.2466588	-1.4448820
Br	6.4683672	-2.3499553	1.9899513
Br	6.4683672	-2.3499553	-1.9899513
Br	3.2775640	-0.6929586	-3.1624191
Br	3.3497924	2.8946769	-1.9876003
Br	3.1352602	-3.0363252	0.0000000
Br	1.1606817	0.3065828	0.0000000
Br	3.3497924	2.8946769	1.9876003
Br	3.2775640	-0.6929586	3.1624191
Br	-1.7883810	-2.2608554	0.0000000
Br	-5.3643749	-3.8036799	0.0000000
Br	-2.0523372	1.1248270	-1.9918068
Br	-4.0980341	-1.8233012	-3.1640124
Br	-7.6501614	-1.2924641	-1.9892521
Br	-4.3516357	3.4107968	0.0000000
Br	-7.6501614	-1.2924641	1.9892521
Br	-4.0980341	-1.8233012	3.1640124
Br	-2.0523372	1.1248270	1.9918068
Br	6.5631753	3.3949418	0.0000000
C	5.5227005	0.6361439	-1.3106415
B	6.5190862	0.1721299	0.0000000
Br	8.4427986	0.2295074	0.0000000
H	6.0201707	0.9310028	-2.2336978
C	-5.1308612	0.5680472	-1.3100109
H	-5.3585763	1.0985486	-2.2337329
B	-6.2095995	0.7777954	0.0000000

Br	-7.7322346	1.9550194	0.0000000
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18.

B	-6.3537642	-0.2993855	0.8930908
B	-4.7859052	-0.9821844	1.4419940
B	-3.4722856	0.1140636	0.8942374
B	-4.2251513	1.4574708	0.0000000
B	-6.3537642	-0.2993855	-0.8930908
B	-5.6004696	-1.6630717	0.0000000
B	-3.8133382	-1.4051911	0.0000000
B	-3.4722856	0.1140636	-0.8942374
C	-5.0294227	0.7144979	1.3028757
H	-5.1113509	1.2860089	2.2184682
B	-4.7859052	-0.9821844	-1.4419940
B	4.9322814	1.8300582	0.0000000
B	3.6936588	0.9118866	0.8922622
B	4.4396625	-0.6248228	1.4411562
B	6.1502730	-0.6453994	0.8929819
B	3.6936588	0.9118866	-0.8922622
B	3.3778910	-0.6145249	0.0000000
B	4.9041041	-1.5797384	0.0000000
B	6.1502730	-0.6453994	-0.8929819
C	5.3587976	0.8227396	1.3025747
H	5.6682152	1.3104253	2.2184118
B	4.4396625	-0.6248228	-1.4411562
C	5.3587976	0.8227396	-1.3025747
B	6.4525393	0.8659915	0.0000000
H	5.6682152	1.3104253	-2.2184118
C	-5.0294227	0.7144979	-1.3028757
H	-5.1113509	1.2860089	-2.2184682
B	-6.0081193	1.2032576	0.0000000
I	-8.1107797	-0.4184950	2.0986400
I	-7.2988708	2.8982447	0.0000000
I	-3.4567452	3.4444038	0.0000000
I	-1.7490425	0.4898518	-2.0922977
I	-1.7490425	0.4898518	2.0922977
I	-2.4193401	-3.0284080	0.0000000
I	-4.6475272	-1.9419834	-3.3441096
I	-4.6475272	-1.9419834	3.3441096
I	-6.4851594	-3.6089515	0.0000000
I	-8.1107797	-0.4184950	-2.0986400
I	3.9166946	-1.4409596	3.3434110
I	1.4411476	-1.5128438	0.0000000
I	2.2827789	1.9722199	2.0944554
I	2.2827789	1.9722199	-2.0944554
I	5.0537336	3.9572485	0.0000000
I	8.3253134	1.8811436	0.0000000
I	7.7041604	-1.4725269	-2.0989549
I	7.7041604	-1.4725269	2.0989549
I	4.9118577	-3.7169622	0.0000000
I	3.9166946	-1.4409596	-3.3434110

19.

B	-6.0668319	-0.7833406	0.8900132
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B	-4.3735305	-1.0228090	1.4340807
B	-3.3997954	0.3824066	0.8901689
B	-4.4825412	1.4700923	0.0000000
B	-6.0668319	-0.7833406	-0.8900132
B	-4.9779741	-1.8996224	0.0000000
B	-3.3189639	-1.1752374	0.0000000
B	-3.3997954	0.3824066	-0.8901689
C	-5.0604731	0.5475573	1.2994555
H	-5.2897973	1.0731278	2.2185580
B	-4.3735305	-1.0228090	-1.4340807
B	5.4933677	1.7384737	0.0000000
B	3.9821729	1.4602960	0.8901846
B	3.9787577	-0.2475454	1.4360504
B	5.5044390	-1.0159874	0.8906698
B	3.9821729	1.4602960	-0.8901846
B	3.0298541	0.2290386	0.0000000
B	3.9755883	-1.3097478	0.0000000
B	5.5044390	-1.0159874	-0.8906698
C	5.4387255	0.6498549	1.3015440
H	5.9293352	0.9511287	2.2187878
B	3.9787577	-0.2475454	-1.4360504
C	5.4387255	0.6498549	-1.3015440
B	6.4348261	0.2069597	0.0000000
H	5.9293352	0.9511287	-2.2187878
C	-5.0604731	0.5475573	-1.2994555
H	-5.2897973	1.0731278	-2.2185580
B	-6.1303911	0.7499246	0.0000000
Br	3.1324537	-3.0328358	0.0000000
Br	3.2390226	-0.6999692	3.1421486
Br	3.2390226	-0.6999692	-3.1421486
Br	1.1143716	0.2545200	0.0000000
Br	3.2566174	2.8594120	1.9755047
Br	3.2566174	2.8594120	-1.9755047
Br	6.4328284	3.4000967	0.0000000
Br	8.3416422	0.2948351	0.0000000
Br	6.4270131	-2.2923984	-1.9772879
Br	6.4270131	-2.2923984	1.9772879
Cl	-5.2455092	-3.6372316	0.0000000
Cl	-1.8622362	-2.1578768	0.0000000
Cl	-2.1309913	1.0547346	1.8934360
Cl	-2.1309913	1.0547346	-1.8934360
Cl	-4.3308241	3.2102809	0.0000000
Cl	-7.4223191	-1.2580025	1.8940003
Cl	-7.4223191	-1.2580025	-1.8940003
Cl	-7.5104629	1.8210037	0.0000000
Cl	-4.0603597	-1.7398020	3.0020584
Cl	-4.0603597	-1.7398020	-3.0020584

19. B3LYP-D3/def2-TZVP

B	-6.0868362	-0.7900954	0.8916132
B	-4.3826409	-1.0265589	1.4380107
B	-3.4054682	0.3887349	0.8918865
B	-4.4950469	1.4791802	0.0000000
B	-6.0868362	-0.7900954	-0.8916132
B	-4.9894527	-1.9065905	0.0000000

B	-3.3232404	-1.1752412	0.0000000
B	-3.4054682	0.3887349	-0.8918865
C	-5.0775640	0.5522946	1.3030988
H	-5.3066037	1.0748185	2.2216357
B	-4.3826409	-1.0265589	-1.4380107
B	5.5124767	1.7473191	0.0000000
B	3.9938339	1.4708660	0.8920684
B	3.9866854	-0.2472492	1.4403853
B	5.5196813	-1.0246536	0.8925330
B	3.9938339	1.4708660	-0.8920684
B	3.0359300	0.2361794	0.0000000
B	3.9831078	-1.3137704	0.0000000
B	5.5196813	-1.0246536	-0.8925330
C	5.4581161	0.6522214	1.3049990
H	5.9467545	0.9508630	2.2216036
B	3.9866854	-0.2472492	-1.4403853
C	5.4581161	0.6522214	-1.3049990
B	6.4577077	0.2014453	0.0000000
H	5.9467545	0.9508630	-2.2216036
C	-5.0775640	0.5522946	-1.3030988
H	-5.3066037	1.0748185	-2.2216357
B	-6.1545002	0.7497457	0.0000000
Br	3.1263295	-3.0498983	0.0000000
Br	3.2387531	-0.7019674	3.1615118
Br	3.2387531	-0.7019674	-3.1615118
Br	1.1037471	0.2664496	0.0000000
Br	3.2646531	2.8822261	1.9891641
Br	3.2646531	2.8822261	-1.9891641
Br	6.4646866	3.4210374	0.0000000
Br	8.3814375	0.2865225	0.0000000
Br	6.4448855	-2.3145120	-1.9908815
Br	6.4448855	-2.3145120	1.9908815
Cl	-5.2532355	-3.6574009	0.0000000
Cl	-1.8568106	-2.1651715	0.0000000
Cl	-2.1319266	1.0670899	1.9052102
Cl	-2.1319266	1.0670899	-1.9052102
Cl	-4.3451901	3.2311662	0.0000000
Cl	-7.4483983	-1.2728166	1.9039538
Cl	-7.4483983	-1.2728166	-1.9039538
Cl	-7.5461422	1.8248082	0.0000000
Cl	-4.0648274	-1.7491520	3.0156053
Cl	-4.0648274	-1.7491520	-3.0156053

19. BP86-D3/def2-TZVP

B	-6.0401387	-0.8171584	0.8949397
B	-4.3283668	-1.0300448	1.4430387
B	-3.3685602	0.4025274	0.8951878
B	-4.4774963	1.4822533	0.0000000
B	-6.0401387	-0.8171584	-0.8949397
B	-4.9239255	-1.9207090	0.0000000
B	-3.2637320	-1.1640769	0.0000000
B	-3.3685602	0.4025274	-0.8951878
C	-5.0476264	0.5434831	1.3081661
H	-5.2857527	1.0674527	2.2332720
B	-4.3283668	-1.0300448	-1.4430387

B	5.5161674	1.7359208	0.0000000
B	3.9853925	1.4991300	0.8950378
B	3.9310698	-0.2215391	1.4447939
B	5.4448985	-1.0425025	0.8954221
B	3.9853925	1.4991300	-0.8950378
B	2.9929530	0.2885308	0.0000000
B	3.8979067	-1.2893717	0.0000000
B	5.4448985	-1.0425025	-0.8954221
C	5.4309036	0.6396126	1.3104754
H	5.9324364	0.9270583	2.2336624
B	3.9310698	-0.2215391	-1.4447939
C	5.4309036	0.6396126	-1.3104754
B	6.4204064	0.1613973	0.0000000
H	5.9324364	0.9270583	-2.2336624
C	-5.0476264	0.5434831	-1.3081661
H	-5.2857527	1.0674527	-2.2332720
B	-6.1305633	0.7277718	0.0000000
Br	2.9920038	-2.9984488	0.0000000
Br	3.1679499	-0.6569538	3.1628066
Br	3.1679499	-0.6569538	-3.1628066
Br	1.0636574	0.3722144	0.0000000
Br	3.2920394	2.9297274	1.9880926
Br	3.2920394	2.9297274	-1.9880926
Br	6.5113983	3.3832130	0.0000000
Br	8.3447048	0.1910603	0.0000000
Br	6.3333803	-2.3594719	-1.9898213
Br	6.3333803	-2.3594719	1.9898213
Cl	-5.1631413	-3.6754315	0.0000000
Cl	-1.7829042	-2.1332888	0.0000000
Cl	-2.1048423	1.0990648	1.9102383
Cl	-2.1048423	1.0990648	-1.9102383
Cl	-4.3506862	3.2373089	0.0000000
Cl	-7.3967464	-1.3208335	1.9053852
Cl	-7.3967464	-1.3208335	-1.9053852
Cl	-7.5388527	1.7830635	0.0000000
Cl	-3.9999850	-1.7502563	3.0207696
Cl	-3.9999850	-1.7502563	-3.0207696

20.

B	-5.9985636	-0.9282516	0.8928325
B	-4.2884520	-0.9697787	1.4409856
B	-3.4864984	0.5401491	0.8930246
B	-4.6913035	1.5017275	0.0000000
B	-5.9985636	-0.9282516	-0.8928325
B	-4.7867947	-1.9074171	0.0000000
B	-3.2266990	-0.9972499	0.0000000
B	-3.4864984	0.5401491	-0.8930246
C	-5.1543039	0.5101675	1.3024784
H	-5.4452946	1.0084663	2.2187005
B	-4.2884520	-0.9697787	-1.4409856
B	5.8168322	1.5218208	0.0000000
B	4.2848639	1.5968674	0.8901694
B	3.8908741	-0.0660495	1.4339437
B	5.2035461	-1.1621293	0.8901698
B	4.2848639	1.5968674	-0.8901694

B	3.0733348	0.6164235	0.0000000
B	3.6465507	-1.1013688	0.0000000
B	5.2035461	-1.1621293	-0.8901698
C	5.5184724	0.4752665	1.3002964
H	6.0635926	0.6562456	2.2187579
B	3.8908741	-0.0660495	-1.4339437
C	5.5184724	0.4752665	-1.3002964
B	6.3847603	-0.1831779	0.0000000
H	6.0635926	0.6562456	-2.2187579
C	-5.1543039	0.5101675	-1.3024784
H	-5.4452946	1.0084663	-2.2187005
B	-6.2457963	0.5933770	0.0000000
I	-7.5821198	-1.6992566	2.0981143
I	-8.0812717	1.6752094	0.0000000
I	-4.7343222	3.6317008	0.0000000
I	-2.0367141	1.5398034	-2.0980953
I	-2.0367141	1.5398034	2.0980953
I	-1.3208008	-1.9584619	0.0000000
I	-3.7985739	-1.8052274	-3.3438606
I	-3.7985739	-1.8052274	3.3438606
I	-4.8724343	-4.0432156	0.0000000
I	-7.5821198	-1.6992566	-2.0981143
Cl	2.5483080	-2.4756777	0.0000000
Cl	3.1426160	-0.3141099	2.9988491
Cl	3.1426160	-0.3141099	-2.9988491
Cl	1.3719573	1.0483796	0.0000000
Cl	3.9322791	2.9900258	1.8932494
Cl	3.9322791	2.9900258	-1.8932494
Cl	7.0073900	2.7999606	0.0000000
Cl	8.1041003	-0.4916322	0.0000000
Cl	5.7573704	-2.4873874	-1.8934661
Cl	5.7573704	-2.4873874	1.8934661

21.

B	-6.1058197	-0.9768797	0.8928381
B	-4.3953206	-0.9977421	1.4410243
B	-3.6120863	0.5218151	0.8929853
B	-4.8281754	1.4688022	0.0000000
B	-6.1058197	-0.9768797	-0.8928381
B	-4.8822634	-1.9412588	0.0000000
B	-3.3334648	-1.0122212	0.0000000
B	-3.6120863	0.5218151	-0.8929853
C	-5.2791974	0.4716717	1.3024755
H	-5.5763561	0.9664744	2.2185837
B	-4.3953206	-0.9977421	-1.4410243
B	5.9469484	1.5492475	0.0000000
B	4.4141053	1.6321708	0.8906497
B	4.0092916	-0.0259145	1.4358567
B	5.3143081	-1.1280751	0.8905740
B	4.4141053	1.6321708	-0.8906497
B	3.1992969	0.6600317	0.0000000
B	3.7605883	-1.0565122	0.0000000
B	5.3143081	-1.1280751	-0.8905740
C	5.6397045	0.5048555	1.3021433
H	6.1876917	0.6829368	2.2191189

B	4.0092916	-0.0259145	-1.4358567
C	5.6397045	0.5048555	-1.3021433
B	6.5040077	-0.1575371	0.0000000
H	6.1876917	0.6829368	-2.2191189
C	-5.2791974	0.4716717	-1.3024755
H	-5.5763561	0.9664744	-2.2185837
B	-6.3714750	0.5415803	0.0000000
I	-7.6799550	-1.7667420	2.0981401
I	-8.2196366	1.6013916	0.0000000
I	-4.8965452	3.5980641	0.0000000
I	-2.1745333	1.5389550	-2.0985433
I	-2.1745333	1.5389550	2.0985433
I	-1.4145537	-1.9475153	0.0000000
I	-3.8950893	-1.8272579	-3.3437121
I	-3.8950893	-1.8272579	3.3437121
I	-4.9414501	-4.0779422	0.0000000
I	-7.6799550	-1.7667420	-2.0981401
Br	2.5550651	-2.5506330	0.0000000
Br	3.1790432	-0.2959839	3.1390302
Br	3.1790432	-0.2959839	-3.1390302
Br	1.3446160	1.1417070	0.0000000
Br	4.0369348	3.1625360	1.9763520
Br	4.0369348	3.1625360	-1.9763520
Br	7.2481048	2.9457046	0.0000000
Br	8.3784989	-0.5176652	0.0000000
Br	5.9124976	-2.5854422	-1.9767772
Br	5.9124976	-2.5854422	1.9767772

22.

B	-0.9189896	-5.8328200	0.8997230
B	-0.9992276	-4.1232015	-1.4559035
B	0.5475047	-4.9978589	-1.4558130
B	0.5475047	-4.9978589	1.4558130
B	-0.9992276	-4.1232015	1.4559035
B	-1.0491658	-3.0677209	0.0000000
B	0.4670626	-3.2881948	-0.8999209
B	0.4670626	-3.2881948	0.8999209
B	0.5803582	5.3753707	-1.4554137
B	-0.1287005	3.7457631	-1.4549630
B	-1.0928274	5.1591064	0.8993953
B	1.5446120	3.9630252	-0.8991664
B	0.4683314	2.8733998	0.0000000
B	-0.1287005	3.7457631	1.4549630
B	0.5803582	5.3753707	1.4554137
B	1.5446120	3.9630252	0.8991664
C	1.4798724	5.4167396	0.0000000
B	-0.0151726	6.2487088	0.0000000
H	2.3754159	6.0275458	0.0000000
C	1.2896408	-4.4893034	0.0000000
H	2.3725728	-4.4374524	0.0000000
B	0.5971003	-6.0543666	0.0000000
C	-1.7415484	-4.6320103	0.0000000
H	-2.8244505	-4.6833074	0.0000000
B	-0.9189896	-5.8328200	-0.8997230
C	-1.0274701	3.7054888	0.0000000

H	-1.9228253	3.0943583	0.0000000
B	-1.0928274	5.1591064	-0.8993953
C1	1.3080435	-2.0322933	1.7847054
C1	-2.0226277	-1.6104382	0.0000000
C1	-1.9187196	-3.7003299	2.8853746
C1	-1.9187196	-3.7003299	-2.8853746
C1	-1.7607659	-7.0893115	1.7832598
C1	-1.7607659	-7.0893115	-1.7832598
C1	1.4671060	-5.4189186	2.8855839
C1	1.4671060	-5.4189186	-2.8855839
C1	1.5653221	-7.5140508	0.0000000
C1	1.3080435	-2.0322933	-1.7847054
C1	0.5783219	1.1282672	0.0000000
C1	2.9722682	3.4632868	1.7831284
C1	2.9722682	3.4632868	-1.7831284
C1	1.0599212	6.2655164	2.8858813
C1	-0.1210148	7.9972716	0.0000000
C1	-2.5208879	5.6572236	1.7833639
C1	-2.5208879	5.6572236	-1.7833639
C1	-0.6079089	2.8520714	-2.8831050
C1	-0.6079089	2.8520714	2.8831050
C1	1.0599212	6.2655164	-2.8858813

23.

B	-0.3649124	-6.0349020	0.8981986
B	-0.9911969	-4.4453923	-1.4533818
B	0.7560757	-4.7712500	-1.4532388
B	0.7560757	-4.7712500	1.4532388
B	-0.9911969	-4.4453923	1.4533818
B	-1.3769380	-3.4643555	0.0000000
B	0.1299992	-3.1818231	-0.8989830
B	0.1299992	-3.1818231	0.8989830
B	0.8516152	5.1084451	-1.4532842
B	-0.6172746	4.1075195	-1.4533719
B	-0.6818885	5.8151916	0.8984759
B	0.9155993	3.4014701	-0.8976201
B	-0.5795570	3.0517651	0.0000000
B	-0.6172746	4.1075195	1.4533719
B	0.8516152	5.1084451	1.4532842
B	0.9155993	3.4014701	0.8976201
C	1.6397232	4.6658014	0.0000000
B	0.8121183	6.1636012	0.0000000
H	2.7226825	4.7063736	0.0000000
C	1.2999033	-4.0490291	0.0000000
H	2.3081179	-3.6513374	0.0000000
B	1.1432490	-5.7532564	0.0000000
C	-1.5354789	-5.1679611	0.0000000
H	-2.5439742	-5.5649429	0.0000000
B	-0.3649124	-6.0349020	-0.8981986
C	-1.4052875	4.5512728	0.0000000
H	-2.4882815	4.5096219	0.0000000
B	-0.6818885	5.8151916	-0.8984759
Br	0.5338432	-1.5836983	1.8663527
Br	-2.8835976	-2.2828043	0.0000000
Br	-2.0760189	-4.3221552	3.0239242

Br	-0.7704862	-7.6319738	1.8693447
Br	1.8403127	-4.8925251	3.0244241
Br	2.6454842	-6.9373677	0.0000000
Br	-0.7704862	-7.6319738	-1.8693447
Br	-2.0760189	-4.3221552	-3.0239242
Br	0.5338432	-1.5836983	-1.8663527
Br	1.8403127	-4.8925251	-3.0244241
Br	-1.4819249	1.3678791	0.0000000
Br	1.9376807	2.1071394	1.8680485
Br	1.7956919	5.6542150	3.0247810
Br	1.7956919	5.6542150	-3.0247810
Br	1.7138158	7.8503161	0.0000000
Br	-1.6955293	7.1140196	1.8697663
Br	-1.6955293	7.1140196	-1.8697663
Br	-1.5585382	3.5579311	3.0248924
Br	-1.5585382	3.5579311	-3.0248924
Br	1.9376807	2.1071394	-1.8680485

24.

B	-0.4426909	-6.3512401	0.8989310
B	-0.9983603	-4.7349092	-1.4549420
B	0.7379982	-5.1354353	-1.4542321
B	0.7379982	-5.1354353	1.4542321
B	-0.9983603	-4.7349092	1.4549420
B	-1.3413825	-3.7389099	0.0000000
B	0.1815517	-3.5188523	-0.8997738
B	0.1815517	-3.5188523	0.8997738
B	0.8502397	5.4618331	-1.4546839
B	-0.5884941	4.4091272	-1.4544131
B	-0.7128547	6.1149673	0.8993809
B	0.9734295	3.7566521	-0.8981730
B	-0.5138799	3.3554838	0.0000000
B	-0.5884941	4.4091272	1.4544131
B	0.8502397	5.4618331	1.4546839
B	0.9734295	3.7566521	0.8981730
C	1.6561396	5.0465772	0.0000000
B	0.7737255	6.5160774	0.0000000
H	2.7366762	5.1259365	0.0000000
C	1.3148788	-4.4367588	0.0000000
H	2.3393838	-4.0840778	0.0000000
B	1.0813758	-6.1345594	0.0000000
I	-0.9613610	-8.1123225	1.9851938
I	2.6867603	-7.5389562	0.0000000
I	1.9299099	-5.3290977	-3.2122709
I	0.6934450	-1.7508566	-1.9760919
I	-2.1894716	-4.5360525	-3.2130600
I	-2.9633470	-2.3489954	0.0000000
I	0.6934450	-1.7508566	1.9760919
I	-2.1894716	-4.5360525	3.2130600
I	1.9299099	-5.3290977	3.2122709
I	-1.4323328	1.4341258	0.0000000
I	-1.6032394	3.7553290	-3.2129072
I	2.1473765	2.3416198	-1.9827058
I	1.8686138	6.1086065	-3.2137620
I	1.7006898	8.4368756	0.0000000
I	1.8686138	6.1086065	3.2137620

I	-1.8825565	7.5286995	1.9866160
I	-1.6032394	3.7553290	3.2129072
I	2.1473765	2.3416198	1.9827058
C	-1.5765014	-5.4340611	0.0000000
H	-2.6010544	-5.7865411	0.0000000
B	-0.4426909	-6.3512401	-0.8989310
I	-0.9613610	-8.1123225	-1.9851938
I	-1.8825565	7.5286995	-1.9866160
C	-1.3938606	4.8256701	0.0000000
H	-2.4743428	4.7459763	0.0000000
B	-0.7128547	6.1149673	-0.8993809

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B	-0.4338239	-6.4074853	0.9053122
B	-1.0029592	-4.7833301	-1.4654530
B	0.7396257	-5.1784907	-1.4642972
B	0.7396257	-5.1784907	1.4642972
B	-1.0029592	-4.7833301	1.4654530
B	-1.3553178	-3.7834465	0.0000000
B	0.1689208	-3.5540938	-0.9060495
B	0.1689208	-3.5540938	0.9060495
B	0.8556664	5.5075189	-1.4647369
B	-0.5895664	4.4555323	-1.4646703
B	-0.7063328	6.1737278	0.9057172
B	0.9707763	3.7898766	-0.9043133
B	-0.5204852	3.3945135	0.0000000
B	-0.5895664	4.4555323	1.4646703
B	0.8556664	5.5075189	1.4647369
B	0.9707763	3.7898766	0.9043133
C	1.6617986	5.0850806	0.0000000
B	0.7837375	6.5696435	0.0000000
H	2.7403678	5.1586984	0.0000000
C	1.3128690	-4.4726207	0.0000000
H	2.3329502	-4.1144449	0.0000000
B	1.0911978	-6.1828440	0.0000000
I	-0.9561804	-8.1927250	2.0028417
I	2.7300861	-7.5890396	0.0000000
I	1.9541111	-5.3635428	-3.2399989
I	0.6848380	-1.7615943	-1.9922699
I	-2.2152902	-4.5925212	-3.2421626
I	-3.0135249	-2.3955757	0.0000000
I	0.6848380	-1.7615943	1.9922699
I	-2.2152902	-4.5925212	3.2421626
I	1.9541111	-5.3635428	3.2399989
I	-1.4700246	1.4607669	0.0000000
I	-1.6270319	3.7996924	-3.2414076
I	2.1570437	2.3529285	-1.9991243
I	1.8974310	6.1558730	-3.2416858
I	1.7386027	8.5061626	0.0000000
I	1.8974310	6.1558730	3.2416858
I	-1.8906181	7.6067956	2.0039133
I	-1.6270319	3.7996924	3.2414076
I	2.1570437	2.3529285	1.9991243
C	-1.5779278	-5.4902620	0.0000000
H	-2.5981144	-5.8480886	0.0000000

B	-0.4338239	-6.4074853	-0.9053122
I	-0.9561804	-8.1927250	-2.0028417
I	-1.8906181	7.6067956	-2.0039133
C	-1.3954606	4.8795782	0.0000000
H	-2.4739752	4.8055545	0.0000000
B	-0.7063328	6.1737278	-0.9057172

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B	-0.4467907	-6.3670010	0.9068433
B	-1.0041710	-4.7359375	-1.4678568
B	0.7403331	-5.1441274	-1.4665673
B	0.7403331	-5.1441274	1.4665673
B	-1.0041710	-4.7359375	1.4678568
B	-1.3490911	-3.7321054	0.0000000
B	0.1811624	-3.5127296	-0.9075689
B	0.1811624	-3.5127296	0.9075689
B	0.8526957	5.4753168	-1.4673959
B	-0.5861345	4.4061661	-1.4670646
B	-0.7210820	6.1264149	0.9074618
B	0.9860153	3.7561099	-0.9056836
B	-0.5057129	3.3442390	0.0000000
B	-0.5861345	4.4061661	1.4670646
B	0.8526957	5.4753168	1.4673959
B	0.9860153	3.7561099	0.9056836
C	1.6689634	5.0610487	0.0000000
B	0.7697502	6.5385620	0.0000000
H	2.7553657	5.1470611	0.0000000
C	1.3239820	-4.4400397	0.0000000
H	2.3551088	-4.0870238	0.0000000
B	1.0846173	-6.1528239	0.0000000
I	-0.9758264	-8.1445608	2.0030029
I	2.7041697	-7.5728461	0.0000000
I	1.9456408	-5.3407658	-3.2405773
I	0.7028223	-1.7273637	-1.9923403
I	-2.2075051	-4.5327566	-3.2426631
I	-2.9918141	-2.3333829	0.0000000
I	0.7028223	-1.7273637	1.9923403
I	-2.2075051	-4.5327566	3.2426631
I	1.9456408	-5.3407658	3.2405773
I	-1.4271637	1.4021127	0.0000000
I	-1.6079114	3.7382675	-3.2417530
I	2.1809994	2.3327589	-1.9983355
I	1.8793396	6.1333390	-3.2429465
I	1.6974184	8.4820897	0.0000000
I	1.8793396	6.1333390	3.2429465
I	-1.9119266	7.5464020	2.0046623
I	-1.6079114	3.7382675	3.2417530
I	2.1809994	2.3327589	1.9983355
C	-1.5898229	-5.4409433	0.0000000
H	-2.6209886	-5.7937463	0.0000000
B	-0.4467907	-6.3670010	-0.9068433
I	-0.9758264	-8.1445608	-2.0030029
I	-1.9119266	7.5464020	-2.0046623
C	-1.4018849	4.8225781	0.0000000
H	-2.4882191	4.7361547	0.0000000

B -0.7210820 6.1264149 -0.9074618

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B -1.0851443 -5.8220772 0.8998752
B -1.0343785 -4.1111651 -1.4558564
B 0.4406788 -5.1017210 -1.4558943
B 0.4406788 -5.1017210 1.4558943
B -1.0343785 -4.1111651 1.4558564
B -1.0031468 -3.0543755 0.0000000
B 0.4916005 -3.3912664 -0.8998776
B 0.4916005 -3.3912664 0.8998776
B 0.5575282 5.4564561 -1.4529148
B 0.0356787 3.7569119 -1.4522801
B -1.0804758 5.0492395 0.8977136
B 1.6739034 4.1651851 -0.8975091
B 0.7269630 2.9594032 0.0000000
B 0.0356787 3.7569119 1.4522801
B 0.5575282 5.4564561 1.4529148
B 1.6739034 4.1651851 0.8975091
C 1.4498425 5.6043132 0.0000000
B -0.1320284 6.2551292 0.0000000
H 2.2704233 6.3129081 0.0000000
C 1.2197701 -4.6513472 0.0000000
H 2.3034447 -4.6830899 0.0000000
B 0.4095395 -6.1588620 0.0000000
C -1.8134104 -4.5618108 0.0000000
H -2.8970257 -4.5293362 0.0000000
B -1.0851443 -5.8220772 -0.8998752
C -0.8559286 3.6104068 0.0000000
H -1.6762159 2.9014532 0.0000000
B -1.0804758 5.0492395 -0.8977136
Cl 1.4273332 -2.2060113 1.7874706
Cl -1.8618543 -1.5270056 0.0000000
Cl -1.9189079 -3.6188516 2.8850976
Cl -1.9189079 -3.6188516 -2.8850976
Cl -2.0198454 -7.0105799 1.7837256
Cl -2.0198454 -7.0105799 -1.7837256
Cl 1.3258684 -5.5915386 2.8854550
Cl 1.3258684 -5.5915386 -2.8854550
Cl 1.2643086 -7.6875523 0.0000000
Cl 1.4273332 -2.2060113 -1.7874706
Br 1.0813144 1.0828270 0.0000000
Br -0.3599028 2.7360052 3.0208656
Br -0.3599028 2.7360052 -3.0208656
Br -2.6840178 5.4305158 1.8684189
Br -2.6840178 5.4305158 -1.8684189
Br 0.9520994 6.4718947 3.0253295
Br 0.9520994 6.4718947 -3.0253295
Br -0.4842289 8.1352996 0.0000000
Br 3.2770984 3.7828222 1.8683639
Br 3.2770984 3.7828222 -1.8683639

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B -0.8307896 -6.2639398 0.8994657

B	-1.0743339	-4.5706793	-1.4556281
B	0.5491149	-5.2927837	-1.4554318
B	0.5491149	-5.2927837	1.4554318
B	-1.0743339	-4.5706793	1.4556281
B	-1.2247286	-3.5261544	0.0000000
B	0.3050862	-3.5998891	-0.8994424
B	0.3050862	-3.5998891	0.8994424
B	0.7902000	5.6504918	-1.4544149
B	-0.2637769	4.2129306	-1.4541251
B	-0.8971971	5.8013318	0.8990862
B	1.4230295	4.0622670	-0.8984821
B	0.1273632	3.2305113	0.0000000
B	-0.2637769	4.2129306	1.4541251
B	0.7902000	5.6504918	1.4544149
B	1.4230295	4.0622670	0.8984821
C	1.6836529	5.4983979	0.0000000
B	0.3985303	6.6324377	0.0000000
H	2.6895228	5.9005695	0.0000000
C	1.2396102	-4.7156501	0.0000000
H	2.3125078	-4.5596756	0.0000000
B	0.6996438	-6.3391928	0.0000000
C	-1.7651709	-5.1477510	0.0000000
H	-2.8381710	-5.3029971	0.0000000
B	-0.8307896	-6.2639398	-0.8994657
C	-1.1569191	4.3658773	0.0000000
H	-2.1629458	3.9639577	0.0000000
B	-0.8971971	5.8013318	-0.8990862
C1	1.0186558	-2.2650516	1.7808087
C1	-2.3285041	-2.1644969	0.0000000
C1	-2.0288323	-4.2360982	2.8853464
C1	-2.0288323	-4.2360982	-2.8853464
C1	-1.5478490	-7.5955358	1.7829070
C1	-1.5478490	-7.5955358	-1.7829070
C1	1.5036321	-5.6241627	2.8858860
C1	1.5036321	-5.6241627	-2.8858860
C1	1.8025058	-7.6998170	0.0000000
C1	1.0186558	-2.2650516	-1.7808087
I	-0.1755228	1.1213235	0.0000000
I	2.9624763	3.0634432	-1.9867577
I	2.9624763	3.0634432	1.9867577
I	1.5662093	6.5766939	3.2121336
I	1.5662093	6.5766939	-3.2121336
I	-1.0383966	3.2837775	3.2108968
I	-1.0383966	3.2837775	-3.2108968
I	-2.4382809	6.7964439	1.9878072
I	-2.4382809	6.7964439	-1.9878072
I	0.7007302	8.7441809	0.0000000

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B	-0.8975699	-6.3182331	0.8981463
B	-1.0530296	-4.6168914	-1.4532249
B	0.5330388	-5.4205676	-1.4532004
B	0.5330388	-5.4205676	1.4532004
B	-1.0530296	-4.6168914	1.4532249
B	-1.1492327	-3.5660487	0.0000000

B	0.3774023	-3.7197927	-0.8979424
B	0.3774023	-3.7197927	0.8979424
B	0.6898742	5.7999438	-1.4543763
B	-0.1694961	4.2377874	-1.4537215
B	-1.0028838	5.7306411	0.8987643
B	1.5230183	4.3075837	-0.8982559
B	0.3461677	3.3148202	0.0000000
B	-0.1694961	4.2377874	1.4537215
B	0.6898742	5.7999438	1.4543763
B	1.5230183	4.3075837	0.8982559
C	1.5957146	5.7650685	0.0000000
B	0.1747626	6.7228948	0.0000000
H	2.5411714	6.2935998	0.0000000
C	1.2578335	-4.8805780	0.0000000
H	2.3371016	-4.7808941	0.0000000
B	0.6291773	-6.4725237	0.0000000
C	-1.7778456	-5.1571822	0.0000000
H	-2.8571236	-5.2566560	0.0000000
B	-0.8975699	-6.3182331	-0.8981463
C	-1.0746226	4.2738939	0.0000000
H	-2.0200157	3.7453207	0.0000000
B	-1.0028838	5.7306411	-0.8987643
I	0.3175723	1.1844228	0.0000000
I	3.1798471	3.5175322	-1.9856861
I	3.1798471	3.5175322	1.9856861
I	1.3407354	6.8161534	3.2132749
I	1.3407354	6.8161534	-3.2132749
I	-0.8205578	3.2162388	3.2096477
I	-0.8205578	3.2162388	-3.2096477
I	-2.6607605	6.5174446	1.9863704
I	-2.6607605	6.5174446	-1.9863704
I	0.2013517	8.8558646	0.0000000
Br	1.2146316	-2.3000482	1.8693836
Br	-2.2582590	-2.0071076	0.0000000
Br	-2.0577406	-4.1939478	3.0246356
Br	-1.7363102	-7.7363507	1.8695532
Br	1.5385120	-5.8397179	3.0251767
Br	1.5385120	-5.8397179	-3.0251767
Br	1.7388242	-8.0304462	0.0000000
Br	-2.0577406	-4.1939478	-3.0246356
Br	-1.7363102	-7.7363507	-1.8695532
Br	1.2146316	-2.3000482	-1.8693836

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B	-0.8965205	-6.3681673	0.9035922
B	-1.0550094	-4.6566088	-1.4619892
B	0.5335414	-5.4638989	-1.4619521
B	0.5335414	-5.4638989	1.4619521
B	-1.0550094	-4.6566088	1.4619892
B	-1.1532964	-3.5996995	0.0000000
B	0.3748728	-3.7529049	-0.9033614
B	0.3748728	-3.7529049	0.9033614
B	0.6927743	5.8431347	-1.4643552
B	-0.1710040	4.2777871	-1.4635577
B	-1.0043685	5.7842478	0.9049378

B	1.5260172	4.3372691	-0.9043820
B	0.3448546	3.3461735	0.0000000
B	-0.1710040	4.2777871	1.4635577
B	0.6927743	5.8431347	1.4643552
B	1.5260172	4.3372691	0.9043820
C	1.6021688	5.8031428	0.0000000
B	0.1776828	6.7745738	0.0000000
H	2.5474717	6.3270138	0.0000000
C	1.2612619	-4.9197904	0.0000000
H	2.3381322	-4.8188354	0.0000000
B	0.6316788	-6.5220318	0.0000000
C	-1.7828029	-5.2011070	0.0000000
H	-2.8596888	-5.3017579	0.0000000
B	-0.8965205	-6.3681673	-0.9035922
C	-1.0796152	4.3192717	0.0000000
H	-2.0248334	3.7953411	0.0000000
B	-1.0043685	5.7842478	-0.9049378
I	0.2992450	1.1906561	0.0000000
I	3.2048287	3.5373964	-2.0032622
I	3.2048287	3.5373964	2.0032622
I	1.3623666	6.8717554	3.2411676
I	1.3623666	6.8717554	-3.2411676
I	-0.8408520	3.2434909	3.2372670
I	-0.8408520	3.2434909	-3.2372670
I	-2.6842624	6.5805198	2.0039999
I	-2.6842624	6.5805198	-2.0039999
I	0.2213704	8.9337619	0.0000000
Br	1.2195036	-2.3205391	1.8830150
Br	-2.2757965	-2.0298062	0.0000000
Br	-2.0702586	-4.2313368	3.0466084
Br	-1.7422648	-7.7994472	1.8831512
Br	1.5495118	-5.8855041	3.0471236
Br	1.5495118	-5.8855041	-3.0471236
Br	1.7544148	-8.0912946	0.0000000
Br	-2.0702586	-4.2313368	-3.0466084
Br	-1.7422648	-7.7994472	-1.8831512
Br	1.2195036	-2.3205391	-1.8830150

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B	-0.8902033	-6.3366515	0.9054407
B	-1.0559234	-4.6221065	-1.4650261
B	0.5415796	-5.4246069	-1.4649503
B	0.5415796	-5.4246069	1.4649503
B	-1.0559234	-4.6221065	1.4650261
B	-1.1585499	-3.5631079	0.0000000
B	0.3756892	-3.7104728	-0.9051804
B	0.3756892	-3.7104728	0.9051804
B	0.6964021	5.8054129	-1.4669572
B	-0.1816911	4.2422559	-1.4660961
B	-1.0060971	5.7569094	0.9064760
B	1.5206397	4.2915145	-0.9058564
B	0.3286808	3.3059736	0.0000000
B	-0.1816911	4.2422559	1.4660961
B	0.6964021	5.8054129	1.4669572
B	1.5206397	4.2915145	0.9058564

C	1.6107463	5.7614361	0.0000000
B	0.1867540	6.7419926	0.0000000
H	2.5671731	6.2830371	0.0000000
C	1.2713683	-4.8762616	0.0000000
H	2.3562634	-4.7698674	0.0000000
B	0.6441207	-6.4846530	0.0000000
C	-1.7857393	-5.1708289	0.0000000
H	-2.8706675	-5.2767442	0.0000000
B	-0.8902033	-6.3366515	-0.9054407
C	-1.0951506	4.2879309	0.0000000
H	-2.0515098	3.7662753	0.0000000
B	-1.0060971	5.7569094	-0.9064760
I	0.2754392	1.1552578	0.0000000
I	3.1861012	3.4773291	-2.0038136
I	3.1861012	3.4773291	2.0038136
I	1.3662521	6.8250104	3.2421674
I	1.3662521	6.8250104	-3.2421674
I	-0.8517726	3.2157330	3.2375232
I	-0.8517726	3.2157330	-3.2375232
I	-2.6731092	6.5664155	2.0047625
I	-2.6731092	6.5664155	-2.0047625
I	0.2385058	8.8955251	0.0000000
Br	1.2111906	-2.2760829	1.8869928
Br	-2.2849682	-1.9976668	0.0000000
Br	-2.0682366	-4.1998207	3.0506161
Br	-1.7260797	-7.7714779	1.8855309
Br	1.5546653	-5.8430579	3.0511115
Br	1.5546653	-5.8430579	-3.0511115
Br	1.7687201	-8.0509060	0.0000000
Br	-2.0682366	-4.1998207	-3.0506161
Br	-1.7260797	-7.7714779	-1.8855309
Br	1.2111906	-2.2760829	-1.8869928