Supporting Information for

Substituent Effects in the Benzene Dimer are Due to Direct Interactions of the Substituents with the Unsubstituted Benzene

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Table S1. Sigma meta constants, sigma para constants, absolute energies (hartree) of substituted benzenes [E(C_6H_5-X)] and dimers of substituted benzenes with benzene [E(dimer)], interaction energies [E(dimerization), kcal mol^{-1}] and interaction energies relative to X = H [E_{int}, kcal mol^{-1}]

X	σ_m	σ_p	E(C_6H_5-X)	E(dimer)	E(dimerization)	E_{int}
H	0.00	0.00	-232.224456	-464.449704	-0.50	0.00
BF_2	0.32	0.48	-456.302043	-688.528465	-1.23	-0.74
CCH	0.21	0.23	-308.367207	-540.593559	-1.19	-0.69
CF_3	0.43	0.54	-569.265344	-801.492320	-1.58	-1.08
CH_3	-0.07	-0.17	-271.535226	-503.760915	-0.77	-0.28
CHO	0.35	0.42	-345.540038	-577.766707	-1.39	-0.89
CN	0.56	0.66	-324.465127	-556.692386	-1.76	-1.26
$COCH_3$	0.38	0.50	-384.857390	-617.084018	-1.36	-0.87
$COOCH_3$	0.37	0.45	-460.085848	-692.312341	-1.28	-0.78
COOH	0.37	0.45	-420.789039	-653.015682	-1.37	-0.88
F	0.34	0.06	-331.460889	-563.686968	-1.02	-0.52
$N(CH3)_2$	-0.15	-0.83	-366.172965	-598.398479	-0.66	-0.17
NH_2	-0.16	-0.66	-287.575100	-519.800708	-0.72	-0.23
$NHCH_3$	-0.30	-0.84	-326.874453	-559.099979	-0.67	-0.17
NHOH	-0.04	-0.34	-362.728620	-594.954244	-0.73	-0.24
NO	0.62	0.91	-361.504375	-593.731438	-1.64	-1.14
NO_2	0.71	0.78	-436.707528	-668.935250	-2.05	-1.55
OCF_3	0.38	0.35	-644.476966	-876.703897	-1.55	-1.06
OH	0.12	-0.37	-307.438898	-539.664749	-0.88	-0.38
OMe	0.12	-0.27	-346.735326	-578.961134	-0.85	-0.35
SCH_3	0.15	0.00	-669.696874	-901.923360	-1.27	-0.78
SH	0.25	0.15	-630.386997	-862.613579	-1.33	-0.84
SiF_3	0.54	0.69	-820.841307	-1053.069084	-2.08	-1.59
SiH_3	0.05	0.10	-522.884409	-755.110803	-1.22	-0.72
CH_2OH	0.00	0.00	-346.738076	-578.963958	-0.89	-0.40

Table S2. Absolute energies (hartree) of H-X [E(H-X)] and dimers of H-X with benzene [E(dimer)], interaction energies [E(dimerization), kcal mol^{-1}] and interaction energies relative to X = H [E_{int}, kcal mol^{-1}]

X	E(H-X)	E(dimer)	E(dimerization)	E_{int}
H	-1.163699	-233.388474	-0.20	0.00
BF_2	-225.240810	-457.466611	-0.84	-0.64
CCH	-77.316621	-309.542423	-0.84	-0.64
CF_3	-338.220680	-570.447153	-1.27	-1.07
CH_3	-40.499069	-272.724010	-0.30	-0.10
CHO	-114.481836	-346.707849	-0.98	-0.78
CN	-93.413125	-325.640024	-1.53	-1.33
$COCH_3$	-153.803632	-386.029709	-1.02	-0.82
$COOCH_3$	-229.032979	-461.258931	-0.94	-0.74
COOH	-189.734971	-421.961156	-1.08	-0.88
F	-100.428751	-332.654856	-1.03	-0.83
$N(CH3)_2$	-135.124479	-367.349759	-0.52	-0.32
NH_2	-56.536241	-288.761543	-0.53	-0.33
$NHCH_3$	-95.828806	-328.054031	-0.48	-0.28
NHOH	-131.686818	-363.912057	-0.49	-0.29
NO	-130.447410	-362.674235	-1.49	-1.29
NO_2	-205.659538	-437.887183	-2.00	-1.80
OCF_3	-413.445872	-645.673029	-1.70	-1.50
OH	-76.404484	-308.630326	-0.87	-0.67
OMe	-115.694834	-347.920702	-0.89	-0.69
SCH_3	-438.655020	-670.881140	-1.04	-0.84
SH	-399.349570	-631.575717	-1.06	-0.86
SiF_3	-589.784606	-822.011698	-1.65	-1.45
SiH_3	-291.834836	-524.060288	-0.63	-0.43
CH_2OH	-115.696172	-347.921460	-0.52	-0.32

Table S3. Absolute energies (hartree) of substituted dimers [E(C_6H_5-X)] and dimers of substituted benzenes with perfluorobenzene [E(dimer)], interaction energies [E(dimerization), kcal mol^{-1}] and interaction energies relative to X = H [E_{int}, kcal mol^{-1}]

X	E(C_6H_5-X)	E(dimer)	E(dimerization)	E_{int}
H	-232.224456	-1059.814232	-4.90	0.00
BF_2	-456.302043	-1283.890808	-4.27	0.63
CCH	-308.367207	-1135.956602	-4.66	0.24
CF_3	-569.265344	-1396.854125	-4.27	0.62
CH_3	-271.535226	-1099.125677	-5.32	-0.42
CHO	-345.540038	-1173.128657	-4.17	0.73
CN	-324.465127	-1152.052859	-3.62	1.28
$COCH_3$	-384.857390	-1212.446830	-4.69	0.21
$COOCH_3$	-460.085848	-1287.675132	-4.59	0.31
COOH	-420.789039	-1248.377986	-4.38	0.52
F	-331.460889	-1159.049548	-4.20	0.70
$N(CH3)_2$	-366.172965	-1193.764926	-6.27	-1.37
NH_2	-287.575100	-1115.166126	-5.68	-0.78
$NHCH_3$	-326.874453	-1154.466042	-6.04	-1.14
NHOH	-362.728620	-1190.319666	-5.70	-0.80
NO	-361.504375	-1189.092384	-3.79	1.11
NO_2	-436.707528	-1264.295074	-3.50	1.40
OCF_3	-644.476966	-1472.066300	-4.62	0.28
OH	-307.438898	-1135.029009	-5.11	-0.21
OMe	-346.735326	-1174.326179	-5.58	-0.68
SCH_3	-669.696874	-1497.287588	-5.49	-0.59
SH	-630.386997	-1457.977054	-5.08	-0.18
SiF_3	-820.841307	-1648.430269	-4.39	0.51
SiH_3	-522.884409	-1350.474672	-5.20	-0.31
CH_2OH	-346.738076	-1174.329011	-5.63	-0.73

Table S4. Absolute energies (hartree) of H-X [E(H-X)] and dimers of H-X with perflurobenzene [E(dimer)], interaction energies [E(dimerization), kcal mol^{-1}] and interaction energies relative to X = H [E_{int}, kcal mol^{-1}]

X	E(H-X)	E(dimer)	E(dimerization)	E_{int}
H	-1.163699	-828.746436	-0.48	0.00
BF_2	-225.240809	-1052.823050	-0.17	0.31
CCH	-77.316622	-904.899081	-0.31	0.17
CF_3	-338.220680	-1165.802502	0.09	0.57
CH_3	-40.499068	-868.082123	-0.68	-0.20
CHO	-114.481835	-942.063843	-0.02	0.46
CN	-93.413125	-920.994202	0.56	1.04
$COCH_3$	-153.803631	-981.386543	-0.59	-0.11
$COOCH_3$	-229.032978	-1056.615544	-0.38	0.11
COOH	-189.734970	-1017.317158	-0.14	0.35
F	-100.428752	-928.009993	0.46	0.94
$N(CH3)_2$	-135.124479	-962.708402	-1.23	-0.74
NH_2	-56.536241	-884.119739	-0.96	-0.48
$NHCH_3$	-95.828806	-923.412589	-1.14	-0.66
NHOH	-131.686818	-959.270192	-0.88	-0.40
NO	-130.447409	-958.029179	0.12	0.61
NO_2	-205.659538	-1033.240671	0.52	1.01
OCF_3	-413.445872	-1241.027999	-0.10	0.38
OH	-76.404484	-903.987246	-0.50	-0.02
OMe	-115.694834	-943.278140	-0.84	-0.36
SCH_3	-438.655019	-1266.238515	-0.96	-0.48
SH	-399.349570	-1226.932526	-0.62	-0.14
SiF_3	-589.784606	-1417.367073	-0.31	0.17
SiH_3	-291.834836	-1119.418460	-1.04	-0.56
CH_2OH	-115.696171	-943.279634	-0.94	-0.46

Table S5. Absolute energies (hartree) of F-X [E(F-X)] and dimers of F-X with benzene [E(dimer)], interaction energies [E(dimerization), kcal mol^{-1}] and interaction energies relative to X = H [E_{int}, kcal mol^{-1}]

X	E(F-X)	E(dimer)	E(dimerization)	E_{int}
H	-100.428752	-332.652418	0.50	0.00
BF_2	-324.555907	-556.781181	-0.51	-1.01
CCH	-176.525196	-408.750508	-0.54	-1.03
CF_3	-437.466218	-669.691769	-0.69	-1.18
CH_3	-139.723575	-371.947622	0.26	-0.24
CHO	-213.744932	-445.970122	-0.46	-0.96
CN	-192.618609	-424.844952	-1.18	-1.68
$COCH_3$	-253.065306	-485.290500	-0.46	-0.96
$COOCH_3$	-328.280768	-560.505904	-0.43	-0.92
COOH	-288.981585	-521.206966	-0.58	-1.08
F	-199.479586	-431.704481	-0.28	-0.77
$N(CH3)_2$	-234.282844	-466.506950	0.22	-0.28
NH_2	-155.680950	-387.905124	0.18	-0.32
$NHCH_3$	-194.981069	-427.205154	0.23	-0.26
NHOH	-230.855517	-463.079604	0.23	-0.26
NO	-229.672721	-461.897897	-0.45	-0.95
NO_2	-304.837221	-537.063396	-1.08	-1.57
OCF_3	-512.526356	-744.752167	-0.85	-1.35
OH	-175.501676	-407.726113	0.01	-0.48
OMe	-214.804264	-447.028594	0.08	-0.42
SCH_3	-537.868810	-770.093520	-0.16	-0.66
SH	-498.551756	-730.776503	-0.18	-0.68
SiF_3	-689.098248	-921.324573	-1.17	-1.67
SiH_3	-391.143650	-623.368431	-0.20	-0.70
CH_2OH	-214.935083	-447.159433	0.07	-0.43

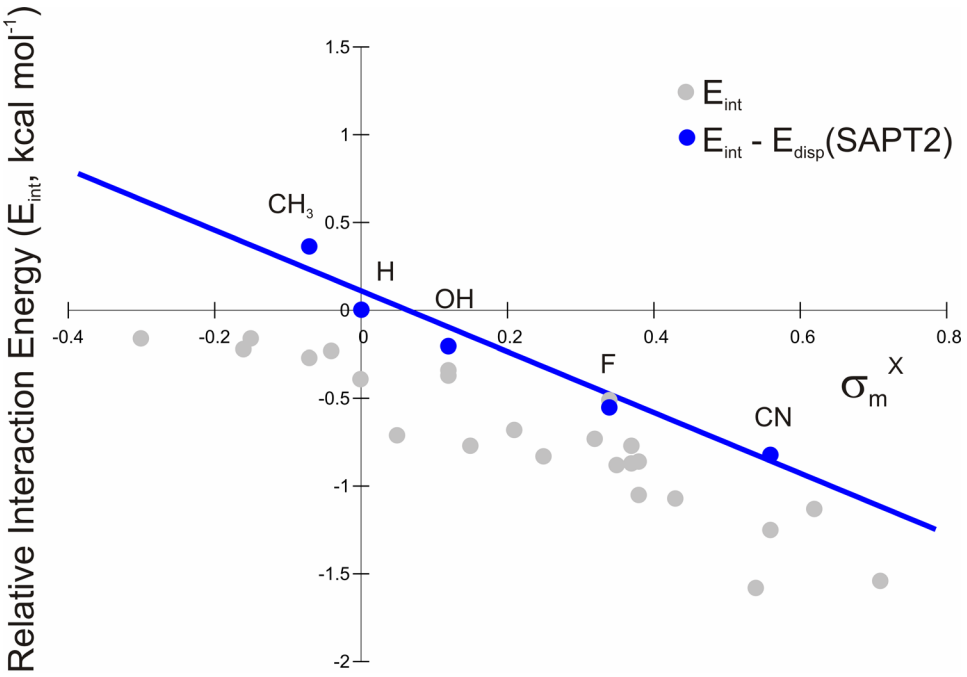

Figure S1. $E_{int}(C_6H_6\cdots C6H5X)$, relative to X = H (gray), versus σ_m and $E_{int}(C_6H_6\cdots C6H5X) - E_{disp}$(SAPT2) for selected dimers (blue). The SAPT2 disperion corrections from from Ref. 8

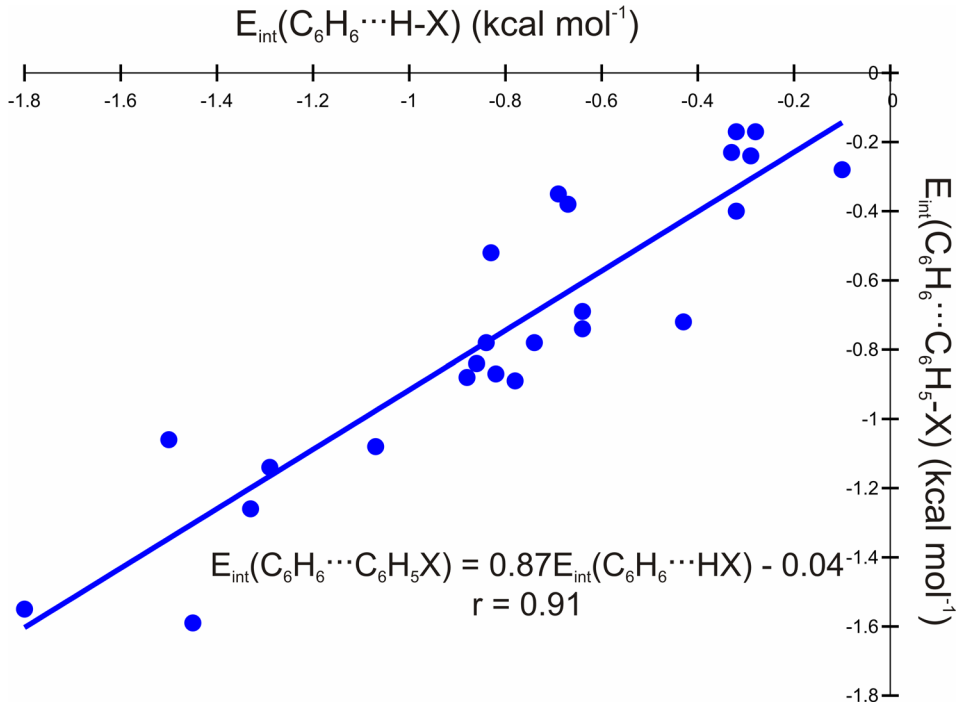

Figure S2. Relative interaction energies of $C_6H_6\cdots C_6H_5X$ versus $C_6H_6\cdots HX$ (kcal mol^{-1})

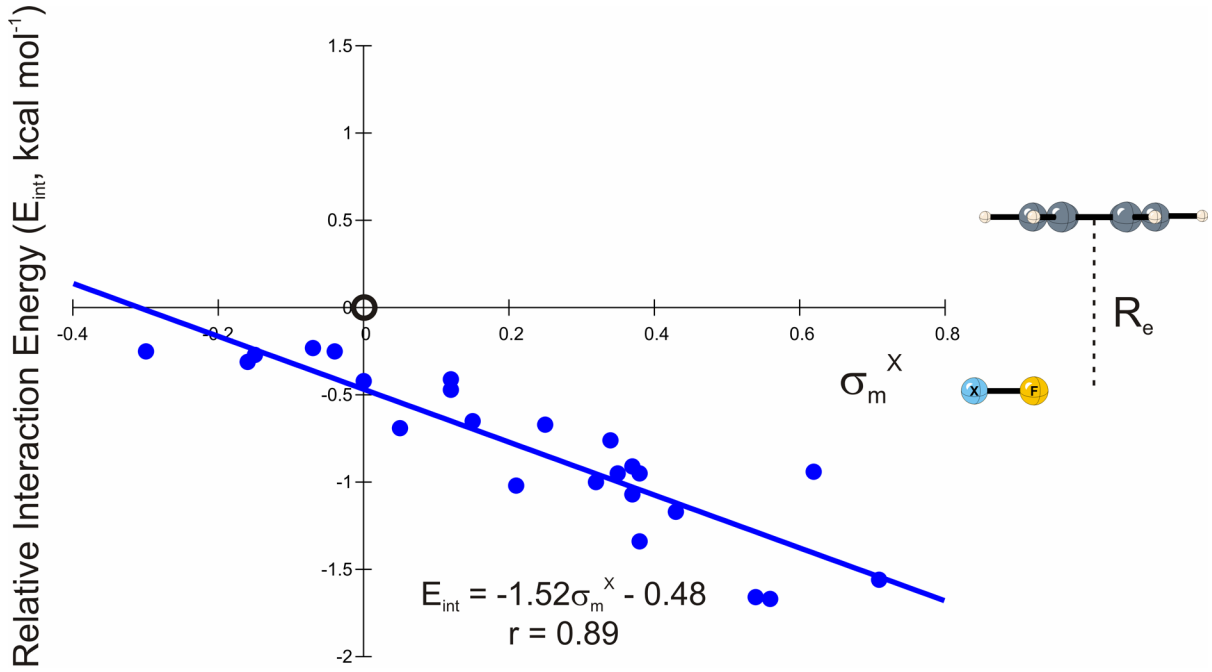

Figure S3. Interaction energies (kcal mol^{-1}), relative to the unsubstituted case (X = H), versus σ_m^X for the dimer of F–X and benzene at the equilibrium separation distances (R_e) of the corresponding substituted dimers in Fig. 1(a). The open circle at the origin corresponds to X = H, and was not included in the least squares fit.

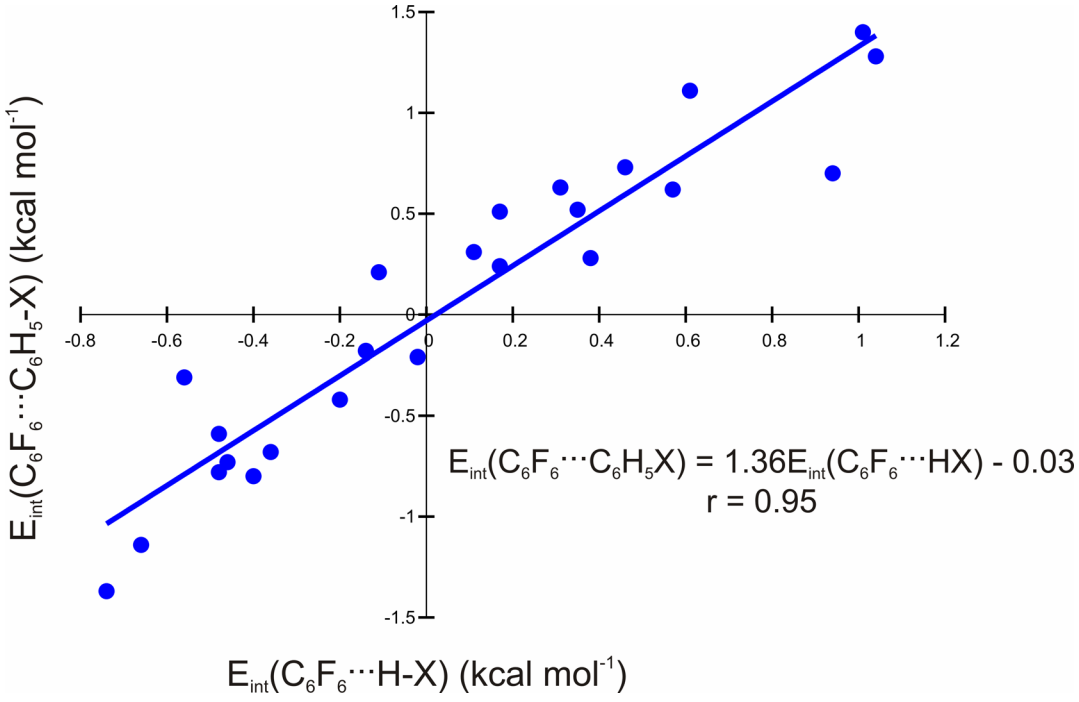

Figure S4. Relative interaction energies of $C_6F_6\cdots C_6H_5X$ versus $C_6F_6\cdots HX$ (kcal mol^{-1})

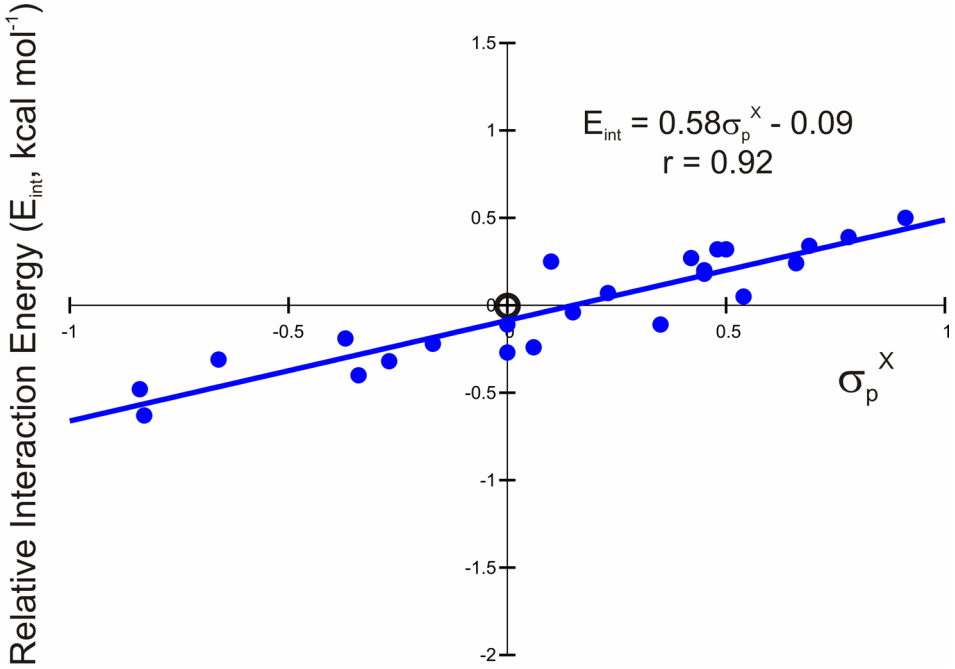

Figure S5. Difference in relative interaction energies (kcal mol^{-1}) between $C_6F_6\cdots C_6H_5$-X and $C_6F_6\ldots$H-X vs. σ_p^X [*i.e.*: $E_{int}(C_6F_6\cdots C_6H_5–X) – E_{int}(C_6F_6\cdots H–X)$ vs. σ_p^X].

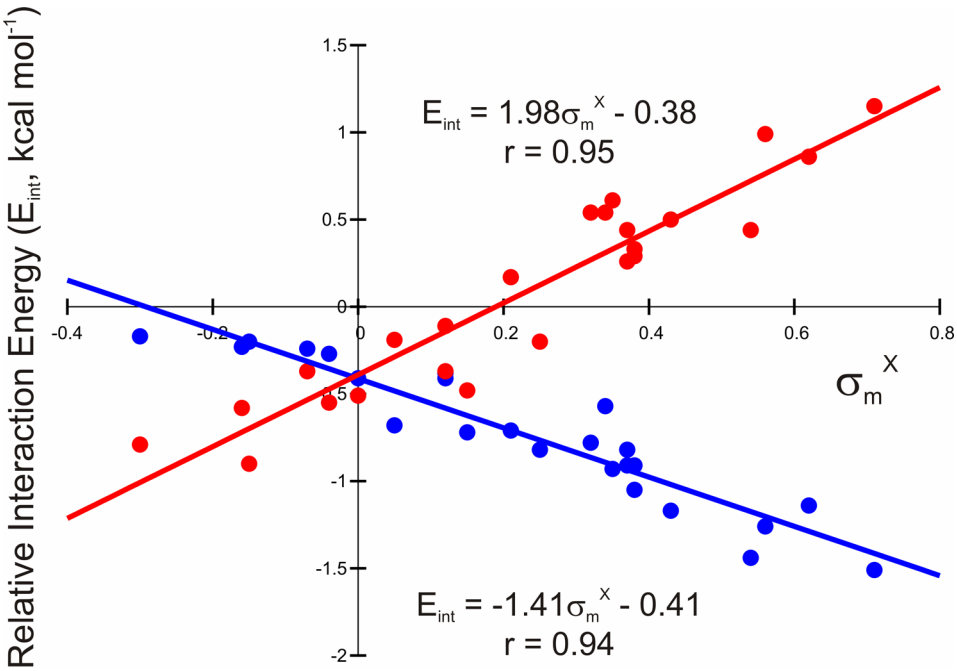

Figure S6. Interaction energies (kcal mol^{-1}), relative to X = H, versus σ_m for $C_6H_6\cdots C_6H_5X$ (blue) and $C_6F_6\cdots C_6H_5X$ (red) dimers with inter-ring separations of 4 Å.

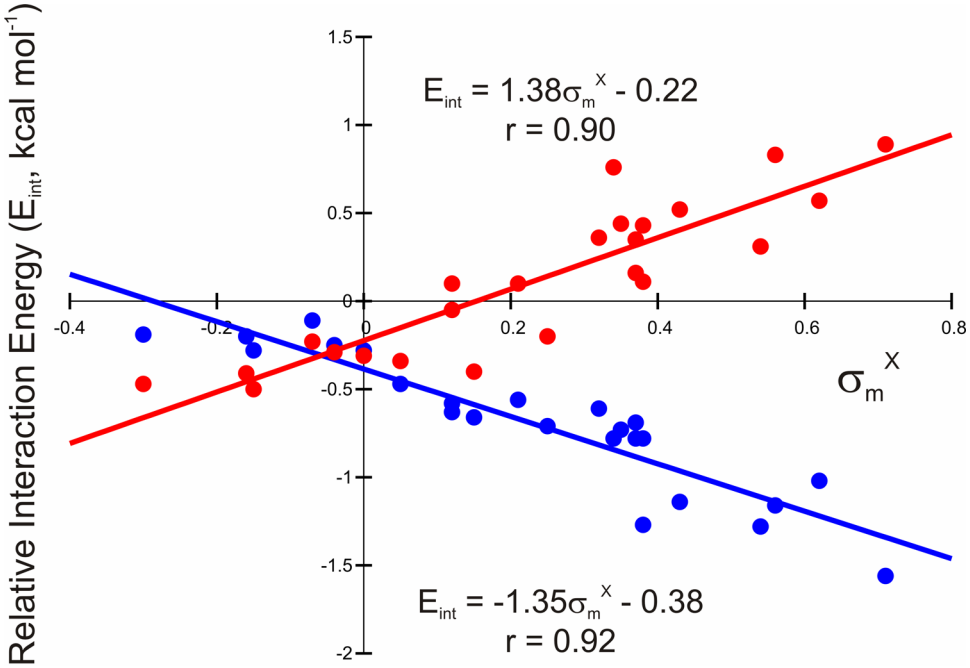

Figure S7. Interaction energies (kcal mol^{-1}), relative to X = H, versus σ_m for $C_6H_6\cdots HX$ (blue) and $C_6F_6\cdots HX$ (red) dimers at 4 Å separations.

Optimized Cartesian Coordinates (Angstrom)

C_6H_5-X···C_6H_6 Dimers

24
C6H5-H...benzene Dimer

C	0.98556144	-0.98556144	-2.02500000
C	-0.36074053	-1.34630197	-2.02500000
C	1.34630197	0.36074053	-2.02500000
C	-0.98556144	0.98556144	-2.02500000
C	0.36074053	1.34630197	-2.02500000
C	-1.34630197	-0.36074053	-2.02500000
H	1.75143711	-1.75143711	-2.02500000
H	-0.64107047	-2.39250758	-2.02500000
H	-2.39250758	-0.64107047	-2.02500000
H	-1.75143711	1.75143711	-2.02500000
H	0.64107047	2.39250758	-2.02500000
H	2.39250758	0.64107047	-2.02500000
C	0.98556144	-0.98556144	2.02500000
C	1.34630197	0.36074053	2.02500000
C	0.36074053	1.34630197	2.02500000
C	-0.98556144	0.98556144	2.02500000
C	-1.34630197	-0.36074053	2.02500000
C	-0.36074053	-1.34630197	2.02500000
H	1.75143711	-1.75143711	2.02500000
H	2.39250758	0.64107047	2.02500000
H	0.64107047	2.39250758	2.02500000
H	-1.75143711	1.75143711	2.02500000
H	-2.39250758	-0.64107047	2.02500000
H	-0.64107047	-2.39250758	2.02500000

26
C6H5-BF2...benzene Dimer

C	2.63906847	-0.09637063	0.00000000
C	2.09595830	0.33466200	-1.20980600
C	2.09595830	0.33466200	1.20980600
C	0.44958877	1.64128269	0.00000000
C	1.00627108	1.19947870	1.20800000
C	1.00627108	1.19947870	-1.20800000
H	0.58128242	1.53676567	-2.14609300
H	2.52126263	-0.00287549	-2.14674300
H	2.52126263	-0.00287549	2.14674300
H	0.58128242	1.53676567	2.14609300
F	-1.30919518	3.03711970	-1.13455100
F	-1.30919518	3.03711970	1.13455100
B	-0.76116592	2.60218309	0.00000000
H	3.48773379	-0.76990330	0.00000000
C	0.18507718	-3.19159769	0.00000000
C	-0.36079685	-2.75837156	1.20705841
C	-1.45254491	-1.89191929	1.20705841
C	-1.99841894	-1.45869316	0.00000000
C	-1.45254491	-1.89191929	-1.20705841
C	-0.36079685	-2.75837156	-1.20705841
H	1.03335241	-3.86482078	0.00000000
H	0.06334076	-3.09498310	2.14492842
H	-1.87668253	-1.55530775	2.14492842
H	-2.84669418	-0.78547007	0.00000000
H	-1.87668253	-1.55530775	-2.14492842
H	0.06334076	-3.09498310	-2.14492842

26
C6H5-CCH...benzene Dimer

C	0.09484676	1.94660902	0.00000000
C	-0.53837103	1.63628894	1.21067500
C	-0.53837103	1.63628894	-1.21067500
C	-2.41371915	0.71723995	0.00000000
C	-1.78693080	1.02440917	-1.20665700
C	-1.78693080	1.02440917	1.20665700
H	-0.04457683	1.87828191	-2.14301400
H	-0.04457683	1.87828191	2.14301400
H	-2.27116346	0.78710201	-2.14584400
H	-2.27116346	0.78710201	2.14584400
C	1.38382668	2.57829744	0.00000000
C	2.46834871	3.10978749	0.00000000
H	3.42529762	3.57875798	0.00000000
H	-3.38630613	0.24060574	0.00000000
C	1.80625058	-1.55783475	0.00000000
C	1.18046211	-1.86451395	1.20705841
C	-0.07111483	-2.47787235	1.20705841
C	-0.69690330	-2.78455155	0.00000000
C	-0.07111483	-2.47787235	-1.20705841
C	1.18046211	-1.86451395	-1.20705841
H	2.77871094	-1.08126259	0.00000000
H	1.66669229	-1.62622787	2.14492842
H	-0.55734501	-2.71615843	2.14492842
H	-1.66936366	-3.26112371	0.00000000
H	-0.55734501	-2.71615843	-2.14492842
H	1.66669229	-1.62622787	-2.14492842

27
C6H5-CF3...benzene Dimer

C	2.66253612	-0.35767743	0.01137271
C	2.15188574	0.11045137	-1.19759077
C	2.11340161	0.07354333	1.21719416
C	0.54814834	1.43801285	0.00512158
C	1.05213712	0.97391367	1.21790040
C	1.09074416	1.01093957	-1.20459788
H	2.51199927	-0.28733323	2.15672883
H	2.58038854	-0.22174483	-2.13453808
C	-0.62883051	2.36661587	0.00055806
F	-0.66252585	3.14830829	1.09781500
F	-1.79973809	1.69163874	-0.02841900
F	-0.62793332	3.18148391	-1.07282136

H	0.62290555	1.31798929	2.14980044
H	0.69125129	1.38353586	-2.13875069
H	3.48986537	-1.05632829	0.01387999
C	0.23249371	-3.41654207	-0.00342213
C	-0.31839876	-2.98391691	1.20157011
C	-1.40862509	-2.11556037	1.19746744
C	-1.94795895	-1.67982901	-0.01162748
C	-1.39706648	-2.11245417	-1.21661972
C	-0.30684015	-2.98081070	-1.21251704
H	1.07958658	-4.09124475	-0.00023440
H	0.10065722	-3.32247499	2.14102246
H	-1.83666198	-1.77941578	2.13373205
H	-2.79505182	-1.00512633	-0.01481521
H	-1.81612246	-1.77389609	-2.15607206
H	0.12119674	-3.31695530	-2.14878166

27
C6H5-CH3...benzene Dimer

C	1.99830194	1.39680916	0.00711381
C	1.31942083	1.56999548	-1.19701495
C	1.30803578	1.53737669	1.20901851
C	-0.74264454	2.02005165	0.00259398
C	-0.04998621	1.84782672	1.20362774
C	-0.03863120	1.88035936	-1.19606094
H	1.82697348	1.40985302	2.15151503
H	1.84726958	1.46800279	-2.13767040
C	-2.22053565	2.32308166	-0.00029184
H	-2.50874272	2.88361325	0.89040859
H	-2.80479608	1.39893570	-0.01558503
H	-2.50037408	2.90758990	-0.87815521
H	-0.58031597	1.95932386	2.14340845
H	-0.56005943	2.01736002	-2.13744925
H	3.05507877	1.15932682	0.00889518
C	1.19271153	-2.44230816	-0.00213543
C	0.50760630	-2.30282355	1.20361255
C	-0.85698141	-2.01901561	1.20100310
C	-1.53646388	-1.87469230	-0.00735434
C	-0.85135864	-2.01417691	-1.21310232
C	0.51322906	-2.29798485	-1.21049287
H	2.25297992	-2.66282354	-0.00010792
H	1.03555608	-2.41496104	2.14249189
H	-1.38930001	-1.91063773	2.13785492
H	-2.59673226	-1.65417692	-0.00938185
H	-1.37930842	-1.90203942	-2.15198166
H	1.04554767	-2.40636273	-2.14734470

26
C6H5-CHO...benzene Dimer

C	-0.07616714	1.91092754	-0.21882198
C	0.33919992	1.70317800	1.09980759
C	0.74170767	1.53271861	-1.28416782
C	2.39194098	0.73832066	0.27836184
C	1.97922972	0.94477887	-1.03622490
C	1.57354746	1.11675695	1.34586919
H	0.40773089	1.69941136	-2.30303548
H	-0.31612932	2.00661450	1.90675128
H	2.61708558	0.64975528	-1.85988990
H	1.90313474	0.95214733	2.36412926
C	-1.38936823	2.53495912	-0.49820250
O	-2.16959635	2.89713755	0.35453920
H	-1.63260554	2.65912953	-1.56860109
H	3.35418468	0.28113650	0.47442877
C	0.70675629	-2.83405867	0.25022485
C	-0.11171615	-2.45554511	1.31299656
C	-1.35030988	-1.86708486	1.06349016
C	-1.77043117	-1.65713816	-0.24878795
C	-0.95195873	-2.03565171	-1.31155965
C	0.28663500	-2.62411197	-1.06205325
H	1.66912886	-3.29128528	0.44408835
H	0.21471309	-2.61867120	2.33262102
H	-1.98625322	-1.57298434	1.88925112
H	-2.73280375	-1.19991155	-0.44265145
H	-1.27838797	-1.87252563	-2.33118411
H	0.92257833	-2.91821249	-1.88781421

25
C6H5-CN...benzene Dimer

C	2.39460020	0.67372350	0.00000000
C	1.77567472	0.98778601	1.20898600
C	1.77567472	0.98778601	-1.20898600
C	-0.08143169	1.93014095	0.00000000
C	0.53596888	1.61685223	-1.21523800
C	0.53596888	1.61685223	1.21523800
C	-1.36537242	2.58165337	0.00000000
N	-2.39641699	3.10483822	0.00000000
H	2.25810021	0.74298795	2.14648100
H	2.25810021	0.74298795	-2.14648100
H	0.04365020	1.86667041	-2.14582200
H	0.04365020	1.86667041	2.14582200
H	3.36022077	0.18373687	0.00000000
C	0.65684914	-2.76178892	0.00000000
C	0.03538525	-2.44643835	1.20705841
C	-1.20754251	-1.81573722	1.20705841
C	-1.82900639	-1.50038665	0.00000000
C	-1.20754251	-1.81573722	-1.20705841
C	0.03538525	-2.44643835	-1.20705841
H	1.62258920	-3.25183619	0.00000000
H	0.51825529	-2.69146199	2.14492842
H	-1.69041254	-1.57071358	2.14492842
H	-2.79474646	-1.01033938	0.00000000
H	-1.69041254	-1.57071358	-2.14492842
H	0.51825529	-2.69146199	-2.14492842

29
C6H5-COCH3...benzene Dimer

C	0.32943943	-1.67336409	0.03326836
C	0.94138238	-1.26399362	1.22233783
C	0.87600445	-1.28552473	-1.19295368
C	2.62742808	-0.09202076	-0.04218091
C	2.02300250	-0.49623241	-1.23003349
C	2.08538358	-0.47675933	1.18492020
H	0.41436347	-1.59403464	-2.12225630

H	0.50216151	-1.57521040	2.16117354
H	2.44245965	-0.19847427	-2.18281435
H	2.55588774	-0.16209299	2.10802797
C	-0.90229459	-2.52147200	0.12519039
O	-1.35281766	-2.84186574	1.20861375
C	-1.57354078	-2.97076629	-1.15315899
H	-0.88689450	-3.56444067	-1.76094553
H	-1.88778448	-2.10928596	-1.74682507
H	-2.44212212	-3.57073168	-0.89197086
H	3.51932623	0.52173237	-0.07148838
C	-1.90577056	1.58321921	0.06515733
C	-1.29952451	1.98868415	1.25289353
C	-0.15174649	2.77851883	1.21520883
C	0.38978549	3.16288857	-0.01021206
C	-0.21646055	2.75742363	-1.19794826
C	-1.36423858	1.96758895	-1.16026356
H	-2.79758041	0.96952708	0.09443790
H	-1.72028841	1.69003344	2.20503096
H	0.31929947	3.09356025	2.13806570
H	1.28159534	3.77658070	-0.03949263
H	0.20430334	3.05607434	-2.15008569
H	-1.83528453	1.65254753	-2.08312043

30
C6H5-COOCH3...benzene Dimer

C	0.81428427	-1.26317906	-0.09942825
C	1.42417504	-0.66590785	-1.20411451
C	1.14414193	-0.85521257	1.19463992
C	2.69577065	0.74928971	0.27673387
C	2.08627614	0.15233459	1.37909979
C	2.36475926	0.34021442	-1.01477527
H	0.66540566	-1.32488896	2.04292918
H	1.14957218	-1.00168814	-2.19572962
H	2.34450290	0.47121841	2.38124139
H	2.83895957	0.80475580	-1.87028038
C	-0.18574265	-2.33542663	-0.35731713
O	-0.50358844	-2.72206935	-1.46022491
O	-0.71051073	-2.84135077	0.77103399
C	-1.68090234	-3.87939461	0.57486495
H	-1.99751023	-4.17044359	1.57164812
H	-2.51988734	-3.49966255	-0.00520921
H	-1.22771634	-4.71795711	0.04949492
H	3.42867081	1.53324149	0.42392296
C	-2.06087520	1.44256955	-0.22147764
C	-1.72818041	1.85334740	1.06818475
C	-0.78506182	2.86212255	1.25674072
C	-0.17463802	3.46011986	0.15563430
C	-0.50733281	3.04934202	-1.13402809
C	-1.45045140	2.04056686	-1.32258406
H	-2.79366711	0.65876327	-0.36798339
H	-2.20247243	1.38871061	1.92373132
H	-0.52656193	3.18129205	2.25879303
H	0.55815389	4.24392614	0.30214004
H	-0.03304079	3.51397880	-1.98957467
H	-1.70895129	1.72139737	-2.32463638

27
C6H5-COOH...benzene Dimer

C	2.60443401	0.04060334	-0.02192153
C	2.02222871	0.45408160	-1.21904577
C	2.05656502	0.43307132	1.19929623
C	0.34324945	1.65323138	0.02400422
C	0.92516202	1.23996598	1.22397883
C	0.88940498	1.26198119	-1.20010718
H	2.44978881	0.14780718	-2.16524517
H	2.51081156	0.11046004	2.12742469
H	0.42886575	1.58908888	-2.12212593
H	0.47954720	1.55909719	2.15701891
C	-0.86361877	2.51401816	0.10027606
O	-1.38457792	2.88701517	1.12655915
O	-1.34942934	2.85873132	-1.11164493
H	-2.12847178	3.41453694	-0.95019838
H	3.48601910	-0.58812470	-0.04022801
C	0.34368339	-3.13729016	-0.01744562
C	-0.20655449	-2.74313684	1.20096924
C	-1.34116776	-1.93395514	1.22401379
C	-1.92554315	-1.51892676	0.02864347
C	-1.37530527	-1.91308008	-1.18977139
C	-0.24069200	-2.72226178	-1.21281594
H	1.22526438	-3.76601470	-0.03535096
H	0.24749822	-3.06560894	2.12975774
H	-1.76869604	-1.62770270	2.17070763
H	-2.80712414	-0.89020221	0.04654881
H	-1.82935799	-1.59060797	-2.11855989
H	0.18683627	-3.02851422	-2.15950977

24
C6H5-F...benzene Dimer

C	0.70908851	2.00325917	0.00000000
C	0.06314069	1.86063520	1.21658000
C	0.06314069	1.86063520	-1.21658000
C	-1.97938639	1.40964937	0.00000000
C	-1.29733710	1.56024447	-1.20644900
C	-1.29733710	1.56024447	1.20644900
F	2.03096993	2.29512791	0.00000000
H	0.61967023	1.98351579	2.13600000
H	0.61967023	1.98351579	-2.13600000
H	-1.82391309	1.44397756	-2.14537100
H	-1.82391309	1.44397756	2.14537100
H	-3.03611913	1.17632492	0.00000000
C	1.58953425	-1.84747914	0.00000000
C	0.90902926	-1.99773326	1.20705841
C	-0.45198071	-2.29824150	1.20705841
C	-1.13248570	-2.44849562	0.00000000
C	-0.45198071	-2.29824150	-1.20705841
C	0.90902926	-1.99773326	-1.20705841
H	2.64702278	-1.61398782	0.00000000
H	1.43777353	-1.88098760	2.14492842
H	-0.98072498	-2.41498716	2.14492842
H	-2.18997423	-2.68198694	0.00000000
H	-0.98072498	-2.41498716	-2.14492842
H	1.43777353	-1.88098760	-2.14492842

32
C6H5-NCH3_2...benzene Dimer

C	0.25126059	-1.60566063	0.00000000
C	0.86881044	-1.21431890	1.20480800
C	0.86881044	-1.21431890	-1.20480800
C	2.62203860	-0.05073878	0.00000000
C	2.02854032	-0.44711079	-1.19537800
C	2.02854032	-0.44711079	1.19537800
H	0.44757517	-1.50308136	2.15666650
H	2.47276271	-0.16204554	2.14181049
H	2.47276271	-0.16204554	-2.14181049
H	0.44757517	-1.50308136	-2.15666650
N	-0.92754448	-2.34099153	0.00000000
C	-1.32491078	-2.98916826	-1.23492798
H	-2.24434978	-3.54390735	-1.05913547
H	-1.53186779	-2.24849395	-2.00861248
H	-0.56074889	-3.68305886	-1.61084497
C	-1.32491078	-2.98916826	1.23492798
H	-1.53186779	-2.24849395	2.00861248
H	-2.24434978	-3.54390735	1.05913547
H	-0.56074889	-3.68305886	1.61084497
H	3.52624029	0.54397292	0.00000000
C	-1.88712797	1.70868571	0.00000000
C	-1.30438835	2.09088707	1.20705841
C	-0.13890911	2.85528978	1.20705841
C	0.44383050	3.23749113	0.00000000
C	-0.13890911	2.85528978	-1.20705841
C	-1.30438835	2.09088707	-1.20705841
H	-2.79269145	1.11475392	0.00000000
H	-1.75717009	1.79392117	2.14492842
H	0.31387263	3.15225567	2.14492842
H	1.34939398	3.83142292	0.00000000
H	0.31387263	3.15225567	-2.14492842
H	-1.75717009	1.79392117	-2.14492842

26
C6H5-NH2...benzene Dimer

C	-0.75640823	-1.95874583	0.00000000
C	-0.05958644	-1.80713175	-1.20529550
C	-0.05958644	-1.80713175	1.20529550
C	1.99359430	-1.36820436	0.00000000
C	1.30019429	-1.51611293	1.19985750
C	1.30019429	-1.51611293	-1.19985750
H	-0.59022184	-1.91222054	2.14520650
H	1.82079752	-1.40602759	2.14355150
H	1.82079752	-1.40602759	-2.14355150
H	-0.59022184	-1.91222054	-2.14520650
H	-2.48756796	-2.63868091	0.83449000
H	-2.48756796	-2.63868091	-0.83449000
N	-2.13251336	-2.19770111	0.00000000
H	3.05219712	-1.14336414	0.00000000
C	-1.55132059	1.80931242	0.00000000
C	-0.86995827	1.95562963	1.20705841
C	0.49276637	2.24826405	1.20705841
C	1.17412869	2.39458126	0.00000000
C	0.49276637	2.24826405	-1.20705841
C	-0.86995827	1.95562963	-1.20705841
H	-2.61014139	1.58193895	0.00000000
H	-1.39936867	1.84194290	2.14492842
H	1.02217678	2.36195078	2.14492842
H	2.23294950	2.62195473	0.00000000
H	1.02217678	2.36195078	-2.14492842
H	-1.39936867	1.84194290	-2.14492842

29
C6H5-NHCH3...benzene Dimer

C	-0.02062998	-1.81908963	-0.27186531
C	0.37387746	-1.61115596	1.05724234
C	0.83859759	-1.39458139	-1.30065758
C	2.43634561	-0.56998813	0.31823753
C	2.04723370	-0.78208407	-1.00621101
C	1.58942937	-0.98861318	1.33842495
H	0.54113766	-1.54262960	-2.33344269
H	2.69116202	-0.46528812	-1.81802154
H	1.87249485	-0.83603899	2.37320882
H	-0.26182672	-1.92854415	1.87283017
N	-1.24007379	-2.39844291	-0.59495725
H	-1.27126793	-2.80123954	-1.51720819
C	-2.00595393	-3.10829863	0.40818750
H	-2.86265569	-3.57419235	-0.07580422
H	-2.38626510	-2.41060667	1.15649378
H	-1.42150998	-3.88349532	0.91954015
H	3.37960083	-0.09043365	0.54544008
C	-1.76619496	1.66721694	-0.29699366
C	-1.38796890	1.86934951	1.02918159
C	-0.17305376	2.48700006	1.32097321
C	0.66363532	2.90251804	0.28658956
C	0.28540926	2.70038548	-1.03958570
C	-0.92950588	2.08273493	-1.33137731
H	-2.71016955	1.18730982	-0.52371227
H	-2.03806635	1.54649698	1.83288537
H	0.12082338	2.64405465	2.35139559
H	1.60760991	3.38242516	0.51330817
H	0.93550671	3.02323800	-1.84328947
H	-1.22338302	1.92568033	-2.36179969

27
C6H5-NHOH...benzene Dimer

C	2.42121109	0.62619501	-0.32694698
C	2.03797777	0.82483272	0.99987970
C	1.57044070	1.04108721	-1.34684510
C	-0.02680684	1.84082408	0.26807179
C	0.34839794	1.64813919	-1.06049190
C	0.82225914	1.42575979	1.30000701
H	0.52122118	1.56539795	2.33273383
H	2.68798824	0.50889808	1.80687350
H	1.85724078	0.89840791	-2.38183991
H	-0.30308794	1.98460824	-1.85378082
N	-1.28335809	2.38589923	0.62647735
H	-1.18628882	3.03967970	1.39446273
O	-1.87155144	3.11311195	-0.42575542
H	-2.70955639	2.65931823	-0.58007228

H	3.36891687	0.15723186	-0.55890568
C	0.66469778	-2.91151865	-0.29988022
C	0.28813658	-2.71617338	1.02778512
C	-0.93183249	-2.11086331	1.32431256
C	-1.77524037	-1.70089851	0.29317467
C	-1.39867918	-1.89624377	-1.03449066
C	-0.17871010	-2.50155384	-1.33101811
H	1.61259921	-3.38183736	-0.53027850
H	0.94345446	-3.03471115	1.82896698
H	-1.22441606	-1.95908237	2.35589271
H	-2.72314181	-1.23057979	0.52357296
H	-2.05399705	-1.57770600	-1.83567253
H	0.11387346	-2.65333479	-2.36259826

25
C6H5-NO...benzene Dimer

C	-0.07782611	-1.85902425	-0.21588508
C	0.71803550	-1.47475866	-1.29186253
C	0.32327913	-1.64670096	1.10528788
C	2.35469424	-0.64678256	0.26559770
C	1.54711494	-1.03688417	1.33960237
C	1.94469384	-0.86344696	-1.04816962
H	-0.32410962	-1.95994981	1.91358339
H	0.36039725	-1.66234094	-2.29688237
H	1.87932263	-0.86181992	2.35509377
H	2.57589580	-0.55839656	-1.87283160
N	-1.32568230	-2.48200531	-0.57418109
O	-2.01168044	-2.81315415	0.36039747
H	3.30836620	-0.17147552	0.45900813
C	-1.78278431	1.53687845	-0.25144955
C	-1.36196338	1.75887677	1.05861909
C	-0.13362198	2.37101828	1.30175179
C	0.67389851	2.76116147	0.23481584
C	0.25307758	2.53916316	-1.07525280
C	-0.97526383	1.92702165	-1.31838549
H	-2.73719095	1.06125180	-0.44036076
H	-1.98939718	1.45574016	1.88761561
H	0.19335087	2.54350833	2.31965952
H	1.62830514	3.23678813	0.42372705
H	0.88051137	2.84229977	-1.90424932
H	-1.30223668	1.75453160	-2.33629322

26
C6H5-NO2...benzene Dimer

C	-0.30650962	1.64474005	0.00000000
C	-0.85226001	1.26539301	-1.21951500
C	-0.85226001	1.26539301	1.21951500
C	-2.56322810	0.07611184	0.00000000
C	-1.99427038	0.47159011	-1.21000200
C	-1.99427038	0.47159011	1.21000200
H	-2.43871173	0.16266223	-2.14716400
H	-0.38783093	1.58821420	-2.13988900
H	-0.38783093	1.58821420	2.13988900
H	-2.43871173	0.16266223	2.14716400
O	1.36392878	2.80584934	-1.07799600
O	1.36392878	2.80584934	1.07799600
N	0.90109843	2.48413941	0.00000000
H	-3.45213298	-0.54175933	0.00000000
C	1.91474329	-1.49999825	0.00000000
C	1.34250807	-1.89775469	1.20705841
C	0.19803762	-2.69326758	1.20705841
C	-0.37419760	-3.09102402	0.00000000
C	0.19803762	-2.69326758	-1.20705841
C	1.34250807	-1.89775469	-1.20705841
H	2.80398319	-0.88189422	0.00000000
H	1.78712802	-1.58870268	2.14492842
H	-0.24658233	-3.00231959	2.14492842
H	-1.26343750	-3.70912805	0.00000000
H	-0.24658233	-3.00231959	-2.14492842
H	1.78712802	-1.58870268	-2.14492842

28
C6H5-OCF3...benzene Dimer

C	0.94324845	-0.90617515	-0.36872532
C	1.55812456	-0.14627576	-1.35633656
C	1.15023372	-0.65459745	0.98145595
C	2.62772834	1.16696511	0.36417320
C	2.00122058	0.39277971	1.33501445
C	2.40238918	0.89277390	-0.98411252
H	0.67216325	-1.24542159	1.74816424
H	1.36536819	-0.38110909	-2.39475496
H	2.16917142	0.59702845	2.38480481
H	2.88352818	1.48737647	-1.75023505
C	-0.54646396	-2.74206428	-0.03949544
O	0.11906386	-1.92017329	-0.86693758
F	-1.40634477	-2.08778277	0.76230325
F	0.27254427	-3.45071309	0.75887968
F	-1.24257509	-3.59768299	-0.78277825
H	3.28531370	1.97626654	0.65375311
C	-2.05616833	1.50759589	-0.36744030
C	-1.83222467	1.78006773	0.98098903
C	-0.98461730	2.82324371	1.34976943
C	-0.36095360	3.59394786	0.37012048
C	-0.58489726	3.32147602	-0.97830886
C	-1.43250463	2.27830004	-1.34708925
H	-2.71474915	0.69706059	-0.65397827
H	-2.31680393	1.18123980	1.74216460
H	-0.81061574	3.03495109	2.39748296
H	0.29762722	4.40448317	0.65665845
H	-0.10031799	3.92030396	-1.73948442
H	-1.60650618	2.06659267	-2.39480278

25
C6H5-OH...benzene Dimer

C	-0.75082593	-1.97830694	0.00211294
C	-0.07496521	-1.83581517	1.21300112
C	-0.07112111	-1.83447740	-1.20587506
C	1.97806025	-1.40191339	0.00479676
C	1.29244022	-1.54646834	-1.19776101
C	1.28494658	-1.54857389	1.20701157
H	-0.60192575	-1.94638940	-2.14581347
H	1.81560087	-1.43576180	-2.13977687

H	1.80729635	-1.43844830	2.14956067
H	-0.62753971	-1.95273041	2.13626604
O	-2.08679922	-2.26050340	0.06081505
H	-2.44612490	-2.33620604	-0.83147169
H	3.03702321	-1.17824021	0.00715424
C	-1.55992017	1.83684381	0.00336936
C	-0.87915232	1.98037276	1.21109777
C	0.48455011	2.26841309	1.21243895
C	1.16748469	2.41292448	0.00605172
C	0.48671684	2.26939553	-1.20167669
C	-0.87698559	1.98135520	-1.20301787
H	-2.61950071	1.61303990	0.00232728
H	-1.40978436	1.86808913	2.14844629
H	1.01349861	2.37993338	2.15082955
H	2.22706523	2.63672839	0.00709380
H	1.01734888	2.38167916	-2.13902521
H	-1.40593409	1.86983492	-2.14140847

28
C6H5-OMe...benzene Dimer

C	-0.05556317	-1.86154030	-0.25239338
C	0.33528705	-1.66202812	1.07184166
C	0.79072406	-1.47762295	-1.29806258
C	2.42235376	-0.69297672	0.30449447
C	2.01892671	-0.89835902	-1.01760166
C	1.57627967	-1.07695751	1.33686808
H	-0.30259440	-1.95097073	1.89514028
H	1.87399383	-0.92472030	2.36727869
H	2.66688279	-0.60461363	-1.83442973
H	0.46013800	-1.64510699	-2.31508497
O	-1.24016538	-2.42150876	-0.62610690
C	-2.12958190	-2.82589624	0.39922891
H	-2.43350843	-1.97346764	1.01201121
H	-1.67459725	-3.59220230	1.03189944
H	-2.99806807	-3.23927669	-0.10606516
H	3.38151702	-0.24062926	0.52124524
C	-1.73068714	1.71539130	-0.29738154
C	-1.33629739	1.91653066	1.02422848
C	-0.10091972	2.49912372	1.30186256
C	0.74006821	2.88057741	0.25788664
C	0.34567846	2.67943804	-1.06372337
C	-0.88969921	2.09684499	-1.34135746
H	-2.69056087	1.26272343	-0.51309991
H	-1.98973499	1.62014569	1.83538534
H	0.20551641	2.65540661	2.32873780
H	1.69994194	3.33324527	0.47360502
H	0.99911606	2.97582302	-1.87488024
H	-1.19613534	1.94056209	-2.36823270

28
C6H5-SCH3...benzene Dimer

C	0.43930155	-1.56125676	-0.20540925
C	0.79718937	-1.24754680	1.10709838
C	1.17701662	-1.01551199	-1.26463576
C	2.60950035	0.14127200	0.29996798
C	2.25105724	-0.17284664	-1.01166374
C	1.87821915	-0.39967740	1.35128989
H	0.24727598	-1.65305642	1.94531648
H	2.14412111	-0.16529320	2.37515109
H	2.81048873	0.24027430	-1.84228033
H	0.90364704	-1.25564007	-2.28596424
S	-0.90805499	-2.62178108	-0.65043288
C	-1.58234629	-3.10346780	0.95714979
H	-1.94812600	-2.23911314	1.51076025
H	-0.84915914	-3.65119164	1.54860859
H	-2.42170123	-3.76254687	0.73922434
H	3.44718778	0.79847608	0.49635760
C	-1.91733098	1.48214537	-0.28649766
C	-1.56513505	1.79142840	1.02611629
C	-0.48648223	2.63763542	1.27730368
C	0.23997468	3.17455942	0.21587712
C	-0.11222125	2.86527639	-1.09673683
C	-1.19087408	2.01906937	-1.34792422
H	-2.75543138	0.82465260	-0.48166727
H	-2.12958341	1.37424486	1.85083208
H	-0.21283019	2.87794465	2.29718909
H	1.07807507	3.83205219	0.41104673
H	0.45222711	3.28245993	-1.92145263
H	-1.46452612	1.77876014	-2.36780963

25
C6H5-SH...benzene Dimer

C	-0.03431113	-1.84160932	-0.01161781
C	0.57723970	-1.52323191	1.20406096
C	0.60012531	-1.51013639	-1.21027354
C	2.44611037	-0.54793342	0.02067375
C	1.83481576	-0.86618004	-1.18908230
C	1.81051551	-0.88000873	1.21556816
H	0.13638953	-1.75154724	-2.15933104
H	2.31689620	-0.61429593	-2.12564360
H	2.27502079	-0.63819600	2.16349460
H	0.08880503	-1.77842841	2.13700831
S	-1.60720382	-2.66199796	0.04873154
H	-1.77910908	-2.75101992	-1.27820015
H	3.40567110	-0.04746970	0.03285285
C	-1.81037707	1.57425216	-0.00956026
C	-1.20462980	1.88960297	1.20546133
C	0.03109523	2.53410137	1.22154871
C	0.66107299	2.86324896	0.02261450
C	0.05532572	2.54789815	-1.19240708
C	-1.18039931	1.90339974	-1.20849446
H	-2.77052070	1.07348458	-0.02205996
H	-1.69411502	1.63385921	2.13701892
H	0.50175364	2.77912519	2.16560601
H	1.62121662	3.36401654	0.03511421
H	0.54481094	2.80364190	-2.12396468
H	-1.65105772	1.65837592	-2.15255177

27
C6H5-SiF3...benzene Dimer

C	0.81220072	-1.09263900	0.00103032
C	1.30286634	-0.58100492	1.21003047

C	1.31142210	-0.58794178	-1.20741039
C	2.75014208	0.92175340	0.00207751
C	2.27506043	0.41624501	-1.20647139
C	2.26654416	0.42318874	1.21010050
Si	-0.47015616	-2.39910678	0.00019594
F	-1.96363035	-1.83109257	-0.01490981
F	-0.35485786	-3.31369256	1.30473037
F	-0.33603864	-3.33133260	-1.28997701
H	0.95385056	-0.98372686	-2.15103720
H	0.93857848	-0.97137194	2.15332628
H	2.65665521	0.80000411	-2.14409493
H	2.64153827	0.81231458	2.14817568
H	3.50094750	1.70215616	0.00247922
C	-2.02650614	1.65069758	-0.00210136
C	-1.54435374	2.15325422	1.20521767
C	-0.57803943	3.15768925	1.20573983
C	-0.09387753	3.65956764	-0.00105704
C	-0.57602993	3.15701100	-1.20837606
C	-1.54234424	2.15257597	-1.20889822
H	-2.77732085	0.87026352	-0.00250707
H	-1.92054177	1.76330069	2.14288446
H	-0.20341276	3.54816978	2.14381233
H	0.65693718	4.44000170	-0.00065133
H	-0.19984190	3.54696453	-2.14604285
H	-1.91697091	1.76209545	-2.14697073

27
C6H5-SiH3...benzene Dimer

C	-0.05637032	-1.90948611	-0.00073901
C	0.59834270	-1.61120061	1.20154816
C	0.59375892	-1.60331153	-1.20356664
C	2.48736876	-0.71468351	-0.00169242
C	1.85393374	-1.00921585	-1.20717308
C	1.85857343	-1.01712485	1.20421768
Si	-1.76702416	-2.68049541	-0.00002369
H	-2.83312421	-1.64017218	-0.00226459
H	-1.93758506	-3.51685302	1.21942655
H	-1.93730913	-3.52121664	-1.21652396
H	0.11617146	-1.83347702	-2.15013523
H	0.12434789	-1.84757925	2.14837648
H	2.34148307	-0.78067985	-2.14711724
H	2.34972375	-0.79477442	2.14376944
H	3.46820812	-0.25511689	-0.00207251
C	-1.76077743	1.76236926	0.00169438
C	-1.12931668	2.05815982	1.20851608
C	0.13224120	2.65071770	1.20804324
C	0.76233833	2.94748502	0.00074870
C	0.13087758	2.65169446	-1.20607300
C	-1.13068030	2.05913658	-1.20560016
H	-2.74099287	1.30195884	0.00206177
H	-1.61889464	1.82757514	2.14656956
H	0.62287868	2.88054344	2.14572932
H	1.74255377	3.40789543	0.00038131
H	0.62045555	2.88227913	-2.14412648
H	-1.62131778	1.82931084	-2.14328625

28
C6H5-CH2OH...benzene Dimer

C	2.44196307	0.62445021	0.36824681
C	1.57685331	1.04845714	1.37247204
C	2.09158607	0.81574352	-0.96828453
C	0.01373610	1.85352387	-0.28345587
C	0.88421463	1.42683631	-1.28952213
C	0.36557206	1.66152562	1.05047952
H	2.75773097	0.48943294	-1.75757280
H	1.84244877	0.90314893	2.41255751
C	-1.28715294	2.51241984	-0.67150728
H	-1.87040252	1.81995104	-1.28856121
H	-1.07321078	3.40435753	-1.27077733
H	0.61502286	1.57396811	-2.33086414
H	-0.31029923	1.99287805	1.82657961
H	3.38134874	0.14895412	0.62176814
O	-2.01002591	2.86300155	0.49834018
H	-2.83850794	3.28271292	0.24336840
C	0.66307605	-2.90207068	0.32663220
C	-0.19801524	-2.48016751	1.33815226
C	-1.40739028	-1.86802910	1.01357266
C	-1.75567403	-1.67779385	-0.32252701
C	-0.89458273	-2.09969702	-1.33404707
C	0.31479231	-2.71183543	-1.00946747
H	1.60274605	-3.37769494	0.57882669
H	0.07259708	-2.62797804	2.37628579
H	-2.07644796	-1.54021536	1.79951170
H	-2.69534403	-1.20216959	-0.57472149
H	-1.16519505	-1.95188649	-2.37218060
H	0.98384999	-3.03964917	-1.79540651

C_6H_5-X···C_6F_6 Dimers

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   24
C6H5-H...perfluorobenzene Dimer
C                    0.98556382    -0.98556382    -2.42045455
C                   -0.36074140    -1.34630522    -2.42045455
C                    1.34630522     0.36074140    -2.42045455
C                   -0.98556382     0.98556382    -2.42045455
C                    0.36074140     1.34630522    -2.42045455
C                   -1.34630522    -0.36074140    -2.42045455
H                    1.75154749    -1.75154749    -2.42045455
H                   -0.64111088    -2.39265837    -2.42045455
H                   -2.39265837    -0.64111088    -2.42045455
H                   -1.75154749     1.75154749    -2.42045455
H                    0.64111088     2.39265837    -2.42045455
H                    2.39265837     0.64111088    -2.42045455
C                    0.98143937    -0.98143937     1.12954545
C                   -0.35923174    -1.34067111     1.12954545
C                   -1.34067111    -0.35923174     1.12954545
C                   -0.98143937     0.98143937     1.12954545
C                    0.35923174     1.34067111     1.12954545
C                    1.34067111     0.35923174     1.12954545
F                    1.92276136    -1.92276136     1.12954545
F                   -0.70377950    -2.62654087     1.12954545
F                   -2.62654087    -0.70377950     1.12954545
F                   -1.92276136     1.92276136     1.12954545
F                    0.70377950     2.62654087     1.12954545
F                    2.62654087     0.70377950     1.12954545


   26
C6H5-BF2...perfluorobenzene Dimer
C                   -2.80825992     0.14147238     0.00000000
C                   -2.36658720    -0.39302085    -1.20980600
C                   -2.36658720    -0.39302085     1.20980600
C                   -1.02771245    -2.01326917     0.00000000
C                   -1.48042241    -1.46541915     1.20800000
C                   -1.48042241    -1.46541915    -1.20800000
H                   -1.13480948    -1.88366497    -2.14609300
H                   -2.71245684     0.02553563    -2.14674300
H                   -2.71245684     0.02553563     2.14674300
H                   -1.13480948    -1.88366497     2.14609300
F                    0.40258094    -3.74414836    -1.13455100
F                    0.40258094    -3.74414836     1.13455100
B                   -0.04309212    -3.20481410     0.00000000
H                   -3.49841881     0.97667282     0.00000000
C                   -0.06921953     2.39982858     0.00000000
C                    0.37284558     1.86486050    -1.20201300
C                    1.25697452     0.79492589    -1.20201300
C                    1.69903963     0.25995781     0.00000000
C                    1.25697452     0.79492589     1.20201300
C                    0.37284558     1.86486050     1.20201300
F                   -0.91720908     3.42602886     0.00000000
F                   -0.05114983     2.37796142    -2.35489200
F                    1.68096994     0.28182497    -2.35489200
F                    2.54702919    -0.76624247     0.00000000
F                    1.68096994     0.28182497     2.35489200
F                   -0.05114983     2.37796142     2.35489200


   26
C6H5-CCH...perfluorobenzene Dimer
C                   -0.90300959     2.30322449     0.00000000
C                   -1.37795766     1.78198783     1.21067500
C                   -1.37795766     1.78198783    -1.21067500
C                   -2.78457158     0.23828485     0.00000000
C                   -2.31444595     0.75422908    -1.20665700
C                   -2.31444595     0.75422908     1.20665700
H                   -1.00758493     2.18845721    -2.14301400
H                   -1.00758493     2.18845721     2.14301400
H                   -2.67764699     0.35563035    -2.14584400
H                   -2.67764699     0.35563035     2.14584400
C                    0.06379602     3.36425530     0.00000000
C                    0.87724701     4.25698550     0.00000000
H                    1.59501116     5.04470318     0.00000000
H                   -3.51406515    -0.56230540     0.00000000
C                    1.71346727    -0.09608266     0.00000000
C                    1.24605324    -0.60905102    -1.20201300
C                    0.31122654    -1.63498625    -1.20201300
C                   -0.15618749    -2.14795460     0.00000000
C                    0.31122654    -1.63498625     1.20201300
C                    1.24605324    -0.60905102     1.20201300
F                    2.61008228     0.88791674     0.00000000
F                    1.69436142    -0.11705057    -2.35489200
F                   -0.13708164    -2.12698669    -2.35489200
F                   -1.05280250    -3.13195401     0.00000000
F                   -0.13708164    -2.12698669     2.35489200
F                    1.69436142    -0.11705057     2.35489200


   27
C6H5-CF3...perfluorobenzene Dimer
C                    2.84515553    -0.19927723    -0.06161244
C                    2.32617261     0.29022487    -1.25850236
C                    2.41025640     0.32201029     1.15519793
C                    0.94066949     1.81728619    -0.02182335
C                    1.45535565     1.33420983     1.17899328
C                    1.37100331     1.30232290    -1.24241690
H                    2.81075079    -0.06030429     2.08540069
H                    2.66132730    -0.11678941    -2.20393873
C                   -0.04863069     2.94356473    -0.00219083
F                   -0.80846367     2.93200475     1.11076533
```

F	0.56290434	4.14859647	-0.03936302
F	-0.88404534	2.90343369	-1.05889607
H	1.10819914	1.74134215	2.11962663
H	0.95887051	1.68489305	-2.16699824
H	3.58638422	-0.98853957	-0.07703977
C	0.15671081	-2.58268112	-0.00012572
C	-0.32940227	-2.06499612	-1.19266250
C	-1.25010113	-1.02652648	-1.17426434
C	-1.68468823	-0.50574034	0.03667063
C	-1.19857514	-1.02342533	1.22920742
C	-0.27787629	-2.06189497	1.21080925
F	1.03977545	-3.57870258	-0.01777185
F	0.08742082	-2.56449480	-2.35409878
F	-1.71634401	-0.53000220	-2.31805446
F	-2.56775287	0.49028113	0.05431676
F	-1.61539823	-0.52392666	2.39064370
F	0.18836659	-2.55841926	2.35459938

26

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C6H5-CH3...perfluorobenzene Dimer

C	2.58381160	0.94656939	0.03385434
C	2.03851210	1.37495010	-1.17442442
C	1.99314246	1.34430440	1.23123413
C	0.30776164	2.59591947	0.01194079
C	0.86613748	2.16302034	1.21723488
C	0.91138741	2.19358512	-1.18207987
H	2.41167567	1.02127259	2.17692896
H	2.49255572	1.07590482	-2.11158811
C	-0.93241938	3.45486867	-0.00050714
H	-0.98559779	4.08165041	0.89107738
H	-1.83241107	2.83435604	-0.02538510
H	-0.95224862	4.10417672	-0.87721084
H	0.41355147	2.47178281	2.15355785
H	0.49427408	2.52630838	-2.12663281
H	3.46244951	0.31324371	0.04235752
C	0.55970097	-1.93643238	0.00085044
C	0.00488452	-1.53603225	-1.20675302
C	-1.13386283	-0.74257823	-1.21812146
C	-1.71779538	-0.34952319	-0.02188647
C	-1.16297894	-0.74992331	1.18571699
C	-0.02423159	-1.54337734	1.19708544
F	1.65190122	-2.69745341	0.01175420
F	0.56494845	-1.91302092	-2.35409019
F	-1.66600080	-0.35854472	-2.37636241
F	-2.80999564	0.41149785	-0.03279022
F	-1.72304287	-0.37293465	2.33305417
F	0.50790639	-1.92741085	2.35532638

C6H5-CHO...perfluorobenzene Dimer

C	0.85472742	2.27470977	-0.17654354
C	1.11841953	1.92780581	1.15183808
C	1.52882767	1.63809038	-1.21924559
C	2.73195836	0.30649086	0.38548376
C	2.47013787	0.65123244	-0.93878856
C	2.05736774	0.94349516	1.43033156
H	1.31505527	1.91649437	-2.24599330
H	0.58026503	2.43849463	1.94068211
H	2.99556058	0.15464539	-1.74480055
H	2.26778980	0.66858811	2.45635609
C	-0.14345900	3.32212416	-0.49041124
O	-0.77961224	3.93151484	0.34088270
H	-0.28526271	3.52905253	-1.56624031
H	3.46374190	-0.46088883	0.60682918
C	0.18470685	-2.16229206	0.24720311
C	-0.08179216	-1.81315466	-1.06943238
C	-1.01992199	-0.82955438	-1.35030064
C	-1.69155417	-0.19509008	-0.31453381
C	-1.42505516	-0.54422748	1.00210168
C	-0.48692533	-1.52782776	1.28296994
F	1.08448996	-3.10568699	0.51659067
F	0.56238647	-2.42168471	-2.06286065
F	-1.27552783	-0.49468808	-2.61311688
F	-2.59133728	0.74830485	-0.58392137
F	-2.06923379	0.06430256	1.99552995
F	-0.23131949	-1.86269406	2.54578618

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C6H5-CN...perfluorobenzene Dimer

C	-2.77102869	-0.27892347	0.00000000
C	-2.29826802	-0.78705865	1.20898600
C	-2.29826802	-0.78705865	-1.20898600
C	-0.87973399	-2.31173509	0.00000000
C	-1.35132987	-1.80485185	-1.21523800
C	-1.35132987	-1.80485185	1.21523800
C	0.10099259	-3.36584495	0.00000000
N	0.88854672	-4.21232815	0.00000000
H	-2.66676440	-0.39098939	2.14648100
H	-2.66676440	-0.39098939	-2.14648100
H	-0.97527667	-2.20904339	-2.14582200
H	-0.97527667	-2.20904339	2.14582200
H	-3.50860928	0.51384690	0.00000000
C	-0.17135675	2.13855591	0.00000000
C	0.30135896	1.63046905	-1.20201300
C	1.24678903	0.61429679	-1.20201300
C	1.71950474	0.10620993	0.00000000
C	1.24678903	0.61429679	1.20201300
C	0.30135896	1.63046905	1.20201300
F	-1.07814169	3.11319142	0.00000000

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F                    -0.15203419     2.11778754    -2.35489200
F                     1.70018218     0.12697830    -2.35489200
F                     2.62628968    -0.86842558     0.00000000
F                     1.70018218     0.12697830     2.35489200
F                    -0.15203419     2.11778754     2.35489200


   29
C6H5-COCH3...perfluorobenzene Dimer
C                     0.98393696    -2.00214107    -0.14682163
C                     1.65487819    -1.44685150     0.94745251
C                     1.19475892    -1.47671274    -1.42441795
C                     2.73268351     0.14156765    -0.51218390
C                     2.06771138    -0.40672809    -1.60621084
C                     2.52547603    -0.37965688     0.76570623
H                     0.68312989    -1.89519951    -2.28173859
H                     1.47755766    -1.86848737     1.92825013
H                     2.22751455    -0.00334115    -2.59824788
H                     3.04284766     0.04717404     1.61579975
C                     0.05533862    -3.15184311     0.09974627
O                    -0.10610159    -3.58587935     1.22445910
C                    -0.67621785    -3.76127982    -1.07499881
H                     0.03190740    -4.14518332    -1.81291046
H                    -1.30282302    -3.01466301    -1.56821900
H                    -1.29770317    -4.57454318    -0.70761620
H                     3.41140507     0.97358679    -0.65401241
C                    -1.65486801     0.24563991     0.33720708
C                    -1.44863356     0.76418868    -0.93362815
C                    -0.57883749     1.83043206    -1.11535298
C                     0.08472539     2.37812820    -0.02624284
C                    -0.12150906     1.85957943     1.24459239
C                    -0.99130513     0.79333605     1.42631722
F                    -2.48911056    -0.77702002     0.51150377
F                    -2.08507271     0.23887998    -1.97821929
F                    -0.38103282     2.32778483    -2.33424107
F                     0.91896795     3.40078813    -0.20053954
F                     0.51493009     2.38488812     2.28918352
F                    -1.18910979     0.29598328     2.64520531


   30
C6H5-COOCH3...perfluorobenzene Dimer
C                     1.19779733    -1.69408576     0.21840117
C                     1.98211156    -1.03087026    -0.72712925
C                     1.14501825    -1.23687114     1.53674268
C                     2.66317352     0.54899015     0.96190810
C                     1.87977298    -0.11387792     1.90527395
C                     2.71435056     0.09054536    -0.35419078
H                     0.53411799    -1.75844605     2.26071746
H                     2.00444372    -1.40703381    -1.74175130
H                     1.84120650     0.24348110     2.92677426
H                     3.32330893     0.60638399    -1.08606088
C                     0.43355084    -2.88931925    -0.23284109
O                     0.44808741    -3.32238244    -1.36384466
O                    -0.28614245    -3.45070677     0.75275651
C                    -1.04137714    -4.60770359     0.36719706
H                    -1.55527633    -4.92994606     1.26752709
H                    -1.75191308    -4.34482797    -0.41422049
H                    -0.37201549    -5.38407956     0.00144627
H                     3.23381837     1.42277566     1.25216832
C                    -1.55813045     0.38405841    -0.61146839
C                    -0.77755310     1.04531506    -1.54949093
C                    -0.04608581     2.16498429    -1.17835689
C                    -0.09519483     2.62339850     0.13080024
C                    -0.87577218     1.96214185     1.06882278
C                    -1.60723947     0.84247261     0.69768874
F                    -2.25969850    -0.68984356    -0.96743207
F                    -0.73045177     0.60563875    -2.80513454
F                     0.70258461     2.79921157    -2.07803628
F                     0.60637322     3.69730047     0.48676392
F                    -0.92287351     2.40181816     2.32446639
F                    -2.35590989     0.20824533     1.59736813


   27
C6H5-COOH...perfluorobenzene Dimer
C                     2.79647268    -0.03694050    -0.05882999
C                     2.30834872     0.49748491    -1.25011426
C                     2.36763566     0.47033423     1.16768357
C                     0.96168045     2.04741052     0.00937771
C                     1.44960383     1.51326023     1.20351499
C                     1.38908907     1.54170980    -1.22001236
H                     2.64310453     0.10161753    -2.20044711
H                     2.74840184     0.05335542     2.09125608
H                     1.00329454     1.96450031    -2.13741367
H                     1.10002217     1.92574522     2.14086758
C                    -0.01693582     3.15999318     0.09753775
O                    -0.42646267     3.64210089     1.12886801
O                    -0.42700902     3.60553842    -1.10949206
H                    -1.05725539     4.32392760    -0.94038114
H                     3.51181176    -0.84958291    -0.08582367
C                     0.13173306    -2.38217909    -0.01983775
C                    -0.35608228    -1.84799199    -1.20437479
C                    -1.27289217    -0.80648245    -1.17029273
C                    -1.70188803    -0.29915851     0.04832642
C                    -1.21407268    -0.83334561     1.23286345
C                    -0.29726280    -1.87485514     1.19878139
F                     1.01106769    -3.38111620    -0.05252668
F                     0.05537812    -2.33457875    -2.37318115
F                    -1.74076772    -0.29413061    -2.30641011
F                    -2.58122266     0.69977860     0.08101535
F                    -1.62553309    -0.34675884     2.40166981
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F                     0.17061275    -2.38720699     2.33489877

   24
C6H5-F...perfluorobenzene Dimer
C                    -0.26986707     2.56733855     0.00000000
C                    -0.81914001     2.19870673     1.21658000
C                    -0.81914001     2.19870673    -1.21658000
C                    -2.55597513     1.03307004     0.00000000
C                    -1.97600379     1.42230438    -1.20644900
C                    -1.97600379     1.42230438     1.20644900
F                     0.85417682     3.32171457     0.00000000
H                    -0.34590269     2.51630900     2.13600000
H                    -0.34590269     2.51630900    -2.13600000
H                    -2.42377053     1.12179610    -2.14537100
H                    -2.42377053     1.12179610     2.14537100
H                    -3.45455344     0.43001001     0.00000000
C                     1.72806863    -0.36716540     0.00000000
C                     1.15182883    -0.75389540    -1.20201300
C                    -0.00064911    -1.52735429    -1.20201300
C                    -0.57688891    -1.91408429     0.00000000
C                    -0.00064911    -1.52735429     1.20201300
C                     1.15182883    -0.75389540     1.20201300
F                     2.83343823     0.37467782     0.00000000
F                     1.70451446    -0.38297324    -2.35489200
F                    -0.55333474    -1.89827646    -2.35489200
F                    -1.68225851    -2.65592751     0.00000000
F                    -0.55333474    -1.89827646     2.35489200
F                     1.70451446    -0.38297324     2.35489200


   32
C6H5-NCH3_2...perfluorobenzene Dimer
C                     0.84825225    -2.00260390     0.00149463
C                     1.34877580    -1.47168847     1.20718069
C                     1.35301297    -1.47169771    -1.20243158
C                     2.76500209     0.08651772     0.00485358
C                     2.28901705    -0.44337930    -1.19136234
C                     2.28480395    -0.44335639     1.19938995
H                     1.00961909    -1.85498943     2.15844788
H                     2.64382550    -0.05799493     2.14645360
H                     2.65137932    -0.05803545    -2.13716074
H                     1.01716888    -1.85498934    -2.15487851
N                    -0.11407777    -3.00470716    -0.00021600
C                    -0.33778814    -3.73081762    -1.23545265
H                    -1.09320728    -4.49429828    -1.06096447
H                    -0.71879808    -3.06377247    -2.00998468
H                     0.57407005    -4.21590240    -1.60954324
C                    -0.34270533    -3.73032745     1.23439852
H                    -0.72644421    -3.06287829     2.00723309
H                    -1.09770056    -4.49362633     1.05730190
H                     0.56756340    -4.21557803     1.61214030
H                     3.49562940     0.88491912     0.00613294
C                    -1.70250366     0.38576778    -0.00300093
C                    -1.23122097     0.89712418    -1.20418989
C                    -0.29288227     1.91984694    -1.20254553
C                     0.17417510     2.43121477     0.00028780
C                    -0.29710758     1.91985837     1.20147676
C                    -1.23544629     0.89713561     1.19983239
F                    -2.60248711    -0.59515047    -0.00457808
F                    -1.67918708     0.40665884    -2.35785569
F                     0.15913643     2.41030132    -2.35463417
F                     1.07415856     3.41213302     0.00186495
F                     0.15085852     2.41032371     2.35514255
F                    -1.68746499     0.40668123     2.35192104


   26
C6H5-NH2...perfluorobenzene Dimer
C                     0.24795283    -2.58438577     0.00000000
C                     0.83820383    -2.18419682    -1.20529550
C                     0.83820383    -2.18419682     1.20529550
C                     2.58027990    -1.01228412     0.00000000
C                     1.99182475    -1.40775986     1.19985750
C                     1.99182475    -1.40775986    -1.19985750
H                     0.38486271    -2.47932290     2.14520650
H                     2.43399461    -1.11173229     2.14355150
H                     2.43399461    -1.11173229    -2.14355150
H                     0.38486271    -2.47932290    -2.14520650
H                    -1.10551606    -3.86006116     0.83449000
H                    -1.10551606    -3.86006116    -0.83449000
N                    -0.94020561    -3.31858224     0.00000000
H                     3.47902605    -0.40941729     0.00000000
C                    -1.72040949     0.37117067     0.00000000
C                    -1.14494882     0.75905909    -1.20201300
C                     0.00597085     1.53483481    -1.20201300
C                     0.58143152     1.92272323     0.00000000
C                     0.00597085     1.53483481     1.20201300
C                    -1.14494882     0.75905909     1.20201300
F                    -2.82428452    -0.37289468     0.00000000
F                    -1.69688717     0.38702586    -2.35489200
F                     0.55790919     1.90686804    -2.35489200
F                     1.68530655     2.66678857     0.00000000
F                     0.55790919     1.90686804     2.35489200
F                    -1.69688717     0.38702586     2.35489200


   29
C6H5-NHCH3...perfluorobenzene Dimer
C                     0.83824257    -2.19482448    -0.21596001
C                     1.06990235    -1.86038906     1.12563843
C                     1.56117427    -1.51394223    -1.21128003
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C	2.70567718	-0.19593639	0.46399542
C	2.48023289	-0.53247577	-0.87259457
C	1.99284333	-0.86721818	1.45118592
H	1.38523219	-1.75803362	-2.25363772
H	3.02463640	-0.02368560	-1.65923113
H	2.15362009	-0.62364039	2.49473914
H	0.53323920	-2.36697988	1.91645888
N	-0.10047760	-3.14878733	-0.58452633
H	0.05305926	-3.54386800	-1.49781856
C	-0.63935356	-4.06779743	0.39618772
H	-1.26559219	-4.79486827	-0.11804571
H	-1.26910209	-3.53255694	1.10914449
H	0.14128787	-4.60149915	0.95273745
H	3.42256294	0.57147069	0.72569197
C	-1.66985173	0.23918149	-0.38372051
C	-0.96780732	0.90127495	-1.38132443
C	-0.04826643	1.88554468	-1.04650851
C	0.16923140	2.20772237	0.28591181
C	-0.53281300	1.54562891	1.28351572
C	-1.45235390	0.56135918	0.94869980
F	-2.55180575	-0.70485552	-0.70485060
F	-1.17641498	0.59226635	-2.65928029
F	0.62508127	2.52057452	-2.00333380
F	1.05118542	3.15175938	0.60704189
F	-0.32420535	1.85463751	2.56147158
F	-2.12570160	-0.07367065	1.90552509

27
C6H5-NHOH...perfluorobenzene Dimer

C	2.69407136	0.23954362	-0.46306934
C	2.46637438	0.56085263	0.87547778
C	1.97816580	0.90828992	-1.45119665
C	0.82062001	2.20119588	0.21829945
C	1.04263781	1.88815928	-1.12173926
C	1.53547530	1.53291386	1.21853081
H	1.35069571	1.76979579	2.26083155
H	3.01510670	0.05104682	1.65813874
H	2.14840846	0.67325644	-2.49503698
H	0.50001859	2.41789272	-1.89108928
N	-0.16429330	3.13442950	0.62265481
H	0.18291763	3.72272387	1.37099110
O	-0.53095614	4.01040235	-0.41668801
H	-1.47869943	3.85989300	-0.52215992
H	3.41967937	-0.51869554	-0.72848201
C	0.18568149	-2.19556780	-0.29743049
C	-0.52252047	-1.53673591	-1.29283903
C	-1.45225121	-0.56323403	-0.95469867
C	-1.67378133	-0.24856263	0.37885072
C	-0.96557936	-0.90739453	1.37425926
C	-0.03584862	-1.88089641	1.03611890
F	1.07740884	-3.12927711	-0.62174912
F	-0.31004535	-1.83854504	-2.57187782
F	-2.13150478	0.06866755	-1.90941834
F	-2.56550868	0.68514668	0.70316936
F	-1.17805449	-0.60558539	2.65329805
F	0.64340494	-2.51279799	1.99083857

25
C6H5-NO...perfluorobenzene Dimer

C	0.78949950	-2.29965911	-0.16856337
C	1.47461686	-1.69464143	-1.21896855
C	1.04826268	-1.96734295	1.16337963
C	2.70846916	-0.39502170	0.38679473
C	2.01409184	-1.00920912	1.43487087
C	2.44226313	-0.73416793	-0.93802319
H	0.49406702	-2.46047512	1.95094963
H	1.23586312	-1.98840221	-2.23378792
H	2.23206391	-0.73513226	2.45937185
H	2.98430052	-0.25390335	-1.74243629
N	-0.18974266	-3.27835336	-0.56463011
O	-0.78061527	-3.79974748	0.34789816
H	3.46058740	0.35176152	0.60916278
C	-1.69493148	0.23149600	-0.32183144
C	-1.00382988	0.84317428	-1.35849721
C	-0.03886554	1.80093157	-1.07923237
C	0.23499859	2.14701196	0.23669866
C	-0.45610301	1.53533369	1.27336443
C	-1.42106735	0.57757639	0.99409958
F	-2.62045223	-0.68711230	-0.58968114
F	-1.26649981	0.51124003	-2.62063778
F	0.62398667	2.38760700	-2.07352283
F	1.16051934	3.06562026	0.50454836
F	-0.19343308	1.86726793	2.53550500
F	-2.08391956	-0.00909904	1.98839005

26
C6H5-NO2...perfluorobenzene Dimer

C	-0.91800139	2.06602865	0.00000000
C	-1.36814865	1.57703468	-1.21951500
C	-1.36814865	1.57703468	1.21951500
C	-2.77939382	0.04400220	0.00000000
C	-2.31010463	0.55379001	-1.21000200
C	-2.31010463	0.55379001	1.21000200
H	-2.67668991	0.15556923	-2.14716400
H	-0.98507705	1.99316451	-2.13988900
H	-0.98507705	1.99316451	2.13988900
H	-2.67668991	0.15556923	2.14716400
O	0.45981398	3.56274641	-1.07799600
O	0.45981398	3.56274641	1.07799600

N	0.07806104	3.14804904	0.00000000
H	-3.51258267	-0.75245921	0.00000000
C	1.70955124	-0.32123049	0.00000000
C	1.23953126	-0.83181214	-1.20201300
C	0.29949266	-1.85297398	-1.20201300
C	-0.17052732	-2.36355563	0.00000000
C	0.29949266	-1.85297398	1.20201300
C	1.23953126	-0.83181214	1.20201300
F	2.61116510	0.65819064	0.00000000
F	1.69033887	-0.34210084	-2.35489200
F	-0.15131495	-2.34268528	-2.35489200
F	-1.07214119	-3.34297676	0.00000000
F	-0.15131495	-2.34268528	2.35489200
F	1.69033887	-0.34210084	2.35489200

28
C6H5-OCF3...perfluorobenzene Dimer

C	1.23426631	-1.45596286	-0.37799875
C	1.80133388	-0.66451670	-1.36943358
C	1.43729478	-1.19422047	0.97085041
C	2.81257471	0.70267160	0.34433298
C	2.23452416	-0.10364776	1.31907109
C	2.59242045	0.41738150	-1.00250576
H	0.99638738	-1.80957213	1.74053159
H	1.61384158	-0.90887514	-2.40661729
H	2.39893429	0.10886113	2.36778178
H	3.03619758	1.03666753	-1.77162042
C	-0.15450072	-3.36772518	-0.03944999
O	0.46102237	-2.51175398	-0.87103714
F	-1.04189030	-2.75977670	0.76881905
F	0.70626284	-4.03255279	0.75266793
F	-0.80991321	-4.25855530	-0.77835430
H	3.42873801	1.54534722	0.62978774
C	-1.64197355	0.62474126	-0.35471027
C	-1.06904698	1.42408223	-1.33412684
C	-0.27818392	2.50573669	-0.97218304
C	-0.06024630	2.78805175	0.36917785
C	-0.63317287	1.98871078	1.34859443
C	-1.42403593	0.90705632	0.98665063
F	-2.40050953	-0.41269981	-0.70185937
F	-1.27807640	1.15330677	-2.62065784
F	0.27132378	3.27240387	-1.91156442
F	0.69828968	3.82549282	0.71632695
F	-0.42414345	2.25948624	2.63512542
F	-1.97354362	0.14038914	1.92603200

25
C6H5-OH...perfluorobenzene Dimer

C	0.32759702	-2.54236752	-0.00059936
C	0.88831564	-2.13721399	1.20968451
C	0.88816763	-2.13373126	-1.20919258
C	2.58485772	-0.90412744	-0.00035044
C	2.01607793	-1.31514386	-1.20229521
C	2.01318775	-1.32081068	1.20248156
H	0.44780803	-2.45193440	-2.14865639
H	2.44752557	-1.00061547	-2.14477688
H	2.44655732	-1.00768454	2.14456360
H	0.43251191	-2.46939138	2.13344152
O	-0.77740132	-3.34442536	0.05929475
H	-1.07585286	-3.55970711	-0.83267046
H	3.46080500	-0.26839780	0.00106215
C	-1.72607336	0.29178555	0.00403510
C	-1.16518292	0.70064408	-1.19791509
C	-0.04188110	1.51589685	-1.19779122
C	0.52053188	1.92229227	0.00428284
C	-0.04035856	1.51343375	1.20623304
C	-1.16366038	0.69818097	1.20610917
F	-2.80345943	-0.49014320	0.00391630
F	-1.70460691	0.31086033	-2.35085266
F	0.49608259	1.90804303	-2.35060998
F	1.59791795	2.70422102	0.00440165
F	0.49906543	1.90321749	2.35917060
F	-1.70162407	0.30603480	2.35892793

28
C6H5-OMe...perfluorobenzene Dimer

C	0.87173112	-2.19960963	-0.17085266
C	1.06614663	-1.86071297	1.16837067
C	1.59132128	-1.53901851	-1.17226568
C	2.70251443	-0.19771154	0.50470173
C	2.49842769	-0.54667609	-0.83299997
C	1.98410010	-0.85838011	1.49286962
H	0.52108052	-2.35797033	1.95820561
H	2.13052985	-0.59983293	2.53463139
H	3.05061631	-0.04120078	-1.61589458
H	1.41901887	-1.82373407	-2.20227614
O	0.00470319	-3.15865535	-0.60097213
C	-0.74594054	-3.85428950	0.37807416
H	-1.38415077	-3.16890822	0.94149959
H	-0.08858304	-4.39496674	1.06368136
H	-1.36394535	-4.56173717	-0.16787600
H	3.41109162	0.57721443	0.76738289
C	-1.65940992	0.20587989	-0.40959880
C	-0.94694545	0.85950048	-1.40540108
C	-0.03801494	1.85338397	-1.07001323
C	0.15845241	2.19364830	0.26117737
C	-0.55401206	1.54002771	1.25697965
C	-1.46294257	0.54614423	0.92159180
F	-2.53118725	-0.74737791	-0.73127744

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F                    -1.13538227     0.53314455    -2.68217749
F                     0.64532688     2.48028727    -2.02511053
F                     1.03022975     3.14690611     0.58285601
F                    -0.36557523     1.86638365     2.53375606
F                    -2.14628439    -0.08075908     1.87668910



   28
C6H5-SCH3...perfluorobenzene Dimer
C                     1.01589252    -1.98473404    -0.04283796
C                     1.12041429    -1.59717815     1.29434174
C                     1.77394617    -1.31255786    -1.01111247
C                     2.72397528     0.11453446     0.69153134
C                     2.61887157    -0.27352475    -0.64484174
C                     1.97234071    -0.55173457     1.65268027
H                     0.54832937    -2.09660010     2.06424363
H                     2.04297878    -0.26215106     2.69435354
H                     3.19767170     0.23528543    -1.40619517
H                     1.69681494    -1.60922117    -2.05108648
S                    -0.02564292    -3.29247127    -0.62863212
C                    -0.81068337    -3.88533978     0.88900793
H                    -1.41009928    -3.10559883     1.35814857
H                    -0.07480091    -4.27402577     1.59241999
H                    -1.46807075    -4.69801739     0.58275582
H                     3.38309819     0.92488739     0.97629689
C                    -1.62313196     0.34438733    -0.50487125
C                    -0.87713100     1.00292366    -1.47247661
C                    -0.03171274     2.04195991    -1.10899937
C                     0.06770577     2.42246133     0.22208375
C                    -0.67829519     1.76392501     1.18968911
C                    -1.52371345     0.72488875     0.82621187
F                    -2.43399315    -0.65217759    -0.85349111
F                    -0.97248597     0.63797536    -2.74914995
F                     0.68379470     2.67357803    -2.03705233
F                     0.87856696     3.41902625     0.57070361
F                    -0.58294022     2.12887330     2.46636245
F                    -2.23922089     0.09327063     1.75426483



   25
C6H5-SH...perfluorobenzene Dimer
C                     0.78421120    -2.26867743    -0.01573676
C                     1.27451956    -1.78182088     1.19908910
C                     1.28765232    -1.76190040    -1.21527148
C                     2.76249254    -0.29062236     0.01310707
C                     2.27240107    -0.77727867    -1.19579645
C                     2.25811957    -0.79832059     1.20888209
H                     0.91579636    -2.13106235    -2.16368216
H                     2.65488930    -0.39218322    -2.13302560
H                     2.63058682    -0.42854422     2.15616064
H                     0.88695597    -2.17198119     2.13271314
S                    -0.47009142    -3.52306383     0.04679868
H                    -0.61000473    -3.65923651    -1.27989092
H                     3.52779773     0.47459618     0.02395239
C                    -1.71834272     0.24921499    -0.00820577
C                    -1.22054727     0.75033342    -1.20299766
C                    -0.23910455     1.73166388    -1.18868799
C                     0.24454414     2.21187733     0.02041360
C                    -0.25325132     1.71075891     1.21520549
C                    -1.23469404     0.72942844     1.20089582
F                    -2.65966829    -0.69200291    -0.02193053
F                    -1.68442651     0.28974899    -2.36267550
F                     0.23834319     2.21229877    -2.33464105
F                     1.18586970     3.15309523     0.03413836
F                     0.21062792     2.17134333     2.37488333
F                    -1.71214178     0.24879356     2.34684888



   27
C6H5-SiF3...perfluorobenzene Dimer
C                     1.11306383    -1.71135991     0.00316285
C                     1.57755036    -1.17758613     1.21293200
C                     1.59035257    -1.18406781    -1.20449137
C                     2.95567250     0.39058470     0.00725393
C                     2.50646891    -0.13634855    -1.20203894
C                     2.49370724    -0.12985816     1.21451552
Si                   -0.10743584    -3.07579031     0.00031288
F                    -1.62557705    -2.57752110    -0.01725311
F                     0.04795376    -3.98408607     1.30508252
F                     0.07179241    -4.00078054    -1.28958985
H                     1.25302244    -1.59596122    -2.14867726
H                     1.23018923    -1.58441855     2.15565500
H                     2.87141504     0.26468409    -2.13906118
H                     2.84875855     0.27618980     2.15317849
H                     3.66954473     1.20490732     0.00883492
C                    -1.69535198     0.77016728    -0.00432552
C                    -1.23491111     1.29175739    -1.20531911
C                    -0.31997360     2.33546678    -1.20328771
C                     0.13452436     2.85758756    -0.00026271
C                    -0.32591650     2.33599744     1.20073088
C                    -1.24085402     1.29228805     1.19869948
F                    -2.57289078    -0.23087976    -0.00627389
F                    -1.67083118     0.79097864    -2.35916875
F                     0.12164645     2.83573656    -2.35518898
F                     1.01206316     3.85863459     0.00168566
F                     0.11000357     2.83677620     2.35458052
F                    -1.68247406     0.79201827     2.35060075



   27
C6H5-SiH3...perfluorobenzene Dimer
C                     0.83044763    -2.24659147     0.00338308
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C                     1.32024596    -1.72324510     1.20726180
C                     1.33322919    -1.72937855    -1.19782744
C                     2.78099837    -0.22335498     0.00872842
C                     2.30161692    -0.72776572    -1.19830765
C                     2.28861459    -0.72157488     1.21305754
Si                   -0.45053150    -3.61767611    -0.00005133
H                     0.19090058    -4.96207599    -0.00084544
H                    -1.30078997    -3.51009620     1.21696595
H                    -1.29775105    -3.50767229    -1.21898539
H                     0.96423534    -2.10706568    -2.14559007
H                     0.94102366    -2.09611795     2.15287594
H                     2.67776114    -0.33953661    -2.13704177
H                     2.65459959    -0.32852816     2.15379934
H                     3.53203427     0.55715023     0.01077405
C                    -1.70983020     0.23603181    -0.00540668
C                    -1.22443168     0.73521743    -1.20609384
C                    -0.26110760     1.73443903    -1.20345392
C                     0.21681935     2.23447646    -0.00012684
C                    -0.26857918     1.73529085     1.20056032
C                    -1.23190326     0.73606925     1.19792040
F                    -2.63377774    -0.72234591    -0.00793869
F                    -1.68282305     0.25561934    -2.36023321
F                     0.20444995     2.21322011    -2.35506127
F                     1.14076688     3.19285418     0.00240517
F                     0.18981220     2.21488893     2.35469968
F                    -1.69746081     0.25728817     2.34952775
C                    -0.56264807    -1.52765949     1.29595594
F                     1.03033793    -3.14691450     0.67407831
F                     0.65655361    -2.55330948    -1.95307580
F                    -1.12722447    -0.63105876    -2.67218274
F                    -2.53721692     0.69758554    -0.76413506
F                    -2.16343260     0.10398052     1.86301905
F                    -0.37965452    -1.81827021     2.58212600
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   28
C6H5-CH2OH...perfluorobenzene Dimer
C                     2.72659697     0.23609672     0.51439671
C                     2.00119084     0.92050309     1.48498362
C                     2.53341428     0.54206717    -0.83272456
C                     0.89079326     2.21441176    -0.22568369
C                     1.62044775     1.52568555    -1.19791052
C                     1.08525139     1.90730199     1.11889993
H                     3.09291048     0.01533057    -1.59608303
H                     2.14607278     0.68812397     2.53304964
C                    -0.09046744     3.27490909    -0.66101453
H                    -0.83814141     2.82275190    -1.32206384
H                     0.44248084     4.04639124    -1.22778618
H                     1.47286372     1.76099946    -2.24736346
H                     0.51901229     2.44213747     1.86873463
H                     3.43671636    -0.52925886     0.80210548
O                    -0.71569455     3.84132882     0.48014966
H                    -1.34016623     4.51684479     0.19508122
C                     0.15705814    -2.20584301     0.32202692
C                    -0.03373394    -1.90284730    -1.01895766
C                    -0.94423093    -0.92166947    -1.38601268
C                    -1.66393714    -0.24348595    -0.41208366
C                    -1.47314505    -0.54648167     0.92890091
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H-X···C_6H_6 Dimers

14
H-H...benzene Dimer

C	0.3172112	-0.5430211	1.2070613
C	-0.0089199	0.8120809	1.2070613
C	0.4802767	-1.2205720	0.0000000
C	-0.0089199	0.8120809	-1.2070613
C	0.3172112	-0.5430211	-1.2070613
C	-0.1719854	1.4896318	0.0000000
H	0.4439287	-1.0695431	2.1450636
H	-0.1356374	1.3386029	2.1450636
H	-0.4254204	2.5426759	0.0000000
H	-0.1356374	1.3386029	-2.1450636
H	0.4439287	-1.0695431	-2.1450636
H	0.7337118	-2.2736161	0.0000000
H	-3.1552462	-3.2095678	0.0000000
H	-3.3283512	-2.4903020	0.0000000

16
H-BF2...benzene Dimer

F	0.0439425	3.4777580	1.1345510
F	0.0439425	3.4777580	-1.1345510
B	0.5434198	2.9878311	0.0000000
C	0.8778294	-2.8731792	0.0000000
C	0.3803163	-2.3851791	-1.2070584
C	-0.6147098	-1.4091789	-1.2070584
C	-1.1122228	-0.9211788	0.0000000
C	-0.6147098	-1.4091789	1.2070584
C	0.3803163	-2.3851791	1.2070584
H	1.6509528	-3.6315197	0.0000000
H	0.7668780	-2.7643493	-2.1449284
H	-1.0012715	-1.0300086	-2.1449284
H	-1.8853462	-0.1628382	0.0000000
H	-1.0012715	-1.0300086	2.1449284
H	0.7668780	-2.7643493	2.1449284
H	1.3905961	2.1568537	0.0000000

16
H-CCH...benzene Dimer

C	-0.7821343	3.4439793	0.0000000
C	0.0434238	4.3255255	0.0000000
C	1.0796103	-0.2735384	0.0000000
C	0.6032486	-0.7822062	-1.2070584
C	-0.3494748	-1.7995417	-1.2070584
C	-0.8258364	-2.3082095	0.0000000
C	-0.3494748	-1.7995417	1.2070584
C	0.6032486	-0.7822062	1.2070584
H	1.8198649	0.5169191	0.0000000
H	0.9733759	-0.3869774	-2.1449284
H	-0.7196021	-2.1947705	-2.1449284
H	-1.5660911	-3.0986671	0.0000000
H	-0.7196021	-2.1947705	2.1449284
H	0.9733759	-0.3869774	2.1449284
H	0.7718709	5.1033747	0.0000000
H	-1.5110081	2.6656744	0.0000000

17
H-CF3...benzene Dimer

C	-0.0001136	2.6033790	0.3641009
F	-1.0964285	3.3871077	0.3678682
F	0.0222056	1.9769062	-0.8336019
F	1.0743950	3.4162415	0.3930817
C	-0.0000113	-3.2102122	0.9877744
C	-1.2070720	-2.7539391	0.4610175
C	-1.2070765	-1.8416509	-0.5927299
C	-0.0000203	-1.3856357	-1.1197204
C	1.2070403	-1.8419088	-0.5929635
C	1.2070448	-2.7541970	0.4607839
H	-0.0000078	-3.9190492	1.8065236
H	-2.1449402	-3.1082574	0.8704828
H	-2.1449482	-1.4871322	-1.0020137
H	-0.0000238	-0.6767987	-1.9384696
H	2.1449086	-1.4875904	-1.0024288
H	2.1449166	-3.1087157	0.8700677
H	-0.0001982	1.8983789	1.1860591

17
H-CH3...benzene Dimer

C	-0.0000127	3.9409218	0.5540618
H	-0.8902255	4.5689066	0.6153991
H	0.0120953	3.4763276	-0.4357087
H	0.8783975	4.5837451	0.6300702
C	-0.0001086	-1.9123931	0.8669585
C	-1.2071134	-1.4255934	0.3681411
C	-1.2070061	-0.4521262	-0.6293633
C	0.0001060	0.0345412	-1.1280503
C	1.2071107	-0.4522586	-0.6292329
C	1.2070034	-1.4257258	0.3682715
H	-0.0001920	-2.6687655	1.6420075
H	-2.1450251	-1.8037281	0.7556149
H	-2.1448344	-0.0738885	-1.0169385
H	0.0001893	0.7909136	-1.9030993
H	2.1450224	-0.0741238	-1.0167067
H	2.1448318	-1.8039634	0.7558467
H	-0.0001331	3.1837104	1.3343582

16
H-CHO...benzene Dimer

C	-0.5045020	3.4082737	-0.5537152
O	0.4222865	3.9964288	-0.0416273
H	-1.5422988	3.6142410	-0.2360816
C	0.1582100	-2.3568813	-0.8762593
C	1.2974598	-1.7427431	-0.3589611
C	1.1769202	-0.7819346	0.6435211
C	-0.0828693	-0.4352642	1.1287051
C	-1.2221191	-1.0494024	0.6114069
C	-1.1015795	-2.0102109	-0.3910753
H	0.2518679	-3.1034180	-1.6551760
H	2.2763012	-2.0121018	-0.7359432
H	2.0621037	-0.3047565	1.0454557
H	-0.1765272	0.3112725	1.9076218
H	-2.2009606	-0.7800437	0.9883891
H	-1.9867630	-2.4873890	-0.7930098
H	-0.3986248	2.6514179	-1.3445076

15
H-CN...benzene Dimer

C	-0.7219643	3.4370631	0.0000000
N	0.0726297	4.2769415	0.0000000
C	-0.8263385	-2.2752798	0.0000000
C	-0.3473957	-1.7690416	1.2070584
C	0.6104901	-0.7565653	1.2070584
C	1.0894329	-0.2503272	0.0000000
C	0.6104901	-0.7565653	-1.2070584
C	-0.3473957	-1.7690416	-1.2070584
H	-1.5706043	-3.0619618	0.0000000
H	-0.7195286	-2.1623827	2.1449284
H	0.9826230	-0.3632243	2.1449284
H	1.8336988	0.5363548	0.0000000
H	0.9826230	-0.3632243	-2.1449284
H	-0.7195286	-2.1623827	-2.1449284
H	-1.4570777	2.6600550	0.0000000

19
H-COCH3...benzene Dimer

C	0.1465015	-2.9713785	-0.5333791
O	1.2027267	-3.3639114	-0.0754099
C	-1.1670666	-3.5215111	-0.0249433
H	-1.7270347	-3.9931356	-0.8357102
H	-1.7855081	-2.7217479	0.3888753
H	-0.9549634	-4.2563587	0.7481172
C	-0.0066070	0.9134626	1.1230100
C	1.2128767	1.4099250	0.6658032
C	1.2394909	2.3772922	-0.3372649
C	0.0466216	2.8481971	-0.8831262
C	-1.1728621	2.3517348	-0.4259194
C	-1.1994764	1.3843675	0.5771487
H	-0.0272860	0.1618298	1.9023820
H	2.1397220	1.0440375	1.0899310
H	2.1870152	2.7630375	-0.6925091
H	0.0673005	3.5998300	-1.6624982
H	-2.0997074	2.7176223	-0.8500471
H	-2.1470007	0.9986222	0.9323930
H	0.1297288	-2.2080796	-1.3266513

20
H-COOCH3...benzene Dimer

C	0.4863046	2.4315008	-0.7114219
O	1.4773354	2.8211469	-0.1343969
O	-0.7367086	2.9371220	-0.4809806
C	-0.7852830	3.9786779	0.5041484
H	-1.8295298	4.2689803	0.5657924
H	-0.4281385	3.6027235	1.4610624
H	-0.1656569	4.8166920	0.1905018
C	-0.1013878	-1.3405875	1.0868540
C	-1.2698177	-1.7547502	0.4497559
C	-1.2205728	-2.7669350	-0.5071716
C	-0.0028980	-3.3649570	-0.8270011
C	1.1655320	-2.9507943	-0.1899030
C	1.1162871	-1.9386096	0.7670246
H	-0.1396505	-0.5541320	1.8303753
H	-2.2159366	-1.2900942	0.6982596
H	-2.1284290	-3.0887345	-1.0021893
H	0.0353648	-4.1514125	-1.5705224
H	2.1116509	-3.4154503	-0.4384066
H	2.0241433	-1.6168101	1.2620422
H	0.4833960	1.6431120	-1.4652960

17
H-COOH...benzene Dimer

C	0.1028553	-2.9467461	0.5169227
O	1.1243068	-3.3926583	0.0461985
O	-1.1134694	-3.3581778	0.0987486
H	-0.9591835	-4.0222122	-0.5920092
C	-0.0077865	2.8205274	0.8843974
C	1.2055190	2.3492818	0.3859288
C	1.2181445	1.3825984	-0.6180717
C	0.0174647	0.8871606	-1.1236038
C	-1.1958407	1.3584062	-0.6251353
C	-1.2084663	2.3250896	0.3788653
H	-0.0175964	3.5716289	1.6644938
H	2.1384329	2.7342310	0.7787212
H	2.1608684	1.0164461	-1.0053759
H	0.0272746	0.1360591	-1.9037003

```
H       -2.1287547        0.9734570       -1.0179276
H       -2.1511902        2.6912418        0.7661694
H        0.0549946       -2.1917250        1.3013744


14
H-F...benzene Dimer
F       -0.4187881       -3.8617588        0.0000000
C        1.1722208       -0.0114667        0.0000000
C        0.6461457        0.4455981        1.2070584
C       -0.4060046        1.3597279        1.2070584
C       -0.9320797        1.8167927        0.0000000
C       -0.4060046        1.3597279       -1.2070584
C        0.6461457        0.4455981       -1.2070584
H        1.9897291       -0.7217346        0.0000000
H        1.0548998        0.0904642        2.1449284
H       -0.8147587        1.7148618        2.1449284
H       -1.7495880        2.5270606        0.0000000
H       -0.8147587        1.7148618       -2.1449284
H        1.0548998        0.0904642       -2.1449284
H       -1.1233009       -3.2496637        0.0000000


22
H-NCH3_2...benzene Dimer
N        0.3882151       -2.7677906        0.0000000
C        0.0907220       -3.4674554        1.2349280
H       -0.7369137       -4.1516503        1.0591355
H       -0.2231413       -2.7653732        2.0086125
H        0.9488095       -4.0411396        1.6108450
C        0.0907220       -3.4674554       -1.2349280
H       -0.2231413       -2.7653732       -2.0086125
H       -0.7369137       -4.1516503       -1.0591355
H        0.9488095       -4.0411396       -1.6108450
C       -1.1577623        1.0962280        0.0000000
C       -0.6377188        1.5601441       -1.2070584
C        0.4023682        2.4879762       -1.2070584
C        0.9224117        2.9518923        0.0000000
C        0.4023682        2.4879762        1.2070584
C       -0.6377188        1.5601441        1.2070584
H       -1.9658975        0.3753136        0.0000000
H       -1.0417864        1.1996869       -2.1449284
H        0.8064358        2.8484335       -2.1449284
H        1.7305468        3.6728068        0.0000000
H        0.8064358        2.8484335        2.1449284
H       -1.0417864        1.1996869        2.1449284
H        1.1528542       -2.1163127        0.0000000


16
H-NH2...benzene Dimer
H        0.4435332        4.3292393        0.8344900
H        0.4435332        4.3292393       -0.8344900
N        0.5091224        3.7669005        0.0000000
C       -1.1334490        0.0661030        0.0000000
C       -0.6347394       -0.4206742        1.2070584
C        0.3626798       -1.3942287        1.2070584
C        0.8613893       -1.8810060        0.0000000
C        0.3626798       -1.3942287       -1.2070584
C       -0.6347394       -0.4206742       -1.2070584
H       -1.9084318        0.8225433        0.0000000
H       -1.0222308       -0.0424541        2.1449284
H        0.7501712       -1.7724488        2.1449284
H        1.6363721       -2.6374462        0.0000000
H        0.7501712       -1.7724488       -2.1449284
H       -1.0222308       -0.0424541       -2.1449284
H        1.2557995        3.0937041        0.0000000


19
H-NHCH3...benzene Dimer
N        0.6052095        3.1426292       -0.4683775
H        1.5268831        3.5459581       -0.4282726
C       -0.4686574        4.0321496       -0.0780823
H       -0.0883991        4.7271787        0.6686312
H       -1.2811886        3.4649757        0.3796073
H       -0.8748773        4.6040414       -0.9218307
C        0.1188570       -0.6071629        1.1433595
C       -1.1511565       -0.9206837        0.6622944
C       -1.2981912       -1.8614892       -0.3555067
C       -0.1752123       -2.4887739       -0.8922428
C        1.0948013       -2.1752531       -0.4111778
C        1.2418359       -1.2344476        0.6066234
H        0.2331012        0.1238317        1.9341789
H       -2.0236978       -0.4332909        1.0793320
H       -2.2849766       -2.1050910       -0.7292886
H       -0.2894565       -3.2197685       -1.6830622
H        1.9673425       -2.6626459       -0.8282153
H        2.2286214       -0.9908457        0.9804052
H        0.4776458        2.4873306       -1.2188356


17
H-NHOH...benzene Dimer
N        0.6184157        3.1790370       -0.3838323
H        1.4096138        3.7884524       -0.5549207
O       -0.4803230        4.0295795       -0.1572175
H       -0.7518766        3.8207461        0.7453577
C       -0.1933769       -2.4574661       -0.9191097
C        1.0803986       -2.1543535       -0.4413314
C        1.2354907       -1.2358861        0.5954991
C        0.1168073       -0.6205314        1.1545512
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C       -1.1569682       -0.9236440        0.6767730
C       -1.3120603       -1.8421114       -0.3600576
H       -0.3138816       -3.1711043       -1.7247147
H        1.9496023       -2.6324768       -0.8757083
H        2.2251991       -1.0003712        0.9667271
H        0.2373120        0.0931068        1.9601562
H       -2.0261719       -0.4455207        1.1111498
H       -2.3017687       -2.0776262       -0.7312856
H        0.4682438        2.5566932       -1.1669369


15
H-NO...benzene Dimer
N        0.5770619        3.3095052       -0.4914911
O       -0.4236091        3.8261706       -0.0609049
C        0.0857262       -0.3778691        1.1291211
C       -1.1697581       -0.7310820        0.6375386
C       -1.2802583       -1.6931251       -0.3649164
C       -0.1352743       -2.3019553       -0.8757890
C        1.1202099       -1.9487425       -0.3842065
C        1.2307102       -0.9866994        0.6182485
H        0.1715836        0.3696269        1.9080167
H       -2.0593970       -0.2580282        1.0344805
H       -2.2557546       -1.9675673       -0.7468702
H       -0.2211317       -3.0494513       -1.6546846
H        2.0098488       -2.4217963       -0.7811484
H        2.2062065       -0.7122572        1.0002023
H        0.4146960        2.5954792       -1.2436811


16
H-NO2...benzene Dimer
O       -0.0430560        3.3252244        1.0779960
O       -0.0430560        3.3252244       -1.0779960
N       -0.4532710        2.9386589        0.0000000
C        1.1379356       -0.8519730        0.0000000
C        0.6307532       -1.3299158       -1.2070584
C       -0.3836117       -2.2858014       -1.2070584
C       -0.8907941       -2.7637442        0.0000000
C       -0.3836117       -2.2858014        1.2070584
C        0.6307532       -1.3299158        1.2070584
H        1.9260851       -0.1092613        0.0000000
H        1.0248279       -0.9585600       -2.1449284
H       -0.7776864       -2.6571573       -2.1449284
H       -1.6789435       -3.5064559        0.0000000
H       -0.7776864       -2.6571573        2.1449284
H        1.0248279       -0.9585600        2.1449284
H       -1.2062945        2.2290480        0.0000000


18
H-OCF3...benzene Dimer
C       -0.0233340        2.6637272        0.1151640
O       -0.8554882        1.9002823        0.8416376
F        0.7807542        1.9401269       -0.6849643
F        0.7730311        3.4352214        0.8773711
F       -0.7616779        3.4612084       -0.6516446
C       -0.3541079       -1.6941214       -1.0450563
C        0.9927255       -1.9499549       -0.7935757
C        1.3554956       -2.9213427        0.1377980
C        0.3714322       -3.6368969        0.8176913
C       -0.9754011       -3.3810635        0.5662107
C       -1.3381712       -2.4096757       -0.3651630
H       -0.6359759       -0.9393647       -1.7687226
H        1.7573310       -1.3939778       -1.3218447
H        2.4019690       -3.1201222        0.3331954
H        0.6533002       -4.3916536        1.5413576
H       -1.7400066       -3.9370406        1.0944797
H       -2.3846447       -2.2108961       -0.5605604
H       -0.5158876        1.2488638        1.4666986


15
H-OH...benzene Dimer
O        0.0664761        3.8321015        0.4937551
H       -0.8280522        4.0809674        0.2312551
C       -0.0036432        0.0431464       -1.1518626
C        1.2083479       -0.4285453       -0.6506265
C        1.2183077       -1.3744203        0.3730310
C        0.0162763       -1.8486035        0.8954524
C       -1.1957148       -1.3769119        0.3942163
C       -1.2056746       -0.4310369       -0.6294412
H       -0.0113819        0.7780799       -1.9472323
H        2.1423120       -0.0601105       -1.0565417
H        2.1600105       -1.7409191        0.7624855
H        0.0240150       -2.5835371        1.6908221
H       -2.1296789       -1.7453466        0.8001315
H       -2.1473774       -0.0645381       -1.0188957
H        0.0311049        3.1799039        1.1999087


18
H-OMe...benzene Dimer
O        0.6650040       -3.2106439        0.5292241
C       -0.4797996       -3.8605144        0.0067325
H       -1.1741595       -3.1383915       -0.4302010
H       -0.9883199       -4.4399278        0.7814552
H       -0.1148082       -4.5294070       -0.7677594
C        0.0684030        0.5711090       -1.1455972
C       -1.1723513        0.8997381       -0.6022879
C       -1.2573358        1.8411561        0.4219987
C       -0.1015660        2.4539451        0.9029760
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C        1.1391884        2.1253159        0.3596667
C        1.2241728        1.1838979       -0.6646199
H        0.1344349       -0.1603616       -1.9414557
H       -2.0703707        0.4236085       -0.9760016
H       -2.2213871        2.0964970        0.8441435
H       -0.1675979        3.1854156        1.6988345
H        2.0372078        2.6014456        0.7333804
H        2.1882242        0.9285570       -1.0867647
H        0.5328740       -2.5720756        1.2354267
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18
H-SCH3...benzene Dimer
S        0.6561372       -2.9806860        0.2607837
C       -1.0435348       -3.5268922       -0.0286755
H       -1.6715321       -2.7070899       -0.3764280
H       -1.4727636       -3.9825681        0.8632384
H       -0.9815980       -4.2798344       -0.8132998
C        0.0367222        0.9814645       -1.1216011
C       -1.1876794        1.3375893       -0.5588675
C       -1.2389443        2.3042432        0.4439312
C       -0.0658074        2.9147725        0.8839965
C        1.1585942        2.5586477        0.3212629
C        1.2098591        1.5919937       -0.6815359
H        0.0765544        0.2303859       -1.9007638
H       -2.0991928        0.8632154       -0.9007929
H       -2.1902898        2.5809480        0.8811685
H       -0.1056396        3.6658511        1.6631591
H        2.0701076        3.0330216        0.6631883
H        2.1612046        1.3152890       -1.1187731
H        0.5099732       -2.0622698        1.2291673
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15
H-SH...benzene Dimer
S        0.0536782        3.4975344        0.2321510
H       -1.2740484        3.6304805        0.0991421
C       -0.0123139       -0.5181761       -1.1317430
C        1.2055639       -0.9883842       -0.6435511
C        1.2275170       -1.9488492        0.3662402
C        0.0315924       -2.4391061        0.8878395
C       -1.1862854       -1.9688979        0.3996476
C       -1.2082385       -1.0084329       -0.6101437
H       -0.0293712        0.2280938       -1.9163388
H        2.1347831       -0.6074605       -1.0488276
H        2.1737936       -2.3141954        0.7455595
H        0.0486497       -3.1853760        1.6724353
H       -2.1155046       -2.3498216        0.8049240
H       -2.1545151       -0.6430868       -0.9894630
H        0.0137439        2.5742965        1.2031150
```

```
17
H-SiF3...benzene Dimer
Si      -0.0001241        2.4185999       -0.3076051
F        0.0138481        1.7836320        1.1586671
F       -1.3043691        3.3378049       -0.3822911
F        1.2903544        3.3555990       -0.3985815
C        0.0001914       -1.6974365        1.0640328
C       -1.2069202       -2.1773617        0.5588529
C       -1.2070265       -3.1370752       -0.4518911
C       -0.0000213       -3.6168635       -0.9574550
C        1.2070902       -3.1369383       -0.4522751
C        1.2071966       -2.1772248        0.5584689
H        0.0002741       -0.9517505        1.8493688
H       -2.1447489       -1.8045718        0.9516700
H       -2.1449379       -3.5099713       -0.8444099
H       -0.0001040       -4.3625495       -1.7427910
H        2.1449189       -3.5097281       -0.8450922
H        2.1451079       -1.8043287        0.9509877
H       -0.0003447        1.4232420       -1.3771661
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17
H-SiH3...benzene Dimer
Si      -0.0000031        3.6249760       -0.2633734
H        0.0032990        2.9716256        1.0752711
H       -1.2196853        4.4723862       -0.3629493
H        1.2162627        4.4769085       -0.3662841
C        0.0000561       -0.5955579        1.1244962
C       -1.2070282       -1.0747463        0.6185523
C       -1.2070801       -2.0331615       -0.3934228
C       -0.0000476       -2.5123883       -0.8994541
C        1.2070367       -2.0331998       -0.3935102
C        1.2070886       -1.0747846        0.6184649
H        0.0000964        0.1491193        1.9107888
H       -2.1448781       -0.7023928        1.0117326
H       -2.1449703       -2.4054852       -0.7865351
H       -0.0000879       -3.2570654       -1.6857467
H        2.1448866       -2.4055533       -0.7866905
H        2.1449787       -0.7024609        1.0115773
H       -0.0000104        2.6211953       -1.3570848
```

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18
H-CH2OH...benzene Dimer
C       -0.6762112        3.2838253       -0.5035072
H       -1.1767533        2.8034674        0.3445274
H       -1.3311156        4.0774607       -0.8799269
O        0.5738150        3.8219494       -0.1011977
H        0.4282548        4.4724326        0.5939530
C        0.2144780       -2.4760529       -0.8867296
```

C	1.3257015	-1.8269583	-0.3514616
C	1.1603125	-0.8784234	0.6562990
C	-0.1163001	-0.5789833	1.1287917
C	-1.2275236	-1.2280779	0.5935237
C	-1.0621346	-2.1766127	-0.4142369
H	0.3429833	-3.2130531	-1.6697476
H	2.3176142	-2.0596197	-0.7185828
H	2.0237199	-0.3740847	1.0721958
H	-0.2448054	0.1580170	1.9118097
H	-2.2194364	-0.9954164	0.9606449
H	-1.9255420	-2.6809515	-0.8301338
H	-0.5204724	2.5488933	-1.2878065

F-X···C_6H_6 Dimers

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14
F-H...benzene Dimer
C       -0.7056126       -0.5160857        1.2070613
C        0.5526843       -1.1155450        1.2070613
C       -1.3347611       -0.2163560        0.0000000
C        0.5526843       -1.1155450       -1.2070613
C       -0.7056126       -0.5160857       -1.2070613
C        1.1818328       -1.4152747        0.0000000
H       -1.1945212       -0.2831670        2.1450636
H        1.0415930       -1.3484637        2.1450636
H        2.1596501       -1.8811121        0.0000000
H        1.0415930       -1.3484637       -2.1450636
H       -1.1945212       -0.2831670       -2.1450636
H       -2.3125784        0.2494813        0.0000000
H       -0.5922116        3.8606222        0.0000000
F        0.2494562        3.4596472        0.0000000


16
F-BF2...benzene Dimer
F       -0.2911978        3.2389880        1.1345510
F       -0.2911978        3.2389880       -1.1345510
B        0.2341500        2.7769104        0.0000000
C        0.8863728       -3.0572885        0.0000000
C        0.3630911       -2.5970281       -1.2070584
C       -0.6834723       -1.6765074       -1.2070584
C       -1.2067540       -1.2162471        0.0000000
C       -0.6834723       -1.6765074        1.2070584
C        0.3630911       -2.5970281        1.2070584
H        1.6995401       -3.7725221        0.0000000
H        0.7696748       -2.9546450       -2.1449284
H       -1.0900559       -1.3188906       -2.1449284
H       -2.0199213       -0.5010134        0.0000000
H       -1.0900559       -1.3188906        2.1449284
H        0.7696748       -2.9546450        2.1449284
F        1.2189983        1.9106722        0.0000000


16
F-CCH...benzene Dimer
C        0.2592683        3.1588229        0.0000000
C       -0.6540566        3.9490807        0.0000000
C       -1.2029887       -0.7331992        0.0000000
C       -0.6759840       -1.1891919        1.2070584
C        0.3780253       -2.1011775        1.2070584
C        0.9050300       -2.5571703        0.0000000
C        0.3780253       -2.1011775       -1.2070584
C       -0.6759840       -1.1891919       -1.2070584
H       -2.0219414       -0.0245973        0.0000000
H       -1.0854604       -0.8348910        2.1449284
H        0.7875016       -2.4554785        2.1449284
H        1.7239826       -3.2657722        0.0000000
H        0.7875016       -2.4554785       -2.1449284
H       -1.0854604       -0.8348910       -2.1449284
H       -1.4599464        4.6463799        0.0000000
F        1.2306625        2.3183204        0.0000000


17
F-CF3...benzene Dimer
C       -0.0001032        2.4461980        0.1488924
F       -1.0964096        3.2295984        0.1254967
F        0.0224085        1.7788691       -1.0265325
F        1.0744101        3.2595700        0.1500554
C       -0.0001730       -3.3424800        0.9723111
C       -1.2071403       -2.9046021        0.4299587
C       -1.2069583       -2.0291265       -0.6545669
C        0.0001911       -1.5915288       -1.1967401
C        1.2071585       -2.0294066       -0.6543878
C        1.2069765       -2.9048822        0.4301378
H       -0.0003144       -4.0227141        1.8149746
H       -2.1450811       -3.2446103        0.8512209
H       -2.1447576       -1.6889006       -1.0759682
H        0.0003326       -0.9112946       -2.0394036
H        2.1450992       -1.6893984       -1.0756499
H        2.1447757       -3.2451081        0.8515392
F       -0.0003803        1.6316682        1.1675091


17
F-CH3...benzene Dimer
C        0.0001301        3.5536519       -0.2542091
H       -0.8900614        4.1830430       -0.2992877
H        0.0124096        2.9295780       -1.1519957
H        0.8785594        4.2000986       -0.2869527
C       -0.0003396       -2.1641888        1.0363323
C       -1.2072195       -1.7679591        0.4626632
C       -1.2068626       -0.9756549       -0.6840309
C        0.0003742       -0.5795803       -1.2570557
C        1.2072541       -0.9758100       -0.6833866
C        1.2068972       -1.7681142        0.4633075
H       -0.0006170       -2.7797998        1.9272999
H       -2.1452282       -2.0757044        0.9078967
H       -2.1445939       -0.6677892       -1.1297649
H        0.0006515        0.0360306       -2.1480233
H        2.1452628       -0.6680647       -1.1286201
H        2.1446285       -2.0759799        0.9090415
F       -0.0002698        2.7734590        0.8817892
```

16
F-CHO...benzene Dimer

C	0.3813085	-3.1286444	0.0095214
O	-0.6776737	-3.6411525	0.2976008
H	1.2845799	-3.3337351	0.6114968
C	0.1278469	2.5990761	-0.9440027
C	-1.1383282	2.0671517	-0.7062837
C	-1.3396000	1.1991880	0.3655288
C	-0.2746967	0.8631488	1.1996224
C	0.9914784	1.3950733	0.9619034
C	1.1927502	2.2630369	-0.1099092
H	0.2842328	3.2734735	-1.7767883
H	-1.9657453	2.3282501	-1.3543644
H	-2.3234030	0.7858890	0.5502337
H	-0.4310825	0.1887514	2.0324079
H	1.8188955	1.1339748	1.6099841
H	2.1765532	2.6763359	-0.2946140
F	0.5602434	-2.3036068	-1.0138249

15
F-CN...benzene Dimer

C	-0.2112777	3.1459753	0.0000000
N	0.6650529	3.9001769	0.0000000
C	-0.8993705	-2.5257338	0.0000000
C	-0.3711607	-2.0711375	1.2070584
C	0.6852588	-1.1619449	1.2070584
C	1.2134686	-0.7073486	0.0000000
C	0.6852588	-1.1619449	-1.2070584
C	-0.3711607	-2.0711375	-1.2070584
H	-1.7201959	-3.2321655	0.0000000
H	-0.7815734	-2.4243534	2.1449284
H	1.0956715	-0.8087290	2.1449284
H	2.0342940	-0.0009168	0.0000000
H	1.0956715	-0.8087290	-2.1449284
H	-0.7815734	-2.4243534	-2.1449284
F	-1.1744521	2.3170328	0.0000000

19
F-COCH3...benzene Dimer

C	0.1270222	-2.7585814	-0.2083701
O	1.1649068	-3.1271513	0.3077512
C	-1.2062688	-3.2702285	0.2887881
H	-1.7423605	-3.7881996	-0.5097409
H	-1.8326224	-2.4436323	0.6319451
H	-1.0247213	-3.9571190	1.1120944
C	-0.0544707	1.2214666	1.2006494
C	1.1827389	1.6831383	0.7547512
C	1.2489225	2.5868373	-0.3043055
C	0.0778965	3.0288647	-0.9174640
C	-1.1593130	2.5671930	-0.4715659
C	-1.2254966	1.6634939	0.5874909
H	-0.1058945	0.5193032	2.0235239
H	2.0926121	1.3396883	1.2311681
H	2.2102196	2.9455507	-0.6507631
H	0.1293204	3.7310280	-1.7403385
H	-2.0691862	2.9106430	-0.9479828
H	-2.1867937	1.3047806	0.9339484
F	0.1446479	-1.8935303	-1.2257501

20
F-COOCH3...benzene Dimer

C	0.4875956	2.3051170	-0.3853265
O	1.3482838	2.6843641	0.3777670
O	-0.7671059	2.7844906	-0.3642994
C	-1.0163119	3.7845368	0.6334386
H	-2.0600141	4.0580304	0.5133811
H	-0.8323001	3.3749653	1.6248866
H	-0.3672484	4.6428278	0.4702474
C	-0.3407219	-1.5442861	1.1325060
C	-1.3643056	-1.9479804	0.2769589
C	-1.1201986	-2.9198156	-0.6918555
C	0.1474921	-3.4879566	-0.8051228
C	1.1710757	-3.0842623	0.0504242
C	0.9269688	-2.1124271	1.0192386
H	-0.5303902	-0.7891817	1.8852632
H	-2.3492862	-1.5065416	0.3649663
H	-1.9155110	-3.2334813	-1.3566053
H	0.3371603	-4.2430610	-1.5578801
H	2.1560563	-3.5257011	-0.0375832
H	1.7222811	-1.7987614	1.6839884
F	0.6696166	1.3931799	-1.3133754

17
F-COOH...benzene Dimer

C	0.0955944	-2.7353152	0.1997016
O	1.1071718	-3.1542881	-0.3150363
O	-1.1292082	-3.1184055	-0.2206456
H	-0.9892259	-3.7401163	-0.9526105
C	0.0095038	2.9997367	0.9141884
C	1.2123349	2.5567448	0.3668229
C	1.2041998	1.6520171	-0.6933916
C	-0.0067664	1.1902813	-1.2062408
C	-1.2095975	1.6332731	-0.6588754
C	-1.2014624	2.5380008	0.4013392
H	0.0158246	3.7026993	1.7379625
H	2.1532412	2.9155080	0.7653006
H	2.1387852	1.3078177	-1.1186881
H	-0.0130873	0.4873186	-2.0300149

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H       -2.1505038        1.2745099       -1.0573531
H       -2.1360479        2.8822002        0.8266356
F        0.0576175       -1.8869394        1.1949468


14
F-F...benzene Dimer
F        0.2362256       -3.4486249        0.0000000
C        1.2932635        0.5811058        0.0000000
C        0.7103368        0.9630218        1.2070584
C       -0.4555165        1.7268538        1.2070584
C       -1.0384432        2.1087698        0.0000000
C       -0.4555165        1.7268538       -1.2070584
C        0.7103368        0.9630218       -1.2070584
H        2.1991177       -0.0123826        0.0000000
H        1.1632639        0.6662776        2.1449284
H       -0.9084436        2.0235980        2.1449284
H       -1.9442974        2.7022581        0.0000000
H       -0.9084436        2.0235980       -2.1449284
H        1.1632639        0.6662776       -2.1449284
F       -0.9136553       -2.6952576        0.0000000


22
F-NCH3_2...benzene Dimer
N        0.1233569       -2.5658345        0.0000000
C       -0.2097281       -3.2492724        1.2349280
H       -1.0714584       -3.8899942        1.0591355
H       -0.4870660       -2.5319765        2.0086125
H        0.6177174       -3.8663311        1.6108450
C       -0.2097281       -3.2492724       -1.2349280
H       -0.4870660       -2.5319765       -2.0086125
H       -1.0714584       -3.8899942       -1.0591355
H        0.6177174       -3.8663311       -1.6108450
C       -1.2218372        1.3725839        0.0000000
C       -0.6786215        1.8091386       -1.2070584
C        0.4078098        2.6822482       -1.2070584
C        0.9510255        3.1188030        0.0000000
C        0.4078098        2.6822482        1.2070584
C       -0.6786215        1.8091386        1.2070584
H       -2.0659814        0.6941881        0.0000000
H       -1.1006936        1.4699408       -2.1449284
H        0.8298819        3.0214460       -2.1449284
H        1.7951697        3.7971987        0.0000000
H        0.8298819        3.0214460        2.1449284
H       -1.1006936        1.4699408        2.1449284
F        1.2150817       -1.7286376        0.0000000


16
F-NH2...benzene Dimer
H       -0.3283431        3.9275535        0.8344900
H       -0.3283431        3.9275535       -0.8344900
N       -0.1800233        3.3811761        0.0000000
C       -1.2551679       -0.5224128        0.0000000
C       -0.6897383       -0.9297857        1.2070584
C        0.4411208       -1.7445316        1.2070584
C        1.0065504       -2.1519045        0.0000000
C        0.4411208       -1.7445316       -1.2070584
C       -0.6897383       -0.9297857       -1.2070584
H       -2.1338321        0.1106351        0.0000000
H       -1.1290704       -0.6132618        2.1449284
H        0.8804529       -2.0610555        2.1449284
H        1.8852146       -2.7849524        0.0000000
H        0.8804529       -2.0610555       -2.1449284
H       -1.1290704       -0.6132618       -2.1449284
F        0.9636220        2.6241369        0.0000000


19
F-NHCH3...benzene Dimer
N        0.4712576        2.8939993        0.0304859
H        1.3367631        3.3205147        0.3181485
C       -0.7060230        3.7170249        0.2132594
H       -0.5471017        4.3619227        1.0758681
H       -1.5754558        3.0911433        0.4223808
H       -0.9282243        4.3413916       -0.6612570
C       -0.2012624       -0.9845682        1.2135356
C       -1.3048411       -1.2972044        0.4216858
C       -1.1614773       -2.1584995       -0.6647169
C        0.0854650       -2.7071584       -0.9592699
C        1.1890437       -2.3945222       -0.1674200
C        1.0456800       -1.5332271        0.9189827
H       -0.3126543       -0.3153522        2.0576576
H       -2.2737004       -0.8709029        0.6505499
H       -2.0189448       -2.4014141       -1.2799748
H        0.1968570       -3.3763744       -1.8033919
H        2.1579031       -2.8208237       -0.3962842
H        1.9031474       -1.2903126        1.5342406
F        0.5878763        2.0770184       -1.0676197


17
F-NHOH...benzene Dimer
N        0.4733379        2.9156796        0.1009272
H        1.2546159        3.5586310        0.1545107
O       -0.6852618        3.7149413        0.1297536
H       -1.1420271        3.4308846        0.9314219
C        0.0553073       -2.6852091       -0.9811970
C        1.1751707       -2.3827620       -0.2084842
C        1.0532613       -1.5411428        0.8958113
C       -0.1885114       -1.0019706        1.2273940
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C	-1.3083748	-1.3044176	0.4546812
C	-1.1864655	-2.1460368	-0.6496143
H	0.1500294	-3.3391372	-1.8392214
H	2.1400133	-2.8016924	-0.4661199
H	1.9233818	-1.3061450	1.4962000
H	-0.2832336	-0.3480424	2.0854184
H	-2.2732175	-0.8854872	0.7123169
H	-2.0565860	-2.3810346	-1.2500030
F	0.5503569	2.1477379	-1.0353991

15
F-NO...benzene Dimer

N	0.4406428	3.0396210	0.0698682
O	-0.6556122	3.4850724	0.3011429
C	-0.2232187	-0.7957774	1.2159624
C	-1.3160201	-1.1368996	0.4209314
C	-1.1494869	-2.0035797	-0.6578575
C	0.1098477	-2.5291377	-0.9416155
C	1.2026491	-2.1880155	-0.1465846
C	1.0361159	-1.3213354	0.9322044
H	-0.3526130	-0.1223773	2.0541686
H	-2.2945080	-0.7285473	0.6414081
H	-1.9985805	-2.2686275	-1.2755871
H	0.2392420	-3.2025378	-1.7798217
H	2.1811370	-2.5963678	-0.3670612
H	1.8852095	-1.0562875	1.5499339
F	0.5039826	2.1758499	-1.0381207

16
F-NO2...benzene Dimer

O	0.3026219	3.0845853	1.0779960
O	0.3026219	3.0845853	-1.0779960
N	-0.1309693	2.7244354	0.0000000
C	1.2200192	-1.1583032	0.0000000
C	0.6839348	-1.6035860	-1.2070584
C	-0.3882340	-2.4941518	-1.2070584
C	-0.9243184	-2.9394347	0.0000000
C	-0.3882340	-2.4941518	1.2070584
C	0.6839348	-1.6035860	1.2070584
H	2.0530816	-0.4663442	0.0000000
H	1.1004660	-1.2576065	-2.1449284
H	-0.8047652	-2.8401313	-2.1449284
H	-1.7573808	-3.6313937	0.0000000
H	-0.8047652	-2.8401313	2.1449284
H	1.1004660	-1.2576065	2.1449284
F	-1.1839281	1.8498259	0.0000000

18

F-OCF3...benzene Dimer

C	0.0794759	-2.5687440	0.0841730
O	-1.0164767	-1.8331213	-0.1624841
F	1.1562271	-1.8160012	0.3745959
F	0.4200061	-3.3574466	-0.9513693
F	-0.1759319	-3.3477420	1.1315757
C	0.2656334	1.8197171	1.1580080
C	1.3143559	2.0769256	0.2767145
C	1.1580945	3.0222683	-0.7354925
C	-0.0468895	3.7104025	-0.8664059
C	-1.0956120	3.4531939	0.0148876
C	-0.9393505	2.5078512	1.0270945
H	0.3870467	1.0851971	1.9444807
H	2.2506141	1.5422536	0.3784326
H	1.9729394	3.2221163	-1.4202470
H	-0.1683028	4.4449225	-1.6528786
H	-2.0318702	3.9878660	-0.0868306
H	-1.7541954	2.3080033	1.7118491
F	-1.0463297	-0.9262934	-1.2001036

15
F-OH...benzene Dimer

O	0.0540242	3.4378458	-0.1974040
H	-0.8455348	3.6441330	-0.4789366
C	-0.0255809	-0.5503349	-1.2731516
C	1.1960659	-0.9417271	-0.7281337
C	1.2259921	-1.7285942	0.4219089
C	0.0342715	-2.1240691	1.0269335
C	-1.1873753	-1.7326770	0.4819156
C	-1.2173015	-0.9458099	-0.6681270
H	-0.0488333	0.0610514	-2.1667210
H	2.1220187	-0.6344477	-1.1982307
H	2.1751972	-2.0327012	0.8453813
H	0.0575239	-2.7354555	1.9205029
H	-2.1133280	-2.0399564	0.9520126
H	-2.1665066	-0.6417029	-1.0915994
F	0.0228023	2.6533102	0.9505981

18
F-OMe...benzene Dimer

O	0.5176469	-2.9648369	-0.0338026
C	-0.7607398	-3.5281843	-0.2667652
H	-1.5060730	-2.7480332	-0.4409796
H	-1.0710521	-4.1546590	0.5733203
H	-0.6583596	-4.1398229	-1.1588920
C	-0.2986569	0.9651556	-1.1963091
C	-1.3243376	1.2875277	-0.3093431
C	-1.0744724	2.1395307	0.7650459
C	0.2010734	2.6691615	0.9524689

C	1.2267541	2.3467893	0.0655029
C	0.9768890	1.4947864	-1.0088861
H	-0.4927991	0.3031594	-2.0310966
H	-2.3154215	0.8760109	-0.4549686
H	-1.8714141	2.3900100	1.4542079
H	0.3952157	3.3311576	1.7872563
H	2.2178381	2.7583061	0.2111283
H	1.7738306	1.2443070	-1.6980481
F	0.6649101	-2.1202884	1.0742534

18
F-SCH3...benzene Dimer

S	0.5318102	-2.7882770	-0.1280299
C	-1.2080445	-3.2813540	-0.1561987
H	-1.8600351	-2.4303703	-0.3514504
H	-1.4966861	-3.7765691	0.7705355
H	-1.3001054	-3.9907699	-0.9775679
C	-0.1886946	1.2567042	-1.1826857
C	-1.2912574	1.6070072	-0.4053207
C	-1.1459729	2.5174316	0.6399894
C	0.1018744	3.0775530	0.9079345
C	1.2044372	2.7272499	0.1305694
C	1.0591527	1.8168255	-0.9147407
H	-0.3015789	0.5493153	-1.9948792
H	-2.2608199	1.1717996	-0.6135108
H	-2.0026510	2.7896129	1.2439928
H	0.2147588	3.7849419	1.7201279
H	2.1739997	3.1624576	0.3387595
H	1.9158309	1.5446443	-1.5187441
F	0.5863317	-1.7287501	1.1255718

15
F-SH...benzene Dimer

S	0.0526480	3.2022812	-0.2008085
H	-1.2757505	3.3238498	-0.3379307
C	-0.0190789	-0.9134936	-1.2234255
C	1.2013050	-1.3413903	-0.7035979
C	1.2284695	-2.2139600	0.3829276
C	0.0352500	-2.6586329	0.9496255
C	-1.1851340	-2.2307363	0.4297979
C	-1.2122984	-1.3581666	-0.6567276
H	-0.0401854	-0.2355174	-2.0676428
H	2.1284224	-0.9958847	-1.1439154
H	2.1766933	-2.5464306	0.7868275
H	0.0563565	-3.3366092	1.7938429
H	-2.1122513	-2.5762419	0.8701154
H	-2.1605223	-1.0256960	-1.0606274
F	0.0099619	2.1771227	1.0765237

17
F-SiF3...benzene Dimer

Si	-0.0001153	2.3083961	-0.1266175
F	0.0142745	1.6400134	1.3247236
F	-1.3043703	3.2290784	-0.1798528
F	1.2903485	3.2472254	-0.1964853
C	0.0005463	-1.8379746	1.1503929
C	-1.2067180	-2.3061967	0.6347047
C	-1.2071299	-3.2425099	-0.3977539
C	-0.0002776	-3.7106010	-0.9145243
C	1.2069866	-3.2423788	-0.3988361
C	1.2073986	-2.3060656	0.6336225
H	0.0008664	-1.1104704	1.9526009
H	-2.1444278	-1.9424956	1.0362291
H	-2.1451599	-3.6063130	-0.7984375
H	-0.0005977	-4.4381052	-1.7167323
H	2.1446965	-3.6060800	-0.8003605
H	2.1454286	-1.9422626	1.0343061
F	-0.0007003	1.2642546	-1.3014385

17
F-SiH3...benzene Dimer

Si	0.0000062	3.3257519	0.1986900
H	0.0033433	2.5594349	1.4760286
H	-1.2196760	4.1785924	0.1725704
H	1.2162719	4.1833835	0.1695701
C	0.0000905	-0.9987127	1.2175592
C	-1.2070093	-1.4325012	0.6722236
C	-1.2070922	-2.3001106	-0.4186051
C	-0.0000752	-2.7339315	-0.9640982
C	1.2070247	-2.3001430	-0.4187626
C	1.2071075	-1.4325337	0.6720661
H	0.0001549	-0.3245906	2.0651201
H	-2.1448471	-1.0954275	1.0960653
H	-2.1449944	-2.6371590	-0.8423244
H	-0.0001396	-3.4080536	-1.8116592
H	2.1448625	-2.6372167	-0.8426043
H	2.1450097	-1.0954852	1.0957854
F	-0.0000381	2.3393674	-1.0821763

18
F-CH2OH...benzene Dimer

C	-0.5075821	3.0468490	0.1669130
H	-0.6487996	2.5093663	1.1111686
H	-1.2078298	3.8892909	0.1470794
O	0.8290227	3.5106664	0.0557516
H	1.0199834	4.1020644	0.7915050
C	-0.2128124	-2.6814581	-0.9358072

C	1.0583511	-2.1146353	-0.8615881
C	1.3771172	-1.2531281	0.1866709
C	0.4247197	-0.9584437	1.1607107
C	-0.8464438	-1.5252666	1.0864916
C	-1.1652099	-2.3867738	0.0382326
H	-0.4604899	-3.3508390	-1.7502919
H	1.7983526	-2.3436015	-1.6184054
H	2.3647961	-0.8127135	0.2443383
H	0.6723972	-0.2890629	1.9751955
H	-1.5864453	-1.2963003	1.8433089
H	-2.1528888	-2.8271884	-0.0194348
F	-0.7863191	2.2128067	-0.8652457

H-X···C_6F_6 Dimers

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14
H-H...perfluorobenzene Dimer
H        3.4424315        2.4552290        0.0000000
C       -0.0734559       -0.7535963       -1.2020128
C       -0.0660348       -1.4475391        0.0000000
C       -0.0734559       -0.7535963        1.2020128
C       -0.0882982        0.6342892        1.2020128
C       -0.0957193        1.3282320        0.0000000
C       -0.0882982        0.6342892       -1.2020128
F       -0.0663382       -1.4191734       -2.3548921
F       -0.0517993       -2.7786933        0.0000000
F       -0.0663382       -1.4191734        2.3548921
F       -0.0954159        1.2998663        2.3548921
F       -0.1099548        2.6593862        0.0000000
F       -0.0954159        1.2998663       -2.3548921
H        3.4503482        1.7149407        0.0000000


16
H-BF2...perfluorobenzene Dimer
F        0.8247427        3.9685111        1.1345510
F        0.8247427        3.9685111       -1.1345510
B        1.1955450        3.3752054        0.0000000
C        0.4837020       -2.1841095        0.0000000
C        0.1159016       -1.5956069        1.2020130
C       -0.6196981       -0.4186035        1.2020130
C       -0.9874985        0.1698991        0.0000000
C       -0.6196981       -0.4186035       -1.2020130
C        0.1159016       -1.5956069       -1.2020130
F        1.1892336       -3.3130021        0.0000000
F        0.4686679       -2.1600541        2.3548920
F       -0.9724645        0.1458437        2.3548920
F       -1.6930301        1.2987917        0.0000000
F       -0.9724645        0.1458437       -2.3548920
F        0.4686679       -2.1600541       -2.3548920
H        1.8250374        2.3679800        0.0000000


16
H-CCH...perfluorobenzene Dimer
C       -1.8081330        3.4377550        0.0000000
C       -1.3063211        4.5363243        0.0000000
C        0.8198564        0.6468724        0.0000000
H       -0.8635377        5.5056680        0.0000000
C        0.5315121        0.0156276        1.2020130
C       -0.0451756       -1.2468602        1.2020130
C       -0.3335199       -1.8781050        0.0000000
C       -0.0451756       -1.2468602       -1.2020130
C        0.5315121        0.0156276       -1.2020130
F        1.3729716        1.8577551        0.0000000
F        0.8080701        0.6210699        2.3548920
F       -0.3217336       -1.8523024        2.3548920
F       -0.8866351       -3.0889877        0.0000000
F       -0.3217336       -1.8523024       -2.3548920
F        0.8080701        0.6210699       -2.3548920
H       -2.2510503        2.4681182        0.0000000


17
H-CF3...perfluorobenzene Dimer
C        0.0001530       -3.1139060        0.8726640
F        1.0964729       -3.1726997        0.0911416
F       -0.0224472       -4.2580175        1.5923558
F       -1.0743447       -3.1493810        0.0600444
C        0.0002507        2.4079935        0.5723497
C       -1.2018792        1.8490474        0.1613625
C       -1.2021132        0.7308138       -0.6608282
C       -0.0002172        0.1715246       -1.0720329
C        1.2019128        0.7304707       -0.6610457
C        1.2021467        1.8487044        0.1611450
F        0.0004751        3.4805186        1.3609327
F       -2.3546460        2.3854753        0.5557590
F       -2.3551044        0.1947149       -1.0550160
F       -0.0004416       -0.9010004       -1.8606159
F        2.3546796        0.1940429       -1.0554422
F        2.3551379        2.3848032        0.5553328
H        0.0004245       -2.2383122        1.5102426


17
H-CH3...perfluorobenzene Dimer
C        0.0000120        3.4857370       -2.2529318
H        0.8902248        4.0124641       -2.6003307
H       -0.0120979        3.5369180       -1.1607442
H       -0.8783982        4.0187355       -2.6202349
C        0.0001098       -1.7084273       -0.1761049
C       -1.2019578       -1.0480176        0.0368276
C       -1.2020669        0.2729800        0.4627493
C       -0.0001085        0.9335699        0.6757391
C        1.2019591        0.2731602        0.4628066
C        1.2020682       -1.0478374        0.0368849
F        0.0002145       -2.9754282       -0.5846168
F       -2.3547844       -1.6816054       -0.1674561
F       -2.3549983        0.9063950        0.6669780
F       -0.0002132        2.2005708        1.0842510
F        2.3547857        0.9067480        0.6670903
F        2.3549996       -1.6812524       -0.1673439
H        0.0001344        2.4506997       -2.5898763
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16
H-CHO...perfluorobenzene Dimer

C	-0.4858392	3.4509762	-1.6331037
O	0.3878033	4.2055337	-1.2663759
H	-1.5491294	3.7123831	-1.4867612
C	0.2329715	-1.8953156	-0.3559725
C	-1.0618321	-1.4561632	-0.1170655
C	-1.2765466	-0.2320585	0.5009227
C	-0.1964580	0.5528955	0.8800048
C	1.0983456	0.1137431	0.6410978
C	1.3130602	-1.1103616	0.0231095
F	0.4389094	-3.0693842	-0.9487001
F	-2.0977705	-2.2090316	-0.4806524
F	-2.5184233	0.1891434	0.7300643
F	-0.4023959	1.7269641	1.4727323
F	2.1342840	0.8666115	1.0046846
F	2.5549369	-1.5315635	-0.2060320
H	-0.3047860	2.4814767	-2.1227101

15
H-CN...perfluorobenzene Dimer

C	-1.7643595	-3.4656852	0.0000000
N	-1.2718627	-4.5117360	0.0000000
C	-0.3481736	1.8603847	0.0000000
C	-0.0525610	1.2325108	1.2020130
C	0.5386635	-0.0232351	1.2020130
C	0.8342761	-0.6511089	0.0000000
C	0.5386635	-0.0232351	-1.2020130
C	-0.0525610	1.2325108	-1.2020130
F	-0.9152313	3.0648011	0.0000000
F	-0.3360902	1.8347199	2.3548920
F	0.8221928	-0.6254442	2.3548920
F	1.4013338	-1.8555253	0.0000000
F	0.8221928	-0.6254442	-2.3548920
F	-0.3360902	1.8347199	-2.3548920
H	-2.2197365	-2.4984756	0.0000000

19
H-COCH3...perfluorobenzene Dimer

C	-0.1256026	3.2890906	-1.2660167
O	-1.1995025	3.7755289	-0.9667740
C	1.1662099	3.9722304	-0.8772308
H	1.7544172	4.2179151	-1.7643543
H	1.7715063	3.3200546	-0.2434960
H	0.9229236	4.8837594	-0.3363629
C	-0.0254490	0.2128269	0.9813498
C	1.1834695	-0.3683306	0.6246711
C	1.1975162	-1.5634203	-0.0810251
C	0.0026444	-2.1773544	-0.4300437
C	-1.2062741	-1.5961969	-0.0733650
C	-1.2203208	-0.4011072	0.6323312
F	-0.0389215	1.3590666	1.6582001
F	2.3294993	0.2205085	0.9594233
F	2.3570185	-2.1208227	-0.4231243
F	0.0161169	-3.3235941	-1.1068940
F	-2.3523039	-2.1850360	-0.4081172
F	-2.3798231	0.1562951	0.9744304
H	-0.0765679	2.3404022	-1.8266395

20
H-COOCH3...perfluorobenzene Dimer

C	0.3949321	2.9753719	-1.2123175
O	1.4672161	3.4294235	-0.8791985
O	-0.7728359	3.5610136	-0.8994942
C	-0.6581809	4.7709088	-0.1374673
H	-1.6775515	5.1066704	0.0258562
H	-0.1580767	4.5692308	0.8079427
H	-0.0891305	5.5107404	-0.6972968
C	0.0832710	-0.1575066	1.0042326
C	1.2262295	-0.8476007	0.6249391
C	1.1173458	-2.0184593	-0.1124065
C	-0.1344967	-2.4992255	-0.4704596
C	-1.2774552	-1.8091313	-0.0911662
C	-1.1685714	-0.6382727	0.6461794
F	0.1877041	0.9654924	1.7114387
F	2.4269012	-0.3864861	0.9683567
F	2.2135842	-2.6803454	-0.4761960
F	-0.2389297	-3.6222244	-1.1776657
F	-2.4781268	-2.2702459	-0.4345837
F	-2.2648098	0.0236133	1.0099690
H	0.2675025	2.0582565	-1.7917992

17
H-COOH...perfluorobenzene Dimer

C	0.0988677	3.3234819	-1.2437631
O	1.1232257	3.8707225	-0.9046458
O	-1.1148323	3.8284581	-0.9346953
H	-0.9562543	4.6434192	-0.4321185
C	-0.0159626	-2.1645340	-0.4563314
C	-1.2084693	-1.5589994	-0.0852475
C	-1.1896798	-0.3775559	0.6429573
C	0.0216164	0.1983548	1.0000793
C	1.2141231	-0.4071798	0.6289954
C	1.1953336	-1.5886233	-0.0992094
F	-0.0339840	-3.2976851	-1.1547703
F	-2.3702521	-2.1113693	-0.4277719
F	-2.3334411	0.2032271	0.9988729
F	0.0396378	1.3315059	1.6985182

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F        2.3759058        0.1451901        0.9715198
F        2.3390949       -2.1694063       -0.4551250
H        0.0460717        2.3958244       -1.8156101


14
H-F...perfluorobenzene Dimer
F       -2.1194738        3.4293376        0.0000000
C        0.7308742        0.9299299        0.0000000
C        0.4854802        0.2807811        1.2020130
C       -0.0053071       -1.0175147        1.2020130
C       -0.2507010       -1.6666635        0.0000000
C       -0.0053071       -1.0175147       -1.2020130
C        0.4854802        0.2807811       -1.2020130
F        1.2016001        2.1751569        0.0000000
F        0.7208435        0.9033955        2.3548920
F       -0.2406704       -1.6401291        2.3548920
F       -0.7214270       -2.9118905        0.0000000
F       -0.2406704       -1.6401291       -2.3548920
F        0.7208435        0.9033955       -2.3548920
H       -2.4491593        2.5572098        0.0000000


22
H-NCH3_2...perfluorobenzene Dimer
N        1.0766193       -3.1734437        0.0000000
C        0.9735290       -3.9267069        1.2349280
H        0.3548771       -4.8044161        1.0591355
H        0.4861322       -3.3318338        2.0086125
H        1.9522514       -4.2546247        1.6108450
C        0.9735290       -3.9267069       -1.2349280
H        0.4861322       -3.3318338       -2.0086125
H        0.3548771       -4.8044161       -1.0591355
H        1.9522514       -4.2546247       -1.6108450
C       -1.0503291       -0.0921266        0.0000000
C       -0.6721267        0.4897458        1.2020130
C        0.0842768        1.6534887        1.2020130
C        0.4624792        2.2353611        0.0000000
C        0.0842768        1.6534887       -1.2020130
C       -0.6721267        0.4897458       -1.2020130
F       -1.7758141       -1.2083007        0.0000000
F       -1.0348698       -0.0683422        2.3548920
F        0.4470199        2.2115767        2.3548920
F        1.1879642        3.3515352        0.0000000
F        0.4470199        2.2115767       -2.3548920
F       -1.0348698       -0.0683422       -2.3548920
H        1.6431275       -2.3438097        0.0000000


16
H-NH2...perfluorobenzene Dimer
H        2.3912246        3.9095934        0.8344900
H        2.3912246        3.9095934       -0.8344900
N        2.1902542        3.3803129        0.0000000
C       -0.6863909        0.9414796        0.0000000
C       -0.4690725        0.2824006       -1.2020130
C       -0.0344363       -1.0357554       -1.2020130
C        0.1828821       -1.6948344        0.0000000
C       -0.0344363       -1.0357554        1.2020130
C       -0.4690725        0.2824006        1.2020130
F       -1.1032611        2.2057552        0.0000000
F       -0.6775079        0.9145394       -2.3548920
F        0.1739991       -1.6678941       -2.3548920
F        0.5997522       -2.9591099        0.0000000
F        0.1739991       -1.6678941        2.3548920
F       -0.6775079        0.9145394        2.3548920
H        2.5425547        2.4389319        0.0000000


19
H-NHCH3...perfluorobenzene Dimer
N        0.5817072        3.2816689       -1.4858673
H        1.5053276        3.6409045       -1.6637437
C       -0.4413835        4.2898924       -1.3027339
H        0.0169277        5.1713287       -0.8574659
H       -1.2071795        3.9297960       -0.6133429
H       -0.9270601        4.5785146       -2.2433729
C        0.2410775        0.4440145        0.9252071
C        1.2955124       -0.3609864        0.5170549
C        1.0412893       -1.5654817       -0.1240423
C       -0.2673690       -1.9649780       -0.3569882
C       -1.3218039       -1.1599771        0.0511641
C       -1.0675809        0.0445183        0.6922613
F        0.4849090        1.5992753        1.5400990
F        2.5506775        0.0221804        0.7404790
F        2.0526226       -2.3375775       -0.5155110
F       -0.5112005       -3.1202387       -0.9718800
F       -2.5769691       -1.5431438       -0.1722600
F       -2.0789141        0.8166141        1.0837299
H        0.3746738        2.4269314       -1.9710686


17
H-NHOH...perfluorobenzene Dimer
N       -0.6086988        3.3098983        1.3902164
H       -1.3833774        3.8021732        1.8193915
O        0.4578525        4.2281355        1.3539886
H        0.6422898        4.3309875        0.4119700
C        0.2779049       -1.9424417        0.3878346
C        1.3292377       -1.1423807       -0.0376645
C        1.0703114        0.0494361       -0.7002156
C       -0.2399479        0.4411936       -0.9372686
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C       -1.2912807       -0.3588674       -0.5117695
C       -1.0323545       -1.5506842        0.1507816
F        0.5262473       -3.0855421        1.0233035
F        2.5859384       -1.5181250        0.1896989
F        2.0786694        0.8167939       -1.1083222
F       -0.4882904        1.5842940       -1.5727376
F       -2.5479814        0.0168770       -0.7391329
F       -2.0407124       -2.3180420        0.5588881
H       -0.3798259        2.4745340        1.9129885


15
H-NO...perfluorobenzene Dimer
N       -0.5587337        3.4288035        1.6120121
O        0.3969625        4.0875479        1.2858361
C       -0.1922362        0.5630279       -0.8972900
C       -1.2794861       -0.2099263       -0.5140441
C       -1.0761255       -1.4281879        0.1191439
C        0.2144851       -1.8734972        0.3690870
C        1.3017349       -1.1005430       -0.0141588
C        1.0983744        0.1177186       -0.6473469
F       -0.3872842        1.7314922       -1.5045961
F       -2.5173412        0.2171808       -0.7537707
F       -2.1189324       -2.1695469        0.4867243
F        0.4095331       -3.0419615        0.9763931
F        2.5395900       -1.5276501        0.2255677
F        2.1411812        0.8590776       -1.0149273
H       -0.3258847        2.5189047        2.0861605


16
H-NO2...perfluorobenzene Dimer
O       -0.9081759        3.8084312        1.0779960
O       -0.9081759        3.8084312       -1.0779960
N       -1.2093657        3.3319924        0.0000000
C        1.0178671        0.2115605        0.0000000
C        0.6470376       -0.3750381        1.2020130
C       -0.0946202       -1.5482336        1.2020130
C       -0.4654496       -2.1348322        0.0000000
C       -0.0946202       -1.5482336       -1.2020130
C        0.6470376       -0.3750381       -1.2020130
F        1.7292091        1.3368009        0.0000000
F        1.0027092        0.1875829        2.3548920
F       -0.4502917       -2.1108546        2.3548920
F       -1.1767917       -3.2600725        0.0000000
F       -0.4502917       -2.1108546       -2.3548920
F        1.0027092        0.1875829       -2.3548920
H       -1.7622478        2.4574127        0.0000000


18
H-OCF3...perfluorobenzene Dimer
C        0.0259780        3.4494972       -0.5406877
O        0.8550770        2.5837055       -1.1457432
F       -0.7748632        2.8568033        0.3635954
F       -0.7734609        4.0964253       -1.4082948
F        0.7675324        4.3539718        0.0926734
C        0.3598620       -0.5135914        1.0195054
C        1.3369627       -1.3216703        0.4549433
C        0.9718214       -2.4187496       -0.3128671
C       -0.3704212       -2.7077517       -0.5161165
C       -1.3475219       -1.8996728        0.0484457
C       -0.9823806       -0.8025935        0.8162561
F        0.7100779        0.5386440        1.7559310
F        2.6243394       -1.0444811        0.6498848
F        1.9089816       -3.1937975       -0.8543523
F       -0.7206371       -3.7599871       -1.2525421
F       -2.6348986       -2.1768620       -0.1464959
F       -1.9195408       -0.0275456        1.3577412
H        0.5132169        1.8456808       -1.6623390


15
H-OH...perfluorobenzene Dimer
O        0.0628301       -3.3613277       -2.1923078
H       -0.8295182       -3.7094583       -2.0759416
C        0.0018243       -0.9483053        0.6884322
C       -1.1994029       -0.2896104        0.4656724
C       -1.1978336        1.0258514        0.0229514
C        0.0049628        1.6826202       -0.1970103
C        1.2061900        1.0239253        0.0257496
C        1.2046207       -0.2915365        0.4684706
F        0.0003191       -2.2099967        1.1130566
F       -2.3530333       -0.9195333        0.6766429
F       -2.3499589        1.6576218       -0.1907030
F        0.0064680        2.9443116       -0.6216347
F        2.3598204        1.6538483       -0.1852210
F        2.3567460       -0.9233069        0.6821250
H        0.0216926       -2.4508626       -2.4987642


18
H-OMe...perfluorobenzene Dimer
O       -0.6178795        3.2559679        1.5992871
C        0.4397018        4.1035849        1.1882254
H        1.0756926        3.6062806        0.4515354
H        1.0424730        4.4197004        2.0433546
H       -0.0328169        4.9707643        0.7352356
C       -0.2237089        0.4825078       -0.9064148
C       -1.2936199       -0.3136621       -0.5218998
C       -1.0631971       -1.5305035        0.1047151
C        0.2371370       -1.9511769        0.3468159
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C	1.3070480	-1.1550071	-0.0376991
C	1.0766252	0.0618344	-0.6643140
F	-0.4447130	1.6496100	-1.5074163
F	-2.5408010	0.0898162	-0.7541046
F	-2.0893738	-2.2941293	0.4735127
F	0.4581411	-3.1182792	0.9478174
F	2.5542292	-1.5584853	0.1945058
F	2.1028019	0.8254602	-1.0331116
H	-0.3856576	2.4276258	2.0274163

18
H-SCH3...perfluorobenzene Dimer

S	-0.6412025	3.4635169	1.0653761
C	1.0039554	4.1244077	0.7080363
H	1.5895036	3.4307304	0.1052650
H	1.5387168	4.3777999	1.6230286
H	0.8375088	5.0351176	0.1341927
C	-0.1776273	0.1064089	-1.0104256
C	-1.2763459	-0.6291256	-0.5882242
C	-1.0920266	-1.7934431	0.1444661
C	0.1910117	-2.2222278	0.4549562
C	1.2897304	-1.4866934	0.0327548
C	1.1054110	-0.3223759	-0.6999355
F	-0.3544124	1.2231341	-1.7131667
F	-2.5069383	-0.2178675	-0.8860228
F	-2.1458335	-2.4989120	0.5494097
F	0.3677968	-3.3389531	1.1576973
F	2.5203227	-1.8979514	0.3305534
F	2.1592179	0.3830930	-1.1048791
H	-0.3664270	2.3515712	1.7684137

15
H-SH...perfluorobenzene Dimer

S	0.0490553	3.7491485	1.3231791
H	-1.2780500	3.9184621	1.2318103
C	-0.0117885	0.4811964	-0.9369163
C	-1.2050727	-0.1405315	-0.5963654
C	-1.1878018	-1.3585721	0.0688586
C	0.0227532	-1.9548865	0.3935326
C	1.2160374	-1.3331586	0.0529817
C	1.1987666	-0.1151180	-0.6122423
F	-0.0283534	1.6494487	-1.5749488
F	-2.3661446	0.4314082	-0.9077682
F	-2.3323088	-1.9548865	0.3954892
F	0.0393181	-3.1231389	1.0315651
F	2.3771093	-1.9050983	0.3643845
F	2.3432736	0.4811963	-0.9388729
H	0.0046524	2.5724313	1.9658853

17
H-SiF3...perfluorobenzene Dimer

Si	-0.0000965	3.2164429	-0.7112142
F	0.0136354	2.8027996	0.8321730
F	-1.3043293	4.1148028	-0.9197740
F	1.2903968	4.1300849	-0.9380714
C	-0.0000129	-0.5359220	1.0867421
C	1.2020297	-1.0821838	0.6587942
C	1.2020889	-2.1748425	-0.1970918
C	0.0001054	-2.7212410	-0.6250313
C	-1.2019371	-2.1749792	-0.1970835
C	-1.2019963	-1.0823205	0.6588026
F	-0.0000696	0.5120736	1.9076432
F	2.3548803	-0.5581197	1.0692414
F	2.3549962	-2.6987755	-0.6075470
F	0.0001622	-3.7692366	-1.4459324
F	-2.3547878	-2.6990433	-0.6075307
F	-2.3549037	-0.5583875	1.0692578
H	-0.0001418	2.0741900	-1.6245768

17
H-SiH3...perfluorobenzene Dimer

Si	0.0000034	3.8198459	1.3514946
H	-0.0032705	4.9354641	2.3385265
H	1.2196826	3.9501064	0.5082515
H	-1.2162655	3.9481474	0.5030191
C	-0.0000341	0.4623055	-0.9209158
C	-1.2020311	-0.1507073	-0.5955448
C	-1.2019990	-1.3766838	0.0551670
C	0.0000300	-1.9896492	0.3805087
C	1.2020270	-1.3766364	0.0551377
C	1.2019949	-0.1506600	-0.5955741
F	-0.0000649	1.6381693	-1.5450293
F	-2.3549255	0.4372027	-0.9075879
F	-2.3548626	-1.9646393	0.3672382
F	0.0000608	-3.1655130	1.0046221
F	2.3549214	-1.9645465	0.3671808
F	2.3548585	0.4372955	-0.9076454
H	-0.0000106	2.4949995	2.0282864

18
H-CH2OH...perfluorobenzene Dimer

C	-0.6591009	3.4027017	-1.5514863
H	-1.2452461	3.1913266	-0.6502632
H	-1.2753827	4.0104772	-2.2232409
O	0.5352980	4.0916102	-1.2156108
H	0.3096555	4.9202632	-0.7797548
C	0.3059732	-1.9553247	-0.3571375

C	-1.0113502	-1.5784406	-0.1356313
C	-1.2919739	-0.3750348	0.4964359
C	-0.2552745	0.4514887	0.9069977
C	1.0620490	0.0746046	0.6854914
C	1.3426726	-1.1288012	0.0534243
F	0.5751262	-3.1095404	-0.9633685
F	-2.0056729	-2.3711792	-0.5294110
F	-2.5554499	-0.0135559	0.7088880
F	-0.5244275	1.6057044	1.5132287
F	2.0563716	0.8673433	1.0792712
F	2.6061487	-1.4902800	-0.1590279
H	-0.4127191	2.4655669	-2.0442330