Supporting Information for

Physical Nature of Substituent Effects in XH/π Interactions

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Table S1: Linear Fit Parameters for B97-D vs CCSD(T)

X	slope	intercept	R^2
BH_2	1.04	–0.04	0.71
CH_3	1.21	–0.05	0.86
NH_2	1.07	–0.10	0.94
OH	1.04	–0.10	0.98
F	1.09	–0.15	0.99

Table S2: Linear Fit Parameters for SAPT0 Total Energies vs CCSD(T)

X	slope	intercept	R^2
BH_2	1.27	0.02	0.94
CH_3	1.37	–0.01	0.98
NH_2	1.18	0.01	0.99
OH	1.15	0.03	1.00
F	1.16	0.04	1.00

Table S3: Correlations between pairs of parameters: Hammett constants ($\boldsymbol{\sigma_m}$), molar refractivity (MR), and interaction distance (r).

X	MR,r	σ_m,MR	σ_m,r
BH_2	0.26	0.02	0.33
CH_3	0.32	0.02	0.31
NH_2	0.16	0.02	0.55
OH	0.12	0.02	0.73
F	0.07	0.02	0.81

Table S4: Hammett Constants and Molar Refractivities by Aryl Substituent

Y	MR	σ_m
H	1.03	0
CCH	9.55	0.21
CF_3	5.02	0.43
CH_2OH	7.19	0
CH_3	5.65	–0.07
CHO	6.88	0.35
CN	6.33	0.56
$COCH_3$	11.18	0.38
$COOCH_3$	12.87	0.37
COOH	6.93	0.37
F	0.92	0.34
$N(CH_3)_2$	15.55	–0.15
NH_2	5.42	–0.16
$NHCH_3$	10.33	–0.3
NHOH	7.22	–0.04
NO_2	7.36	0.71
NO	5.2	0.62
OCF_3	7.86	0.38
OH	2.85	0.12
OCH_3	7.87	0.12
SCH_3	13.82	0.15
SH	9.22	0.25

Table S5: Interaction energies (kcal mol^{-1}), components of SAPT0 interaction energies (kcal mol^{-1}), and optimized interaction distances (Å) for $BH_3 \cdots C_6H_5Y$ dimers.

Y	Electronic	Exchange	Induction	Dispersion	SAPT0 AVDZ	CCSD(T) AVTZ	B97-D TZV(2d,2p)	r
H	–0.720	2.451	–0.310	–2.644	–1.223	–0.973	–1.010	3.910
CCH	–0.819	2.496	–0.274	–2.799	–1.397	–1.098	–1.141	3.901
CF_3	–0.853	2.527	–0.241	–2.776	–1.344	–1.101	–1.256	3.899
CH_2OH	–0.783	2.568	–0.335	–2.834	–1.384	–1.102	–1.205	3.893
CH_3	–0.764	2.529	–0.333	–2.800	–1.367	–1.086	–1.186	3.889
CHO	–0.891	2.487	–0.248	–2.744	–1.397	–1.122	–1.172	3.906
CN	–0.826	2.345	–0.215	–2.659	–1.355	–1.102	–1.120	3.924
$COCH_3$	–0.711	2.483	–0.261	–2.792	–1.281	–1.030	–1.088	3.907
$COOCH_3$	–0.867	2.549	–0.269	–2.822	–1.409	–1.133	–1.207	3.896
COOH	–0.776	2.465	–0.247	–2.744	–1.302	–1.056	–1.113	3.908
F	–0.826	2.509	–0.266	–2.658	–1.241	–1.011	–1.125	3.899
$N(CH_3)_2$	–0.836	2.783	–0.395	–3.012	–1.460	–1.161	–1.297	3.864
NH_2	–0.736	2.299	–0.321	–2.648	–1.407	–1.147	–1.228	3.927
$NHCH_3$	–0.841	2.663	–0.373	–2.893	–1.444	–1.157	–1.271	3.877
NHOH	–0.725	2.528	–0.321	–2.800	–1.318	–1.058	–1.157	3.893
NO_2	–0.864	2.399	–0.212	–2.681	–1.358	–1.113	–1.133	3.917
NO	–0.733	2.120	–0.202	–2.520	–1.335	–1.095	–1.119	3.959
OCF_3	–0.821	2.517	–0.252	–2.774	–1.330	–1.100	–1.222	3.898
OH	–0.676	2.382	–0.295	–2.646	–1.236	–1.004	–1.106	3.918
OCH_3	–0.871	2.629	–0.337	–2.844	–1.423	–1.153	–1.250	3.886
SCH_3	–0.890	2.558	–0.307	–2.899	–1.537	–1.231	–1.301	3.890
SH	–0.878	2.515	–0.285	–2.823	–1.470	–1.180	–1.230	3.896

Table S6: Interaction energies (kcal mol^{-1}), components of SAPT0 interaction energies (kcal mol^{-1}), and optimized interaction distances (Å) for $CH_4 \cdots C_6H_5Y$ dimers.

Y	Electronic	Exchange	Induction	Dispersion	SAPT0 AVDZ	CCSD(T) AVTZ	B97-D TZV(2d,2p)	r
H	–0.961	2.387	–0.298	–2.875	–1.747	–1.379	–1.537	3.735
CCH	–1.012	2.657	–0.290	–3.191	–1.837	–1.413	–1.585	3.694
CF_3	–1.011	2.698	–0.255	–3.172	–1.740	–1.375	–1.678	3.690
CH_2OH	–1.162	2.894	–0.366	–3.312	–1.947	–1.501	–1.759	3.670
CH_3	–1.115	2.727	–0.350	–3.195	–1.934	–1.499	–1.718	3.691
CHO	–0.997	2.650	–0.261	–3.128	–1.736	–1.356	–1.524	3.698
CN	–0.948	2.555	–0.234	–3.073	–1.699	–1.332	–1.500	3.706
$COCH_3$	–1.061	2.730	–0.284	–3.235	–1.850	–1.442	–1.640	3.688
$COOCH_3$	–1.024	2.685	–0.279	–3.191	–1.809	–1.417	–1.631	3.692
COOH	–1.005	2.652	–0.264	–3.146	–1.763	–1.383	–1.580	3.696
F	–1.030	2.678	–0.280	–3.030	–1.661	–1.313	–1.538	3.691
$N(CH_3)_2$	–1.211	3.035	–0.415	–3.453	–2.044	–1.596	–1.859	3.655
NH_2	–1.109	2.782	–0.368	–3.206	–1.900	–1.489	–1.731	3.679
$NHCH_3$	–1.172	2.928	–0.397	–3.343	–1.983	–1.551	–1.789	3.663
NHOH	–1.113	2.813	–0.349	–3.253	–1.902	–1.487	–1.715	3.674
NO_2	–0.926	2.550	–0.226	–3.065	–1.666	–1.331	–1.493	3.706
NO	–0.953	2.572	–0.242	–3.066	–1.688	–1.319	–1.453	3.706
OCF_3	–1.035	2.732	–0.270	–3.185	–1.757	–1.397	–1.661	3.685
OH	–1.090	2.724	–0.327	–3.115	–1.808	–1.428	–1.649	3.688
OCH_3	–1.144	2.853	–0.353	–3.256	–1.901	–1.495	–1.720	3.676
SCH_3	–1.067	2.767	–0.325	–3.331	–1.957	–1.527	–1.736	3.680
SH	–1.056	2.711	–0.305	–3.248	–1.898	–1.484	–1.676	3.685

Table S7: Interaction energies (kcal mol^{-1}), components of SAPT0 interaction energies (kcal mol^{-1}), and optimized interaction distances (Å) for $NH_3 \cdots C_6H_5Y$ dimers.

Y	Electronic	Exchange	Induction	Dispersion	SAPT0 AVDZ	CCSD(T) AVTZ	B97-D TZV(2d,2p)	r
H	–2.051	3.404	–0.595	–3.322	–2.563	–2.077	–2.807	3.473
CCH	–1.975	3.433	–0.567	–3.533	–2.642	–2.105	–2.865	3.461
CF_3	–1.704	3.396	–0.512	–3.463	–2.283	–1.851	–2.770	3.466
CH_2OH	–2.254	3.805	–0.673	–3.694	–2.815	–2.289	–3.173	3.434
CH_3	–2.177	3.658	–0.653	–3.586	–2.758	–2.227	–3.047	3.449
CHO	–1.748	3.322	–0.517	–3.419	–2.363	–1.920	–2.683	3.474
CN	–1.575	3.185	–0.479	–3.353	–2.221	–1.781	–2.548	3.482
$COCH_3$	–1.877	3.521	–0.561	–3.582	–2.498	–2.034	–2.854	3.456
$COOCH_3$	–1.944	3.522	–0.560	–3.565	–2.548	–2.081	–2.890	3.454
COOH	–1.887	3.557	–0.550	–3.555	–2.435	–1.982	–2.824	3.450
F	–1.876	3.455	–0.550	–3.348	–2.320	–1.894	–2.722	3.460
$N(CH_3)_2$	–2.485	3.976	–0.745	–3.813	–3.067	–2.544	–3.501	3.422
NH_2	–2.405	3.865	–0.694	–3.666	–2.900	–2.372	–3.238	3.426
$NHCH_3$	–2.211	3.680	–0.688	–3.611	–2.830	–2.335	–3.214	3.445
NHOH	–2.189	3.663	–0.646	–3.605	–2.778	–2.276	–3.111	3.441
NO_2	–1.533	3.270	–0.479	–3.399	–2.142	–1.766	–2.596	3.471
NO	–1.694	3.320	–0.505	–3.406	–2.285	–1.836	–2.638	3.470
OCF_3	–1.830	3.470	–0.538	–3.500	–2.398	–1.968	–2.857	3.458
OH	–2.075	3.609	–0.619	–3.481	–2.566	–2.113	–2.925	3.450
OCH_3	–2.154	3.723	–0.650	–3.615	–2.696	–2.222	–3.063	3.443
SCH_3	–2.078	3.592	–0.619	–3.697	–2.802	–2.273	–3.074	3.447
SH	–2.059	3.520	–0.590	–3.595	–2.725	–2.211	–2.964	3.452

Table S8: Interaction energies (kcal mol^{-1}), components of SAPT0 interaction energies (kcal mol^{-1}), and optimized interaction distances (Å) for $OH_2 \cdots C_6H_5Y$ dimers.

Y	Electronic	Exchange	Induction	Dispersion	SAPT0 AVDZ	CCSD(T) AVTZ	B97-D TZV(2d,2p)	r
H	–2.939	3.778	–1.047	–3.177	–3.386	–2.863	–4.093	3.299
CCH	–2.719	3.703	–1.013	–3.319	–3.348	–2.795	–4.052	3.297
CF_3	–2.167	3.664	–0.948	–3.269	–2.720	–2.310	–3.763	3.300
CH_2OH	–3.464	4.010	–1.129	–3.417	–4.000	–3.378	–4.744	3.279
CH_3	–3.021	3.923	–1.112	–3.362	–3.572	–3.016	–4.311	3.288
CHO	–2.402	3.674	–0.966	–3.253	–2.946	–2.479	–3.674	3.301
CN	–1.922	3.482	–0.904	–3.175	–2.520	–2.114	–3.374	3.312
$COCH_3$	–2.753	3.785	–1.012	–3.346	–3.327	–2.812	–4.070	3.293
$COOCH_3$	–2.516	3.724	–0.997	–3.309	–3.098	–2.653	–3.976	3.297
COOH	–2.329	3.676	–0.970	–3.268	–2.891	–2.466	–3.778	3.300
F	–2.462	3.633	–0.972	–3.121	–2.922	–2.497	–3.830	3.304
$N(CH_3)_2$	–3.494	3.997	–1.181	–3.451	–4.128	–3.589	–5.019	3.283
NH_2	–3.355	3.854	–1.110	–3.321	–3.932	–3.385	–4.732	3.288
$NHCH_3$	–3.291	3.935	–1.150	–3.372	–3.878	–3.352	–4.762	3.286
NHOH	–3.037	3.819	–1.088	–3.341	–3.647	–3.137	–4.491	3.288
NO_2	–1.554	3.414	–0.878	–3.144	–2.163	–1.889	–3.189	3.317
NO	–1.999	3.475	–0.912	–3.156	–2.592	–2.152	–3.353	3.315
OCF_3	–2.304	3.684	–0.975	–3.269	–2.865	–2.448	–3.866	3.298
OH	–3.072	3.851	–1.068	–3.258	–3.546	–3.044	–4.406	3.291
OCH_3	–3.240	3.920	–1.106	–3.345	–3.771	–3.235	–4.592	3.288
SCH_3	–2.479	3.769	–1.064	–3.394	–3.167	–2.716	–4.062	3.293
SH	–2.890	3.772	–1.043	–3.366	–3.527	–2.990	–4.266	3.290

Table S9: Interaction energies (kcal mol^{-1}), components of SAPT0 interaction energies (kcal mol^{-1}), and optimized interaction distances (Å) for $FH\cdots C_6H_5Y$ dimers.

Y	Electronic	Exchange	Induction	Dispersion	SAPT0 AVDZ	CCSD(T) AVTZ	B97-D TZV(2d,2p)	r
H	–3.905	3.721	–1.852	–2.674	–4.711	–4.122	–5.978	3.159
CCH	–2.961	3.555	–1.821	–2.735	–3.962	–3.480	–5.334	3.165
CF_3	–2.149	3.473	–1.715	–2.684	–3.073	–2.699	–4.786	3.171
CH_2OH	–4.193	3.905	–1.967	–2.846	–5.102	–4.423	–6.444	3.144
CH_3	–4.307	3.985	–1.988	–2.857	–5.168	–4.492	–6.438	3.140
CHO	–2.394	3.469	–1.742	–2.668	–3.335	–2.970	–4.710	3.173
CN	–1.648	3.329	–1.673	–2.620	–2.611	–2.332	–4.162	3.181
$COCH_3$	–2.858	3.682	–1.834	–2.782	–3.792	–3.366	–5.194	3.157
$COOCH_3$	–2.777	3.556	–1.792	–2.726	–3.738	–3.357	–5.279	3.166
COOH	–2.488	3.505	–1.756	–2.692	–3.432	–3.082	–5.012	3.170
F	–2.839	3.548	–1.757	–2.616	–3.665	–3.262	–5.249	3.167
$N(CH_3)_2$	–4.594	4.022	–2.065	–2.932	–5.569	–4.996	–7.124	3.136
NH_2	–4.122	3.800	–1.944	–2.777	–5.044	–4.484	–6.580	3.150
$NHCH_3$	–4.373	3.879	–1.998	–2.841	–5.333	–4.765	–6.873	3.145
NHOH	–3.863	3.738	–1.913	–2.780	–4.818	–4.244	–6.347	3.152
NO_2	–1.218	3.292	–1.644	–2.606	–2.176	–2.126	–3.997	3.182
NO	–1.956	3.306	–1.681	–2.598	–2.929	–2.549	–4.162	3.186
OCF_3	–2.491	3.536	–1.761	–2.697	–3.413	–3.012	–5.088	3.166
OH	–3.735	3.819	–1.905	–2.748	–4.569	–4.060	–6.091	3.150
OCH_3	–3.998	3.873	–1.951	–2.811	–4.888	–4.336	–6.370	3.148
SCH_3	–3.556	3.690	–1.900	–2.824	–4.590	–4.065	–6.105	3.155
SH	–3.229	3.601	–1.844	–2.757	–4.229	–3.737	–5.716	3.161

B97-D/TZV(2d,2p) Optimized Geometries:

18
BH3...C6H5CCH

C	-0.8028710	-0.3163750	-0.0040070
C	-0.1185460	-0.4849390	1.2174710
C	-0.1012450	-0.4982620	-1.2137010
C	-2.1870510	0.0336270	-0.0157760
C	1.2332730	-0.8267780	1.2237160
H	-0.6572530	-0.3452730	2.1500430
C	1.2505000	-0.8400430	-1.1969600
H	-0.6266130	-0.3688670	-2.1553210
C	-3.3619430	0.3307090	-0.0257650
C	1.9219010	-1.0053580	0.0191590
H	1.7510450	-0.9542310	2.1709570
H	1.7816910	-0.9778300	-2.1352830
H	-4.3960660	0.5921960	-0.0345570
H	2.9756620	-1.2718110	0.0281190
B	1.5202010	3.1197800	-0.0063060
H	1.2273520	1.9617760	-0.0020440
H	2.2839580	3.5464290	-0.8269110
H	1.0551190	3.8632210	0.8117130

19
BH3...C6H5CF3

C	1.6420730	0.0539270	-0.0081180
C	0.1823060	-0.3413580	0.0011290
F	1.9744370	0.7822860	-1.1087370
F	2.4562950	-1.0447110	-0.0054090
F	1.9848230	0.7954370	1.0803540
C	-0.4959960	-0.5307190	-1.2080990
C	-0.4844610	-0.5162250	1.2189610
C	-1.8433430	-0.8955480	-1.1963380
H	0.0275510	-0.3933410	-2.1486770
C	-1.8318340	-0.8810900	1.2244230
H	0.0480200	-0.3676450	2.1527990
C	-2.5125290	-1.0710840	0.0183340
H	-2.3692700	-1.0423780	-2.1357190
H	-2.3488480	-1.0166750	2.1704160
H	-3.5615660	-1.3551500	0.0250100
B	-2.1835790	3.0576820	-0.0078980
H	-1.8712380	1.9043520	-0.0024940
H	-1.5465430	3.8573200	0.6178060
H	-3.1375010	3.4205820	-0.6372790

20
BH3...C6H5CH2OH

C	2.0746190	0.0617590	-0.6216080
C	0.6548340	-0.3162110	-0.2543010
O	2.8632640	0.2946600	0.5491930
H	2.0475610	0.9646700	-1.2559950
H	2.5116910	-0.7509320	-1.2273560
C	0.2195720	-0.4118280	1.0717600
C	-0.2536380	-0.5792810	-1.2904000
H	3.7494020	0.5294730	0.2545760
C	-1.1047460	-0.7653840	1.3544250
H	0.9169240	-0.2097150	1.8777400
C	-1.5737550	-0.9317200	-1.0088950
H	0.0769300	-0.5071320	-2.3255990
C	-2.0047550	-1.0261490	0.3192240
H	-1.4312180	-0.8364310	2.3892490
H	-2.2654780	-1.1324520	-1.8234110
H	-3.0327200	-1.3005270	0.5422580
B	-1.6934890	3.0852650	-0.0307500
H	-1.3817260	1.9328700	-0.0115120
H	-1.9797450	3.6521680	0.9871070
H	-1.7230790	3.6872970	-1.0680810

19
BH3...C6H5CH3

C	2.4228370	0.8024300	-0.0120450
C	1.1202930	0.0355830	-0.0044780
H	2.5051950	1.4330680	-0.9044650
H	3.2813870	0.1160230	-0.0127130
H	2.5116460	1.4395970	0.8750650
C	0.4964150	-0.3334740	-1.2050330
C	0.5056060	-0.3245420	1.2035480
C	-0.7078370	-1.0424580	-1.2009000
H	0.9607120	-0.0615070	-2.1510750
C	-0.6986000	-1.0334890	1.2139670
H	0.9771560	-0.0455470	2.1439390
C	-1.3102920	-1.3953750	0.0101740
H	-1.1753450	-1.3190750	-2.1429370
H	-1.1588240	-1.3030550	2.1616140
H	-2.2470180	-1.9468550	0.0157770
B	-2.0771410	2.6775530	-0.0020320

H	-1.4713720	1.6486270	-0.0005280
H	-1.5021570	3.7189690	0.1549020
H	-3.2662080	2.6799420	-0.1608190
18			
BH3...C6H5CHO			
C	-0.7543080	-0.2896160	0.1953120
C	-0.2608920	-0.4241720	-1.1144920
C	0.0866180	-0.5440190	1.2892150
C	-2.1580230	0.1193940	0.4450960
C	1.0609480	-0.8095500	-1.3200580
H	-0.9302600	-0.2219660	-1.9460370
C	1.4119000	-0.9303920	1.0820440
H	-0.3068210	-0.4364640	2.2986470
O	-2.9819080	0.3670500	-0.4155130
H	-2.4231260	0.1888250	1.5286400
C	1.8974230	-1.0626750	-0.2228600
H	1.4470380	-0.9149450	-2.3307000
H	2.0636830	-1.1275680	1.9290530
H	2.9291060	-1.3634210	-0.3881920
B	1.6709600	3.0720640	0.0131270
H	1.3352420	1.9251690	0.0044790
H	2.4029580	3.4921160	-0.8385950
H	1.2806440	3.8077130	0.8756310
17			
BH3...C6H5CN			
C	-0.8249120	-0.2916210	-0.0045770
C	-0.1401810	-0.4914800	-1.2179090
C	-0.1588780	-0.4765360	1.2214650
C	-2.2030880	0.1009630	-0.0175450
C	1.2005570	-0.8733710	-1.1980510
H	-0.6629700	-0.3462480	-2.1582380
C	1.1819710	-0.8585150	1.2268400
H	-0.6960040	-0.3198440	2.1518210
N	-3.3214290	0.4195310	-0.0280680
C	1.8623400	-1.0571040	0.0207090
H	1.7295430	-1.0277680	-2.1344530
H	1.6965280	-1.0013790	2.1730610
H	2.9075360	-1.3548360	0.0305440
B	1.5953400	3.0992260	-0.0068000
H	1.2677460	1.9493460	-0.0022660
H	2.3745840	3.4991990	-0.8253260
H	1.1494910	3.8546670	0.8097500
21			
BH3...C6H5COCH3			
C	2.6996470	0.2277040	1.0703800
C	1.8894110	0.0024610	-0.2009880
H	3.7296110	0.4686760	0.7990590
H	2.2683660	1.0465560	1.6605350
H	2.6808290	-0.6699490	1.7017820
C	0.4327470	-0.3441580	-0.0592520
O	2.4129560	0.1018280	-1.3011380
C	-0.3302530	-0.5554360	-1.2218020
C	-0.1902340	-0.4637120	1.1951470
C	-1.6819710	-0.8780540	-1.1307220
H	0.1611500	-0.4605140	-2.1855170
C	-1.5453960	-0.7871510	1.2865320
H	0.3817040	-0.3044410	2.1040060
C	-2.2930210	-0.9947340	0.1240070
H	-2.2635180	-1.0395210	-2.0348330
H	-2.0169040	-0.8770170	2.2617230
H	-3.3483070	-1.2466230	0.1942490
B	-1.8472350	3.1271200	-0.0589380
H	-1.5681090	1.9655090	-0.0310250
H	-2.3253320	3.6554810	0.9059680
H	-1.6525360	3.7701000	-1.0519700
22			
BH3...C6H5COOCH3			
C	3.5871200	0.2900480	0.5271390
O	2.1749740	0.0582700	0.7457980
H	3.7330520	1.1673060	-0.1117420
H	4.0448050	-0.5816100	0.0477790
H	4.0085570	0.4557970	1.5207240
C	1.4492980	-0.1741830	-0.3845130
C	0.0010190	-0.4054810	-0.0899860
O	1.9379200	-0.1886470	-1.4980100
C	-0.8547110	-0.6569880	-1.1750390
C	-0.5242740	-0.3802610	1.2130940
C	-2.2140790	-0.8797920	-0.9611400
H	-0.4350350	-0.6734840	-2.1760640
C	-1.8855410	-0.6038040	1.4226030
H	0.1327700	-0.1864580	2.0538000
C	-2.7324320	-0.8536950	0.3379890

H	-2.8699550	-1.0737480	-1.8058070
H	-2.2862920	-0.5831050	2.4327190
H	-3.7925760	-1.0274550	0.5048130
B	-2.0492310	3.1897830	-0.2238210
H	-1.8404510	2.0185350	-0.1169900
H	-1.1580510	3.9778840	-0.0736290
H	-3.1522210	3.5853770	-0.4796780

19

BH3...C6H5COOH

C	-0.4462660	-0.3377190	0.0253600
C	-1.8924790	0.0173080	0.1152100
C	0.2624920	-0.5120000	1.2258390
C	0.2178020	-0.5004630	-1.2024340
O	-2.4847440	0.1629960	-1.1123100
O	-2.5109980	0.1689140	1.1505940
C	1.6154490	-0.8441470	1.1989270
H	-0.2649260	-0.3827370	2.1659080
C	1.5724310	-0.8330220	-1.2240920
H	-0.3264100	-0.3666420	-2.1311430
H	-3.4111980	0.3904000	-0.9319170
C	2.2729660	-1.0052840	-0.0258520
H	2.1584780	-0.9776790	2.1308490
H	2.0821830	-0.9579460	-2.1758010
H	3.3286360	-1.2644480	-0.0462030
B	1.8475710	3.1232180	0.0005080
H	1.5626720	1.9627420	0.0002380
H	2.5130450	3.5807750	-0.8861710
H	1.4712200	3.8361320	0.8876770

16

BH3...C6H5F

C	-1.0791580	0.3284170	-0.0183830
C	-0.6227250	-0.1260250	1.2158290
C	-0.5950330	-0.1714550	-1.2241510
F	-2.0334410	1.2966570	-0.0472410
C	0.3586600	-1.1218330	1.2355000
H	-1.0313610	0.2951620	2.1291040
C	0.3861240	-1.1668910	-1.1844750
H	-0.9826660	0.2152740	-2.1615060
C	0.8641970	-1.6433590	0.0403850
H	0.7271270	-1.4889920	2.1897550
H	0.7759920	-1.5691570	-2.1157970
H	1.6265620	-2.4168740	0.0634400
B	2.6628420	2.0866920	-0.0086520
H	1.8119430	1.2482350	-0.0026970
H	3.5416440	2.0492410	-0.8237650
H	2.6451240	2.9706070	0.8016660

16

BH3...C6H5H

C	-0.6258790	0.8635790	-1.1004340
C	-0.6258730	1.3847940	0.1976650
C	-0.6258810	-0.5212150	-1.2980970
H	-0.6258810	1.5348340	-1.9557950
C	-0.6258700	0.5212150	1.2981000
H	-0.6258720	2.4611870	0.3513080
C	-0.6258780	-1.3847930	-0.1976620
H	-0.6258850	-0.9263530	-2.3071020
C	-0.6258720	-0.8635780	1.1004360
H	-0.6258660	0.9263530	2.3071040
H	-0.6258790	-2.4611860	-0.3513050
H	-0.6258700	-1.5348330	1.9557980
B	3.2838960	-0.0000040	-0.0000130
H	2.0896000	-0.0000020	-0.0000090
H	3.8888470	1.0359820	0.0000110
H	3.8888450	-1.0359780	0.0000070

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BH3...C6H5NCH32

C	2.4891450	0.1121780	-1.2617930
N	1.7390160	0.2033800	-0.0160570
H	2.5557380	-0.9228230	-1.6397700
H	3.5005610	0.4930510	-1.0980810
H	2.0206730	0.7280350	-2.0393110
C	2.5027210	0.1874200	1.2246220
C	0.4154530	-0.2261170	0.0040250
H	2.5773330	-0.8239010	1.6621170
H	2.0403120	0.8464540	1.9696280
H	3.5108640	0.5613250	1.0278940
C	-0.2794640	-0.4195230	1.2240390
C	-0.2934910	-0.4882700	-1.1949270
C	-1.6054080	-0.8500580	1.2340750
H	0.2126970	-0.2344710	2.1716710
C	-1.6192970	-0.9182380	-1.1651700
H	0.1877140	-0.3574580	-2.1571160

C	-2.2929350	-1.1050000	0.0446790
H	-2.1038340	-0.9866010	2.1911570
H	-2.1287310	-1.1087500	-2.1071150
H	-3.3259700	-1.4402240	0.0601640
B	-2.1394750	3.0059090	-0.0730340
H	-1.7708630	1.8713760	-0.0429280
H	-3.0224080	3.3377820	-0.8148790
H	-1.6301600	3.8286490	0.6368310

18

BH3...C6H5NH2

N	-2.1794860	1.1470450	-0.0291010
C	-1.1097030	0.2444810	-0.0110490
H	-2.7399100	1.1154470	-0.8691460
H	-2.7524510	1.1340390	0.8029420
C	-0.5518410	-0.2319710	-1.2120000
C	-0.5700380	-0.2050370	1.2084280
C	0.5140540	-1.1312270	-1.1885870
H	-0.9604350	0.1082440	-2.1617660
C	0.4959400	-1.1044160	1.2210150
H	-0.9927920	0.1561470	2.1441530
C	1.0480400	-1.5759810	0.0253900
H	0.9297290	-1.4864590	-2.1286050
H	0.8974110	-1.4386010	2.1748210
H	1.8781660	-2.2763480	0.0394370
B	2.5031550	2.3335580	-0.0071570
H	1.7326250	1.4203580	-0.0027890
H	3.1745800	2.5567770	-0.9768060
H	2.6149910	3.0381980	0.9580730

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BH3...C6H5NHCH3

C	3.0162000	0.2947020	0.3455990
N	1.9357280	0.2629610	-0.6279130
H	2.8075050	1.0417740	1.1216800
H	3.1738150	-0.6782060	0.8424400
H	3.9376130	0.5872020	-0.1663510
C	0.6701750	-0.1978200	-0.2826490
H	2.2212370	0.0123300	-1.5621260
C	0.2630020	-0.3399010	1.0594250
C	-0.2483240	-0.5385950	-1.3003200
C	-1.0188740	-0.8068630	1.3618030
H	0.9450760	-0.0865950	1.8645780
C	-1.5214290	-1.0022850	-0.9847670
H	0.0531140	-0.4336470	-2.3413860
C	-1.9215710	-1.1418290	0.3508150
H	-1.3096140	-0.9078900	2.4049630
H	-2.2081960	-1.2572990	-1.7885660
H	-2.9156150	-1.5055500	0.5944810
B	-1.9604160	2.9705170	0.0158050
H	-1.5507920	1.8496750	0.0214200
H	-2.8702210	3.2802290	-0.7019670
H	-1.4670090	3.8002120	0.7277650

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BH3...C6H5NHOH

N	1.9274820	0.4506380	0.5526040
C	0.6891150	-0.1661270	0.2499070
O	2.9655960	0.1318270	-0.4026480
H	2.2820230	0.1200230	1.4465910
C	-0.1716380	-0.4896610	1.3136220
C	0.2623660	-0.3702230	-1.0703170
H	3.2075190	1.0052680	-0.7369990
C	-1.4474590	-0.9891040	1.0555540
H	0.1620640	-0.3417710	2.3392060
C	-1.0132810	-0.8826180	-1.3144990
H	0.9357550	-0.1416340	-1.8888840
C	-1.8782900	-1.1900690	-0.2602260
H	-2.1021630	-1.2335790	1.8884000
H	-1.3313410	-1.0430750	-2.3418280
H	-2.8697210	-1.5871100	-0.4589970
B	-2.0175630	2.9405890	-0.0922740
H	-1.5807220	1.8297860	-0.0653010
H	-1.3901090	3.8489440	0.3776340
H	-3.0875110	3.1579230	-0.5897510

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BH3...C6H5NO2

N	-1.9101510	0.0588630	-0.0128450
C	-0.4674950	-0.3258100	0.0001260
O	-2.4542160	0.1952500	-1.1075150
O	-2.4681880	0.2163440	1.0719140
C	0.1944480	-0.5120420	-1.2148920
C	0.1787940	-0.4884090	1.2269080
C	1.5423970	-0.8713970	-1.1946430
H	-0.3443700	-0.3757450	-2.1452870

C	1.5268470	-0.8479220	1.2309000
H	-0.3718910	-0.3341970	2.1475060
C	2.2085190	-1.0393490	0.0241880
H	2.0716890	-1.0200330	-2.1315840
H	2.0440660	-0.9783300	2.1772510
H	3.2585340	-1.3193280	0.0336290
B	1.8732360	3.1034480	-0.0180570
H	1.5651020	1.9481510	-0.0088510
H	2.6428900	3.5135030	-0.8406850
H	1.4170240	3.8535130	0.7975040

17

BH3...C6H5NO

C	0.7827240	-0.2584080	-0.2116850
C	-0.0516490	-0.5524420	-1.2987070
C	0.3276140	-0.4010790	1.1103910
N	2.1150110	0.1917210	-0.5704840
C	-1.3548020	-0.9938290	-1.0669780
H	0.3417780	-0.4278400	-2.3045510
C	-0.9715190	-0.8411750	1.3338740
H	1.0045350	-0.1631440	1.9260100
O	2.8529190	0.4515380	0.3668050
C	-1.8120120	-1.1372890	0.2471420
H	-2.0117120	-1.2251230	-1.9009600
H	-1.3416840	-0.9577710	2.3493430
H	-2.8268540	-1.4809910	0.4311530
B	-1.7887400	3.0501180	-0.0156510
H	-1.4035490	1.9183760	-0.0051840
H	-2.2664950	3.5317230	0.9727680
H	-1.7028890	3.7051590	-1.0156000

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BH3...C6H5OCF3

C	-2.0618520	0.0470020	0.0305570
O	-1.0073140	-0.1539320	0.8594450
F	-3.1386690	0.2592660	0.8022970
F	-1.9021040	1.1261990	-0.7807100
F	-2.3185210	-1.0204570	-0.7713110
C	0.2849290	-0.4067800	0.3630170
C	1.2434060	-0.5883360	1.3617590
C	0.6236160	-0.4784010	-0.9892570
C	2.5654690	-0.8463770	1.0005650
H	0.9433390	-0.5255690	2.4031670
C	1.9550280	-0.7381710	-1.3314900
H	-0.1186420	-0.3378090	-1.7645520
C	2.9279910	-0.9226040	-0.3477870
H	3.3116070	-0.9877130	1.7777040
H	2.2238360	-0.7949190	-2.3827980
H	3.9579540	-1.1236260	-0.6278930
B	2.3424550	3.1635830	-0.0072880
H	2.1149290	1.9906730	-0.0021530
H	1.5032280	3.9414330	0.3497110
H	3.4121030	3.5679960	-0.3689660

17

BH3...C6H5OH

C	-1.1087050	0.2720180	0.0082050
C	-0.5872820	-0.1917490	1.2233950
C	-0.5902450	-0.2021190	-1.2044910
O	-2.1279810	1.1916630	0.0663100
C	0.4486200	-1.1261210	1.2154300
H	-1.0005970	0.1860370	2.1540890
C	0.4475450	-1.1381160	-1.1981650
H	-0.9992110	0.1616880	-2.1462200
H	-2.3888640	1.4221280	-0.8342220
C	0.9728290	-1.6054090	0.0091660
H	0.8492950	-1.4824270	2.1612450
H	0.8435110	-1.5003350	-2.1436660
H	1.7794360	-2.3329130	0.0114960
B	2.5542030	2.2437280	-0.0067030
H	1.7541210	1.3566670	-0.0019380
H	3.4218490	2.2714560	-0.8349400
H	2.4967230	3.1147390	0.8159480

20

BH3...C6H5OCH3

C	2.9017240	0.3216990	0.3106410
O	1.9308670	0.0307910	-0.6965320
H	3.8231950	0.5654110	-0.2240270
H	2.5895100	1.1785990	0.9256880
H	3.0679650	-0.5480970	0.9632180
C	0.6712990	-0.3091170	-0.2774490
C	-0.2549460	-0.5879410	-1.2973600
C	0.2734900	-0.3901490	1.0659060
C	-1.5611710	-0.9428330	-0.9728590
H	0.0708180	-0.5201530	-2.3315690

C	-1.0447550	-0.7487230	1.3742660	H	-0.5847230	-0.3070990	2.1523490
H	0.9720960	-0.1791390	1.8679240	H	-2.6425490	0.3222060	1.2367520
C	-1.9672440	-1.0262540	0.3659460	C	1.9559470	-1.0953270	0.0202740
H	-2.2683040	-1.1561180	-1.7708200	H	1.8098230	-1.0578560	-2.1340990
H	-1.3437210	-0.8088780	2.4180380	H	1.7755700	-1.0324610	2.1714430
H	-2.9877140	-1.3036100	0.6147780	H	2.9944280	-1.4144660	0.0304070
B	-1.6845450	3.0760950	-0.0382920	B	1.7580940	3.0408640	-0.0059380
H	-1.3658270	1.9258730	-0.0132920	H	1.4072740	1.8994160	-0.0019960
H	-1.0202830	3.9010230	0.5259670	H	2.1864320	3.5385440	-1.0097360
H	-2.6723200	3.4182020	-0.6267330	H	1.6871300	3.6989240	0.9945510

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BH3...C6H5SCH3

C	2.8743630	0.2764010	0.8517220
S	2.0092810	-0.0064020	-0.7319520
H	3.9111620	0.5020690	0.5853910
H	2.4420920	1.1272370	1.3884540
H	2.8458710	-0.6199530	1.4798930
C	0.3383510	-0.3659970	-0.2244380
C	-0.5896090	-0.6340640	-1.2488610
C	-0.0900020	-0.3950710	1.1115660
C	-1.9159810	-0.9242310	-0.9362690
H	-0.2701900	-0.6146430	-2.2882910
C	-1.4243410	-0.6876820	1.4126570
H	0.6036430	-0.1924520	1.9201400
C	-2.3437350	-0.9533260	0.3967060
H	-2.6194010	-1.1288440	-1.7397690
H	-1.7402280	-0.7062330	2.4530990
H	-3.3788410	-1.1799650	0.6369950
B	-1.8790460	3.1253910	-0.1128840
H	-1.6105660	1.9636570	-0.0520850
H	-1.5564610	3.8682310	0.7723250
H	-2.4746100	3.5602030	-1.0590000

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BH3...C6H5SH

C	-0.7290100	-0.2702050	-0.0057680
C	-0.0437660	-0.4849800	-1.2125430
C	-0.0632790	-0.4706080	1.2126780
S	-2.4352780	0.2539080	-0.0935380
C	1.2902750	-0.8949250	-1.1931090
H	-0.5501870	-0.3326130	-2.1625150
C	1.2716280	-0.8808610	1.2199930

19
CH4...C6H5CCH
C 0.8601050 -0.3406860 0.0000040
C 0.1765220 -0.5496690 -1.2156280
C 0.1765160 -0.5496180 1.2156420
C 2.2255310 0.0766960 -0.0000020
C -1.1569450 -0.9572810 -1.2103750
H 0.7013520 -0.3892600 -2.1527640
C -1.1569510 -0.9572300 1.2103990
H 0.7013420 -0.3891690 2.1527740
C 3.3845040 0.4309690 -0.0000070
C -1.8277490 -1.1623050 0.0000150
H -1.6743180 -1.1154510 -2.1531930
H -1.6743280 -1.1153600 2.1532210
H 4.4046150 0.7427950 -0.0000110
H -2.8672320 -1.4800530 0.0000190
C -1.5678270 2.7794850 -0.0000680
H -1.2482390 1.7339830 -0.0000450
H -2.0284230 3.0221440 0.9636770
H -0.7002580 3.4281100 -0.1617800
H -2.2967390 2.9400870 -0.8017840
20
CH4...C6H5CF3
C -1.6858040 0.0766430 -0.0000460
C -0.2440540 -0.3800970 0.0000300
F -1.9919850 0.8252240 1.0945840
F -2.5457870 -0.9865590 -0.0000320
F -1.9919510 0.8252240 -1.0945710
C 0.4201740 -0.5904820 1.2135880
C 0.4201870 -0.5905670 -1.2135430
C 1.7509060 -1.0120530 1.2104310
H -0.1013160 -0.4252450 2.1508210
C 1.7509160 -1.0121360 -1.2104000
H -0.1013170 -0.4253870 -2.1507800
C 2.4175220 -1.2232740 0.0000350
H 2.2659120 -1.1751730 2.1531700
H 2.2659800 -1.1753380 -2.1530900
H 3.4536110 -1.5515030 0.0000590
C 2.2003630 2.7163510 -0.0000930
H 1.8702100 1.6741900 -0.0000580
H 1.3443800 3.3719430 -0.1922080
H 2.6355050 2.9629580 0.9743060
H 2.9532750 2.8622310 -0.7820650
21
CH4...C6H5CH2OH
C 2.1125690 0.0932080 -0.6253460
C 0.7111100 -0.3451750 -0.2548120
O 2.8926560 0.3614170 0.5436320
H 2.0453850 0.9932940 -1.2607670
H 2.5831390 -0.7006540 -1.2309650
C 0.2828950 -0.4577680 1.0722110
C -0.1871360 -0.6485190 -1.2888180
H 3.7672790 0.6338520 0.2470020
C -1.0244010 -0.8677510 1.3578860
H 0.9724090 -0.2247270 1.8765840
C -1.4902840 -1.0572060 -1.0043110
H 0.1380470 -0.5635130 -2.3247470
C -1.9142880 -1.1684260 0.3247590
H -1.3455390 -0.9514800 2.3934310
H -2.1742500 -1.2886360 -1.8172330
H -2.9290360 -1.4865990 0.5501300
C -1.7139180 2.7398120 -0.0270410
H -1.3831500 1.6978800 -0.0087110
H -1.4333710 3.2309870 0.9109290
H -1.2392860 3.2613470 -0.8655850
H -2.8021570 2.7778590 -0.1463000
20
CH4...C6H5CH3
C -2.3408940 1.0933560 -0.0000170
C -1.1629930 0.1461060 0.0001370
H -2.3339870 1.7330020 0.8897620
H -3.2897230 0.5383900 -0.0000560
H -2.3337460 1.7329520 -0.8897920
C -0.6029130 -0.3043030 1.2043800
C -0.6030280 -0.3042090 -1.2042350
C 0.4860910 -1.1800640 1.2073870
H -1.0259920 0.0359300 2.1476620
C 0.4859570 -1.1799540 -1.2075140
H -1.0262450 0.0361370 -2.1474130
C 1.0350050 -1.6214910 -0.0001050
H 0.9056480 -1.5174660 2.1521870
H 0.9053570 -1.5172280 -2.1524250

H	1.8820950	-2.3027090	-0.0001560
C	2.2527710	2.1356570	0.0000110
H	1.5676090	1.2836620	0.0000100
H	1.6879450	3.0616200	-0.1553450
H	2.7757060	2.1868590	0.9613240
H	2.9853580	2.0182610	-0.8060200

19

CH4...C6H5CHO

C	0.8127620	-0.3094240	-0.1988500
C	0.3369030	-0.4617780	1.1154940
C	-0.0207110	-0.6172930	-1.2846870
C	2.1900140	0.1743980	-0.4618920
C	-0.9602180	-0.9178100	1.3335480
H	1.0000730	-0.2172860	1.9406220
C	-1.3212020	-1.0744960	-1.0649950
H	0.3589650	-0.4953020	-2.2977410
O	3.0051700	0.4729670	0.3908360
H	2.4431190	0.2507500	-1.5478370
C	-1.7893400	-1.2241810	0.2443730
H	-1.3326670	-1.0372320	2.3477420
H	-1.9672020	-1.3131060	-1.9057520
H	-2.8016970	-1.5800380	0.4194510
C	-1.7229810	2.7185140	-0.0180590
H	-1.3584990	1.6877610	-0.0055790
H	-1.5279950	3.1882450	0.9518140
H	-1.2064480	3.2806960	-0.8034000
H	-2.8003660	2.7241910	-0.2156020

18

CH4...C6H5CN

C	0.8831750	-0.3088330	0.0000040
C	0.2190320	-0.5370840	1.2197540
C	0.2190380	-0.5371470	-1.2197380
C	2.2384100	0.1569990	-0.0000050
C	-1.0994420	-0.9902790	1.2125210
H	0.7401650	-0.3579310	2.1551380
C	-1.0994360	-0.9903420	-1.2124870
H	0.7401760	-0.3580430	-2.1551280
N	3.3381350	0.5350040	-0.0000120
C	-1.7593440	-1.2171380	0.0000210
H	-1.6125300	-1.1666160	2.1538810
H	-1.6125200	-1.1667280	-2.1538410
H	-2.7871420	-1.5704200	0.0000280
C	-1.6441590	2.7412360	-0.0000820
H	-1.2887310	1.7071970	-0.0000540
H	-2.1088260	2.9689500	0.9652110
H	-0.8000100	3.4187950	-0.1659650
H	-2.3811720	2.8752900	-0.7991120

22

CH4...C6H5COCH3

C	2.7387760	0.2781610	1.0587940
C	1.9321950	0.0182380	-0.2082750
H	3.7578620	0.5564830	0.7821910
H	2.2796640	1.0824330	1.6480020
H	2.7561830	-0.6173000	1.6933410
C	0.4901180	-0.3820670	-0.0590470
O	2.4470350	0.1331580	-1.3110160
C	-0.2693250	-0.6258790	-1.2175510
C	-0.1226850	-0.5203230	1.1984410
C	-1.6076420	-0.9984600	-1.1195140
H	0.2141340	-0.5161130	-2.1837050
C	-1.4644110	-0.8938520	1.2968010
H	0.4467100	-0.3365320	2.1042640
C	-2.2086280	-1.1333960	0.1382410
H	-2.1865360	-1.1847870	-2.0205400
H	-1.9281300	-0.9977800	2.2743260
H	-3.2534540	-1.4242940	0.2139150
C	-1.8590340	2.7911160	-0.0551350
H	-1.5640010	1.7387380	-0.0270630
H	-1.7636370	3.2257400	0.9458740
H	-1.2117470	3.3351940	-0.7511780
H	-2.8995030	2.8717250	-0.3878210

23

CH4...C6H5COOCH3

C	-3.6243030	0.3372150	-0.5337220
O	-2.2195830	0.0617540	-0.7495320
H	-3.7443810	1.2253190	0.0954840
H	-4.1072940	-0.5153470	-0.0449430
H	-4.0408080	0.5043580	-1.5291520
C	-1.5009100	-0.1794820	0.3834100
C	-0.0600670	-0.4563540	0.0917390
O	-1.9896240	-0.1674190	1.4968960
C	0.7880400	-0.7209440	1.1796610

C	0.4655960	-0.4608180	-1.2114280
C	2.1402680	-0.9858360	0.9685030
H	0.3681710	-0.7141650	2.1807190
C	1.8197000	-0.7264560	-1.4181890
H	-0.1855760	-0.2570530	-2.0543440
C	2.6590200	-0.9891770	-0.3307250
H	2.7902680	-1.1896760	1.8153810
H	2.2207750	-0.7285800	-2.4283860
H	3.7135960	-1.1957600	-0.4954120
C	2.0533470	2.8800310	0.1706200
H	1.8309050	1.8131150	0.0845470
H	1.6302060	3.2688940	1.1029490
H	3.1384920	3.0294190	0.1734180
H	1.6151510	3.4157400	-0.6783870
20			
CH4...C6H5COOH			
C	0.5046890	-0.3744710	-0.0249240
C	1.9349320	0.0377150	-0.1257070
C	-0.2027810	-0.5870320	-1.2199840
C	-0.1458120	-0.5536730	1.2078300
O	2.5272990	0.2172410	1.0972720
O	2.5413830	0.2055420	-1.1657170
C	-1.5410980	-0.9731240	-1.1828420
H	0.3140470	-0.4444080	-2.1639950
C	-1.4858110	-0.9402870	1.2397320
H	0.3974470	-0.3904020	2.1323770
H	3.4428770	0.4802490	0.9098820
C	-2.1851340	-1.1504810	0.0468490
H	-2.0832020	-1.1360840	-2.1106100
H	-1.9851000	-1.0777680	2.1952480
H	-3.2293840	-1.4517420	0.0751830
C	-1.8678150	2.7879620	-0.0136280
H	-1.5645830	1.7375680	-0.0063110
H	-1.8135740	3.1923450	1.0032250
H	-1.1991100	3.3580900	-0.6678610
H	-2.8958980	2.8702350	-0.3835300
17			
CH4...C6H5F			
C	-1.0991990	-0.4232540	-0.0000010
C	-0.6918070	0.1088070	-1.2202760
C	-0.6917820	0.1087620	1.2202840
F	-1.9258980	-1.5028580	-0.0000120
C	0.1582720	1.2189420	-1.2102600
H	-1.0367230	-0.3415970	-2.1458150
C	0.1582970	1.2188990	1.2102900
H	-1.0366780	-0.3416740	2.1458150
C	0.5843370	1.7753110	0.0000210
H	0.4867360	1.6479210	-2.1532680
H	0.4867810	1.6478430	2.1533080
H	1.2447770	2.6377950	0.0000300
C	2.6672250	-1.5763820	-0.0000610
H	1.7992960	-0.9117720	-0.0000400
H	3.1104220	-1.6019820	1.0013570
H	2.3559340	-2.5872430	-0.2847510
H	3.4104800	-1.2100760	-0.7165090
17			
CH4...C6H5H			
C	0.7183510	0.3232840	1.3609600
C	0.7183530	1.3402670	0.4005060
C	0.7183450	-1.0169840	0.9604530
H	0.7183530	0.5745720	2.4188250
C	0.7183510	1.0169810	-0.9604540
H	0.7183570	2.3820500	0.7118170
C	0.7183430	-1.3402700	-0.4005070
H	0.7183430	-1.8074800	1.7070080
C	0.7183450	-0.3232870	-1.3609600
H	0.7183530	1.8074770	-1.7070080
H	0.7183380	-2.3820530	-0.7118180
H	0.7183430	-0.5745750	-2.4188260
C	-3.0165260	0.0000120	0.0000030
H	-1.9233860	0.0000080	0.0000020
H	-3.3826860	1.0272800	-0.1079100
H	-3.3826930	-0.6071060	-0.8356640
H	-3.3826910	-0.4201970	0.9435670
25			
CH4...C6H5NCH32			
C	2.5387050	0.1884910	-1.2441700
N	1.7797360	0.2191310	-0.0008290
H	2.6467450	-0.8332260	-1.6478420
H	3.5339780	0.6034510	-1.0650930
H	2.0506410	0.8056270	-2.0085100
C	2.5376030	0.2007260	1.2433910

C	0.4735430	-0.2610250	0.0008120
H	2.6488830	-0.8178370	1.6555610
H	2.0467260	0.8223760	2.0021880
H	3.5315800	0.6177980	1.0619540
C	-0.2192160	-0.5119240	1.2115490
C	-0.2191330	-0.5194100	-1.2084230
C	-1.5277000	-0.9929520	1.2031080
H	0.2609880	-0.3324320	2.1663580
C	-1.5275940	-1.0003690	-1.1971340
H	0.2612530	-0.3457880	-2.1642270
C	-2.1992960	-1.2435580	0.0037310
H	-2.0250500	-1.1728270	2.1535630
H	-2.0248760	-1.1861200	-2.1464950
H	-3.2187730	-1.6183170	0.0048230
C	-2.1308350	2.6752870	-0.0083810
H	-1.7536990	1.6493540	-0.0051940
H	-3.1792630	2.6810470	-0.3256390
H	-2.0548210	3.0985100	0.9992470
H	-1.5389190	3.2828730	-0.7017870

19

CH4...C6H5NH2

N	-2.1516840	1.2584660	-0.0000360
C	-1.1492370	0.2814880	-0.0000140
H	-2.7185430	1.2768000	-0.8361480
H	-2.7185240	1.2768700	0.8360900
C	-0.6350070	-0.2197300	-1.2103240
C	-0.6350230	-0.2196050	1.2103230
C	0.3638340	-1.1931920	-1.2048750
H	-1.0245180	0.1598420	-2.1531690
C	0.3638210	-1.1930700	1.2049440
H	-1.0245310	0.1600490	2.1531380
C	0.8726890	-1.6890640	0.0000590
H	0.7466800	-1.5663540	-2.1518640
H	0.7466870	-1.5661650	2.1519500
H	1.6505640	-2.4471750	0.0001150
C	2.4311510	1.9290490	-0.0001000
H	1.6681270	1.1461330	-0.0000650
H	1.9546880	2.9060060	-0.1363300
H	2.9692170	1.9173040	0.9540860
H	3.1385650	1.7521780	-0.8176280

22

CH4...C6H5NHCH3

C	3.0465460	0.3739450	0.3685970
N	1.9753190	0.3002460	-0.6128280
H	2.7986640	1.1048890	1.1485000
H	3.2450270	-0.5944550	0.8595660
H	3.9571140	0.7119930	-0.1346330
C	0.7298000	-0.2203500	-0.2799460
H	2.2783440	0.0699010	-1.5467460
C	0.3203890	-0.3909000	1.0581260
C	-0.1652140	-0.5950340	-1.3065820
C	-0.9408610	-0.9180950	1.3479640
H	0.9846750	-0.1127840	1.8699370
C	-1.4179420	-1.1186580	-1.0034850
H	0.1382150	-0.4686540	-2.3446850
C	-1.8204000	-1.2863050	0.3281640
H	-1.2337970	-1.0400860	2.3882640
H	-2.0868460	-1.3987050	-1.8139870
H	-2.7984390	-1.6968010	0.5620930
C	-1.9620440	2.6246990	0.0224640
H	-1.5403450	1.6160900	0.0229350
H	-2.7707360	2.6845160	-0.7141020
H	-2.3590340	2.8574550	1.0166180
H	-1.1817280	3.3491030	-0.2357760

20

CH4...C6H5NHOH

N	1.9505570	0.4854520	0.5685370
C	0.7457340	-0.1885380	0.2527540
O	3.0072340	0.2301460	-0.3854440
H	2.3174110	0.1622450	1.4602620
C	-0.1022440	-0.5671990	1.3085050
C	0.3351830	-0.3978450	-1.0717830
H	3.2067170	1.1184770	-0.7083830
C	-1.3505050	-1.1264180	1.0385440
H	0.2194040	-0.4151380	2.3373250
C	-0.9123180	-0.9701560	-1.3280090
H	0.9997430	-0.1262590	-1.8844070
C	-1.7653080	-1.3328560	-0.2815320
H	-1.9956710	-1.4131110	1.8653490
H	-1.2177090	-1.1339690	-2.3586470
H	-2.7348860	-1.7763570	-0.4896500
C	-2.0206320	2.5835350	-0.0629020

H	-1.5705610	1.5873930	-0.0482260
H	-1.2626260	3.3327150	0.1907480
H	-2.4178980	2.7922880	-1.0621930
H	-2.8351580	2.6292570	0.6681490

19

CH4...C6H5NO2

N	1.9513250	0.0904750	-0.0000100
C	0.5274050	-0.3588010	0.0000040
O	2.4952230	0.2621080	1.0897730
O	2.4952170	0.2620610	-1.0898030
C	-0.1182130	-0.5624810	1.2209920
C	-0.1182200	-0.5625340	-1.2209720
C	-1.4487070	-0.9822790	1.2128760
H	0.4194670	-0.3928130	2.1465460
C	-1.4487140	-0.9823320	-1.2128300
H	0.4194550	-0.3929060	-2.1465360
C	-2.1138570	-1.1921720	0.0000300
H	-1.9651650	-1.1452120	2.1545910
H	-1.9651770	-1.1453060	-2.1545350
H	-3.1502350	-1.5191710	0.0000400
C	-1.9018090	2.7607040	-0.0000570
H	-1.5727950	1.7179350	-0.0000350
H	-2.0681200	3.0923360	1.0304590
H	-1.1326290	3.3874710	-0.4637320
H	-2.8349100	2.8503650	-0.5667590

18

CH4...C6H5NO

C	0.8375970	-0.2759600	-0.2139980
C	0.0133740	-0.6143580	-1.2958460
C	0.3956320	-0.4340350	1.1107830
N	2.1453520	0.2353870	-0.5809300
C	-1.2662570	-1.1161730	-1.0561550
H	0.3959820	-0.4758110	-2.3040370
C	-0.8800830	-0.9344070	1.3422050
H	1.0640540	-0.1604130	1.9222090
O	2.8741880	0.5343280	0.3517860
C	-1.7103170	-1.2751720	0.2606840
H	-1.9150890	-1.3822950	-1.8860660
H	-1.2397940	-1.0638050	2.3598770
H	-2.7068280	-1.6659160	0.4508950
C	-1.7947420	2.6721000	-0.0176990
H	-1.3935960	1.6551380	-0.0052160
H	-1.7238670	3.1062000	0.9852880
H	-1.2189500	3.2844400	-0.7196770
H	-2.8441010	2.6481630	-0.3309010

21

CH4...C6H5OCF3

C	-2.1073050	0.0632800	0.0349860
O	-1.0575230	-0.1710770	0.8611290
F	-3.1758420	0.3050920	0.8095370
F	-1.9173390	1.1395760	-0.7736180
F	-2.3970090	-0.9938530	-0.7693030
C	0.2256910	-0.4606000	0.3613300
C	1.1803650	-0.6732290	1.3575800
C	0.5594260	-0.5383720	-0.9918350
C	2.4935030	-0.9692070	0.9929370
H	0.8843550	-0.6045680	2.3997760
C	1.8818950	-0.8364090	-1.3375410
H	-0.1798900	-0.3737120	-1.7652000
C	2.8509340	-1.0522990	-0.3563690
H	3.2366790	-1.1347310	1.7681360
H	2.1468190	-0.8981020	-2.3895560
H	3.8739460	-1.2828810	-0.6391610
C	2.3402400	2.8399250	-0.0029210
H	2.1004240	1.7732970	-0.0007640
H	1.8494120	3.3279050	0.8459590
H	3.4244880	2.9722200	0.0785350
H	1.9871660	3.2933300	-0.9352970

18

CH4...C6H5OH

C	1.1366530	0.3508070	-0.0254500
C	0.6569460	-0.1881530	-1.2267210
C	0.6845020	-0.1552410	1.2008100
O	2.0494260	1.3743600	-0.1104860
C	-0.2712400	-1.2290320	-1.1913790
H	1.0177690	0.2157120	-2.1682320
C	-0.2455220	-1.1981940	1.2219110
H	1.0606330	0.2673390	2.1316230
H	2.2924380	1.6476250	0.7830490
C	-0.7286100	-1.7409370	0.0286010
H	-0.6399830	-1.6433310	-2.1264970
H	-0.5906480	-1.5844420	2.1777690

H	-1.4514300	-2.5515250	0.0475880
C	-2.5473900	1.7612730	-0.0007360
H	-1.7313590	1.0336120	-0.0001340
H	-3.0560410	1.7435760	0.9693600
H	-2.1453230	2.7639420	-0.1824120
H	-3.2634940	1.5094720	-0.7904500
21			
CH4...C6H5OCH3			
C	2.9231450	0.4133080	0.3325940
O	1.9753960	0.0784770	-0.6829100
H	3.8339240	0.7086570	-0.1943070
H	2.5623650	1.2485110	0.9509080
H	3.1307260	-0.4508660	0.9807860
C	0.7327940	-0.3299330	-0.2744720
C	-0.1709600	-0.6502670	-1.3023370
C	0.3312120	-0.4406820	1.0656340
C	-1.4587600	-1.0754630	-0.9888860
H	0.1573980	-0.5585830	-2.3338810
C	-0.9682950	-0.8700800	1.3628410
H	1.0126070	-0.1985820	1.8736550
C	-1.8684400	-1.1890020	0.3466010
H	-2.1485760	-1.3203100	-1.7929210
H	-1.2703540	-0.9527960	2.4041760
H	-2.8744810	-1.5212520	0.5867990
C	-1.7327740	2.7261590	-0.0263820
H	-1.3860530	1.6894760	-0.0081550
H	-1.6159670	3.1702360	0.9683460
H	-1.1430960	3.2981570	-0.7511510
H	-2.7892100	2.7552870	-0.3145300
21			
CH4...C6H5SCH3			
C	2.9042920	0.3215870	0.8664540
S	2.0558450	0.0219150	-0.7231070
H	3.9328620	0.5882960	0.6062190
H	2.4387180	1.1505320	1.4095480
H	2.9071000	-0.5811850	1.4860160
C	0.3977550	-0.4045760	-0.2253840
C	-0.5160090	-0.6972250	-1.2558230
C	-0.0338300	-0.4624010	1.1086440
C	-1.8317000	-1.0396250	-0.9510430
H	-0.1939470	-0.6559500	-2.2937980
C	-1.3573520	-0.8074290	1.4018690
H	0.6489720	-0.2418180	1.9217330
C	-2.2626750	-1.0974190	0.3799580
H	-2.5242140	-1.2626130	-1.7591150
H	-1.6759200	-0.8477140	2.4408780
H	-3.2894260	-1.3647860	0.6141490
C	-1.8939570	2.7978530	-0.0803560
H	-1.6087830	1.7434980	-0.0337990
H	-1.1685680	3.3995230	0.4781180
H	-1.9103900	3.1281110	-1.1245530
H	-2.8890710	2.9288860	0.3583900
18			
CH4...C6H5SH			
C	-0.7880250	-0.2884040	-0.0039700
C	-0.1194490	-0.5347730	-1.2140540
C	-0.1295810	-0.5284860	1.2112600
S	-2.4643090	0.3260010	-0.0834980
C	1.1909660	-1.0151290	-1.2010630
H	-0.6204130	-0.3521350	-2.1615780
C	1.1816400	-1.0091510	1.2121270
H	-0.6382620	-0.3410160	2.1534490
H	-2.6629430	0.4002280	1.2477920
C	1.8493330	-1.2551890	0.0091040
H	1.6977790	-1.2019160	-2.1445620
H	1.6801740	-1.1908960	2.1611420
H	2.8694030	-1.6291190	0.0142200
C	1.7990790	2.6878820	-0.0014350
H	1.4228150	1.6614610	-0.0003470
H	2.3657070	2.8699580	-0.9210790
H	0.9576540	3.3871510	0.0510860
H	2.4532490	2.8397600	0.8640480

18
NH3...C6H5CCH

C	0.8034640	-0.3732730	0.0102220
C	0.1123460	-0.5630550	-1.2042990
C	0.0967210	-0.4831520	1.2256080
C	2.1995390	-0.0739930	0.0093570
C	-1.2510870	-0.8551570	-1.1982100
H	0.6549770	-0.4788200	-2.1412400
C	-1.2666440	-0.7755990	1.2212070
H	0.6273080	-0.3373190	2.1618840
C	3.3845280	0.1800350	0.0086230
C	-1.9447240	-0.9624070	0.0119230
H	-1.7740170	-0.9995430	-2.1401730
H	-1.8016910	-0.8580140	2.1638260
H	4.4275370	0.4036270	0.0079770
H	-3.0075400	-1.1902450	0.0125810
N	-1.3000400	2.7131080	-0.1047940
H	-1.0867250	1.7181380	-0.0707050
H	-1.2106830	3.0476690	0.8526130
H	-0.5337410	3.1423540	-0.6197900

19
NH3...C6H5CF3

C	-1.6714660	0.0172620	0.0055620
C	-0.2077300	-0.3630820	0.0141150
F	-2.0056710	0.8140840	1.0570920
F	-2.4742090	-1.0872270	0.0809130
F	-2.0275680	0.6809890	-1.1279030
C	0.4787800	-0.4644900	1.2292700
C	0.4544840	-0.6121400	-1.1932440
C	1.8297730	-0.8157440	1.2339440
H	-0.0412740	-0.2699030	2.1616540
C	1.8055360	-0.9630090	-1.1822820
H	-0.0843600	-0.5315750	-2.1317640
C	2.4944300	-1.0652340	0.0297700
H	2.3620740	-0.8942590	2.1779180
H	2.3190110	-1.1562340	-2.1201500
H	3.5463180	-1.3385640	0.0358860
N	2.0136960	2.6338390	-0.1908520
H	1.7578750	1.6507320	-0.1283670
H	1.1389760	3.1428740	-0.3012920
H	2.3696970	2.8880620	0.7283410

20
NH3...C6H5CH2OH

C	2.0866300	-0.0327810	-0.6292840
C	0.6551250	-0.3609280	-0.2595890
O	2.8896520	0.1518130	0.5403570
H	2.0914260	0.8799100	-1.2500900
H	2.4887450	-0.8526220	-1.2494400
C	0.2232110	-0.4594810	1.0673530
C	-0.2681200	-0.5730430	-1.2943140
H	3.7827310	0.3565110	0.2442410
C	-1.1123820	-0.7656640	1.3522380
H	0.9319640	-0.2966410	1.8722790
C	-1.5994780	-0.8782550	-1.0105940
H	0.0597440	-0.4982430	-2.3301850
C	-2.0270770	-0.9758180	0.3183970
H	-1.4361130	-0.8395160	2.3877270
H	-2.3025950	-1.0398060	-1.8240680
H	-3.0637730	-1.2134780	0.5431550
N	-1.4556320	2.6779080	0.0276600
H	-1.2279850	1.6852440	0.0280320
H	-0.8126740	3.1104840	0.6877600
H	-1.1867150	3.0241130	-0.8911280

19
NH3...C6H5CH3

C	-2.5201450	0.4436340	0.0196040
C	-1.1264900	-0.1415650	0.0182420
H	-2.6720590	1.1010860	0.8830740
H	-3.2783010	-0.3505330	0.0721610
H	-2.7084750	1.0183990	-0.8941850
C	-0.4390130	-0.3638580	1.2202070
C	-0.4887710	-0.4757400	-1.1852930
C	0.8495210	-0.9047590	1.2218080
H	-0.9201520	-0.1098260	2.1628140
C	0.7996110	-1.0169220	-1.1899710
H	-1.0089370	-0.3093090	-2.1267070
C	1.4741010	-1.2335870	0.0151710
H	1.3653900	-1.0692940	2.1648460
H	1.2763630	-1.2692020	-2.1342000
H	2.4763480	-1.6544420	0.0140290
N	1.5116960	2.4868300	-0.1586190
H	1.1178970	1.5488730	-0.1068480

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H        0.7457050        3.0942030       -0.4437300
H        1.7314640        2.7490080        0.8004650
18
NH3...C6H5CHO
C       -0.7528660       -0.3498000        0.2004370
C       -0.2661780       -0.4622510       -1.1139610
C        0.1079100       -0.5697660        1.2863380
C       -2.1701720       -0.0002920        0.4634690
C        1.0687390       -0.7916250       -1.3320050
H       -0.9509770       -0.2874940       -1.9391390
C        1.4462930       -0.8999890        1.0666570
H       -0.2804940       -0.4798020        2.2994340
O       -3.0115160        0.2134190       -0.3893120
H       -2.4280850        0.0568930        1.5494610
C        1.9250440       -1.0105050       -0.2427660
H        1.4497000       -0.8797380       -2.3462410
H        2.1134520       -1.0704730        1.9074640
H        2.9668880       -1.2675360       -0.4178360
N        1.4234900        2.6910600       -0.0017100
H        1.1787310        1.7031200       -0.0078160
H        0.8829510        3.1176210       -0.7522930
H        1.0429070        3.0679990        0.8644280
17
NH3...C6H5CN
C        0.8218150       -0.3579740        0.0025750
C        0.1359970       -0.5092690        1.2223030
C        0.1405000       -0.5287420       -1.2171070
C        2.2166930       -0.0293760        0.0025270
C       -1.2210310       -0.8290120        1.2151080
H        0.6706490       -0.3754450        2.1576410
C       -1.2165540       -0.8483700       -1.2098180
H        0.6786070       -0.4098510       -2.1524810
N        3.3485860        0.2372710        0.0024880
C       -1.8980010       -0.9986960        0.0026680
H       -1.7508640       -0.9459040        2.1564520
H       -1.7429110       -0.9802900       -2.1511260
H       -2.9558640       -1.2479020        0.0027040
N       -1.3379020        2.7102810       -0.0259050
H       -1.1045700        1.7198050       -0.0175680
H       -0.9579840        3.0944950        0.8368440
H       -0.7883650        3.1208590       -0.7780860
21
NH3...C6H5COCH3
C        2.7250250        0.1975830        1.0561880
C        1.9081590       -0.0736400       -0.2018910
H        3.7597990        0.4010550        0.7727280
H        2.3131750        1.0549530        1.6040020
H        2.6867880       -0.6661320        1.7324570
C        0.4442280       -0.3795250       -0.0423770
O        2.4323050       -0.0422490       -1.3057880
C       -0.3249490       -0.6323380       -1.1925000
C       -0.1795730       -0.4209730        1.2166190
C       -1.6834880       -0.9192130       -1.0848200
H        0.1671500       -0.5977160       -2.1599060
C       -1.5415730       -0.7085740        1.3246450
H        0.3970670       -0.2286650        2.1160690
C       -2.2952950       -0.9580450        0.1743560
H       -2.2697760       -1.1132530       -1.9794140
H       -2.0136510       -0.7380140        2.3032500
H       -3.3559080       -1.1820720        0.2575590
N       -1.6612770        2.6984210       -0.1854010
H       -1.4459210        1.7063650       -0.1113580
H       -1.2911030        3.1289950        0.6594130
H       -1.0923260        3.0518750       -0.9520190
22
NH3...C6H5COOCH3
C        3.6153310        0.2508350        0.5287460
O        2.2015100        0.0317740        0.7496810
H        3.7676350        1.1183990       -0.1217810
H        4.0672130       -0.6303260        0.0614060
H        4.0374200        0.4270100        1.5202580
C        1.4747950       -0.2108330       -0.3778260
C        0.0248090       -0.4281460       -0.0810560
O        1.9638480       -0.2436360       -1.4907440
C       -0.8321110       -0.6882990       -1.1631280
C       -0.5009320       -0.3817870        1.2212620
C       -2.1930910       -0.8988160       -0.9470430
H       -0.4120720       -0.7211450       -2.1635980
C       -1.8638130       -0.5930890        1.4329670
H        0.1570270       -0.1812440        2.0596690
C       -2.7118830       -0.8516810        0.3513180
H       -2.8498800       -1.0995730       -1.7894070
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H	-2.2649030	-0.5560490	2.4424810
H	-3.7732840	-1.0158580	0.5198470
N	-1.9263470	2.7463570	-0.2190490
H	-1.7553670	1.7482970	-0.1144970
H	-1.2763000	3.2072560	0.4145280
H	-1.6145510	2.9845280	-1.1584960
19			
NH3...C6H5COOH			
C	0.4566640	-0.3712760	-0.0172400
C	1.9107230	-0.0546160	-0.1225290
C	-0.2606850	-0.5654760	-1.2095320
C	-0.2064840	-0.4794860	1.2170510
O	2.5110210	0.1146970	1.0980370
O	2.5287970	0.0495630	-1.1640190
C	-1.6212000	-0.8635090	-1.1681490
H	0.2661360	-0.4784340	-2.1547800
C	-1.5687010	-0.7780530	1.2532020
H	0.3443500	-0.3301550	2.1394700
H	3.4420340	0.3137020	0.9078150
C	-2.2777710	-0.9703660	0.0630600
H	-2.1708560	-1.0126800	-2.0937910
H	-2.0777120	-0.8608280	2.2098940
H	-3.3393410	-1.2029320	0.0947030
N	-1.6539590	2.6966960	-0.0797380
H	-1.4353790	1.7030900	-0.0494100
H	-1.2698590	3.0924710	0.7765170
H	-1.0954750	3.0815050	-0.8395740
16			
NH3...C6H5F			
C	1.1367480	0.0736030	0.0100360
C	0.5970780	-0.3201580	-1.2113710
C	0.5610500	-0.2756830	1.2285170
F	2.2683930	0.8274910	0.0130040
C	-0.5667190	-1.0951840	-1.2044210
H	1.0828730	-0.0224950	-2.1354130
C	-0.6024510	-1.0510730	1.2154630
H	1.0195190	0.0557120	2.1550360
C	-1.1677960	-1.4616570	0.0039910
H	-1.0024370	-1.4119130	-2.1483540
H	-1.0660120	-1.3334330	2.1570370
H	-2.0718540	-2.0639290	0.0016200
N	-1.9248540	2.1907860	-0.0737650
H	-1.3605240	1.3435880	-0.0499890
H	-1.8567610	2.5961210	0.8582350
H	-1.4338200	2.8343380	-0.6921410
16			
NH3...C6H5H			
C	0.7509520	-0.7992760	-1.1121770
C	0.6489150	-1.3938270	0.1498940
C	0.7604760	0.5945510	-1.2299910
H	0.8228630	-1.4205490	-2.0016010
C	0.5564010	-0.5945500	1.2941510
H	0.6415120	-2.4772410	0.2414710
C	0.6679620	1.3938270	-0.0857350
H	0.8397890	1.0566920	-2.2109920
C	0.5659250	0.7992770	1.1763360
H	0.4770880	-1.0566910	2.2751510
H	0.6753650	2.4772420	-0.1773120
H	0.4940150	1.4205500	2.0657600
N	-2.8029440	-0.0000030	-0.2477720
H	-1.7877460	-0.0000020	-0.1656940
H	-3.1230350	-0.8119290	0.2763800
H	-3.1230360	0.8119370	0.2763700
24			
NH3...C6H5NCH32			
C	2.5486940	-0.2946460	-1.2144410
N	1.7874170	0.1871330	-0.0693580
H	2.6240810	-1.3956800	-1.2383360
H	3.5566100	0.1265840	-1.1757110
H	2.0836200	0.0341960	-2.1519100
C	2.5405130	0.5777140	1.1151570
C	0.4660520	-0.2233640	0.0795690
H	2.6167880	-0.2381270	1.8556470
H	2.0681950	1.4379750	1.6051050
H	3.5482880	0.8762020	0.8149030
C	-0.2382690	-0.0188630	1.2923580
C	-0.2311530	-0.8633490	-0.9754850
C	-1.5619220	-0.4335990	1.4320950
H	0.2447370	0.4654680	2.1329550
C	-1.5548410	-1.2711920	-0.8172620
H	0.2575890	-1.0457200	-1.9254060
C	-2.2378320	-1.0635090	0.3839010

H	-2.0678090	-0.2584330	2.3789170
H	-2.0551380	-1.7589950	-1.6508260
H	-3.2691490	-1.3839660	0.4999600
N	-1.9665480	2.3976980	-0.9041010
H	-1.6468350	1.4913670	-0.5656040
H	-2.7969010	2.2040860	-1.4610410
H	-2.2976130	2.8960800	-0.0797980
18			
NH3...C6H5NH2			
N	-2.3819870	0.6561510	0.0136310
C	-1.1491080	-0.0066950	0.0189770
H	-2.9559710	0.4663580	-0.7958560
H	-2.9072360	0.5704780	0.8724250
C	-0.5519310	-0.4220770	-1.1857380
C	-0.4814320	-0.2713470	1.2291820
C	0.6766710	-1.0822000	-1.1749980
H	-1.0584460	-0.2232260	-2.1284220
C	0.7468580	-0.9321460	1.2291210
H	-0.9330100	0.0449110	2.1676990
C	1.3375990	-1.3436460	0.0297880
H	1.1199340	-1.3943120	-2.1177130
H	1.2453210	-1.1263430	2.1759200
H	2.2942840	-1.8579950	0.0339750
N	1.7155440	2.3332500	-0.2107250
H	1.2340400	1.4382250	-0.1408040
H	0.9804410	3.0365760	-0.2539860
H	2.1738020	2.4681960	0.6884230
21			
NH3...C6H5NHCH3			
C	3.0552790	0.2999660	0.3571690
N	1.9889770	0.2000100	-0.6272930
H	2.8362190	1.0997580	1.0757220
H	3.2045790	-0.6356370	0.9233850
H	3.9843380	0.5556570	-0.1606360
C	0.7180360	-0.2352200	-0.2689160
H	2.2876960	-0.1156900	-1.5373400
C	0.2913160	-0.2825820	1.0737710
C	-0.1860200	-0.6465680	-1.2733540
C	-0.9953320	-0.7269900	1.3895690
H	0.9619500	0.0266050	1.8689520
C	-1.4640860	-1.0867870	-0.9445170
H	0.1305760	-0.6150800	-2.3147340
C	-1.8836790	-1.1320750	0.3916180
H	-1.3012580	-0.7544210	2.4329170
H	-2.1394340	-1.3975820	-1.7382960
H	-2.8815580	-1.4776580	0.6457800
N	-1.7651780	2.5418270	-0.1993680
H	-1.4166160	1.5874660	-0.1222560
H	-2.7647230	2.4551030	-0.3727170
H	-1.6814410	2.9401580	0.7338060
19			
NH3...C6H5NHOH			
N	-1.9646140	0.3265200	-0.5748890
C	-0.7041100	-0.2280840	-0.2445540
O	-2.9863570	0.0299420	0.4048600
H	-2.3118130	-0.0689940	-1.4450840
C	0.1621640	-0.5849080	-1.2930330
C	-0.2640960	-0.3380170	1.0824960
H	-3.2568390	0.9129910	0.6881990
C	1.4558060	-1.0238530	-1.0145040
H	-0.1814710	-0.5102160	-2.3232690
C	1.0297550	-0.7907200	1.3479380
H	-0.9410190	-0.0841410	1.8906300
C	1.8997690	-1.1307880	0.3078960
H	2.1145370	-1.2950750	-1.8358130
H	1.3582010	-0.8783830	2.3807750
H	2.9053500	-1.4809010	0.5231040
N	1.7439310	2.5589090	-0.0910240
H	1.4042930	1.5993480	-0.0548920
H	0.9505440	3.1203440	-0.3945860
H	1.9181310	2.8257090	0.8760000
18			
NH3...C6H5NO2			
N	1.9296910	-0.0142800	0.0002590
C	0.4775620	-0.3617250	0.0005970
O	2.4841210	0.1204950	1.0899160
O	2.4846000	0.1163730	-1.0896560
C	-0.1811180	-0.5169520	1.2217300
C	-0.1805810	-0.5215700	-1.2202290
C	-1.5379690	-0.8416160	1.2139170
H	0.3670080	-0.3840050	2.1471600
C	-1.5374360	-0.8462030	-1.2117850

H	0.3679510	-0.3921240	-2.1459140
C	-2.2160250	-1.0062090	0.0012240
H	-2.0648670	-0.9658540	2.1557480
H	-2.0639200	-0.9740040	-2.1533700
H	-3.2729350	-1.2590920	0.0014700
N	-1.6703250	2.6934800	-0.0056530
H	-1.4335730	1.7039900	-0.0037300
H	-1.2162840	3.0927680	0.8132820
H	-1.1953210	3.0946250	-0.8117030

17

NH3...C6H5NO

C	0.7734160	-0.3311680	-0.2159260
C	-0.0858300	-0.5666840	-1.2978120
C	0.3185820	-0.4462020	1.1089360
N	2.1302790	0.0302030	-0.5829070
C	-1.4138830	-0.9209890	-1.0580790
H	0.3083490	-0.4662800	-2.3060660
C	-1.0054290	-0.7994670	1.3403990
H	1.0152030	-0.2555950	1.9203890
O	2.8900110	0.2383210	0.3498420
C	-1.8709180	-1.0366510	0.2588400
H	-2.0902180	-1.1062590	-1.8880190
H	-1.3758030	-0.8934490	2.3581340
H	-2.9051250	-1.3125450	0.4490840
N	-1.4447220	2.6686290	0.0057060
H	-1.1815930	1.6857120	0.0106970
H	-0.9008820	3.1071750	0.7461490
H	-1.0845470	3.0498180	-0.8668460

20

NH3...C6H5OCF3

C	-2.0921370	0.0198340	0.0378160
O	-1.0314330	-0.1482810	0.8661420
F	-3.1649970	0.2533500	0.8089300
F	-1.9425420	1.0716490	-0.8105050
F	-2.3489590	-1.0752730	-0.7258080
C	0.2587830	-0.4120890	0.3701470
C	1.2244190	-0.5555130	1.3681980
C	0.5891950	-0.5279440	-0.9811070
C	2.5453380	-0.8198020	1.0073380
H	0.9306910	-0.4588570	2.4088180
C	1.9195910	-0.7932800	-1.3230200
H	-0.1586190	-0.4169460	-1.7558650
C	2.8996310	-0.9400230	-0.3399970
H	3.2970470	-0.9314650	1.7839380
H	2.1819700	-0.8843920	-2.3735350
H	3.9287110	-1.1458700	-0.6198430
N	2.2154880	2.7201240	-0.1170030
H	2.0262910	1.7206780	-0.0775750
H	1.4256020	3.1338370	-0.6084600
H	2.1509280	3.0537760	0.8426060

17

NH3...C6H5OH

C	1.1512160	-0.0143770	-0.0129230
C	0.5393810	-0.3937320	-1.2151690
C	0.5362280	-0.3098920	1.2112920
O	2.3538950	0.6450770	-0.0949700
C	-0.6827760	-1.0656670	-1.1828410
H	1.0295480	-0.1569320	-2.1550650
C	-0.6881170	-0.9835330	1.2293790
H	1.0161380	-0.0127370	2.1428740
H	2.6592130	0.8447490	0.7989220
C	-1.3045290	-1.3651290	0.0350790
H	-1.1528930	-1.3575790	-2.1187030
H	-1.1578570	-1.2085760	2.1836660
H	-2.2561400	-1.8886200	0.0517230
N	-1.7382290	2.3317650	-0.0957240
H	-1.2471320	1.4400390	-0.0642750
H	-1.7098660	2.6985340	0.8534760
H	-1.1529810	2.9521410	-0.6516880

20

NH3...C6H5OCH3

C	2.9219550	0.1972140	0.3360920
O	1.9520960	-0.0729730	-0.6777920
H	3.8571280	0.4007380	-0.1915470
H	2.6339190	1.0730320	0.9361060
H	3.0502240	-0.6688490	1.0020660
C	0.6768620	-0.3622400	-0.2681780
C	-0.2478510	-0.6221070	-1.2944650
C	0.2622050	-0.4106070	1.0716500
C	-1.5692400	-0.9259980	-0.9797350
H	0.0910630	-0.5801610	-2.3258160
C	-1.0711560	-0.7179730	1.3701580

H	0.9593340	-0.2134430	1.8784630	H	2.6790460	0.1259340	-1.2371740
C	-1.9921930	-0.9765210	0.3554850	C	-1.9803850	-1.0421050	0.0121370
H	-2.2750140	-1.1250760	-1.7825550	H	-1.8475010	-0.8949870	2.1626670
H	-1.3831200	-0.7531080	2.4112650	H	-1.7830610	-1.1017970	-2.1376340
H	-3.0244630	-1.2140980	0.5966850	H	-3.0306540	-1.3201720	0.0097830
N	-1.4565600	2.6766690	-0.0842140	N	-1.5048050	2.6500440	-0.1580570
H	-1.2199590	1.6866960	-0.0467270	H	-1.2446260	1.6669060	-0.1068780
H	-1.1313410	3.0735520	0.7952600	H	-1.6557660	2.9457230	0.8040880
H	-0.8621120	3.0772090	-0.8074150	H	-0.6683550	3.1407690	-0.4687950

20

NH3...C6H5SCH3

C	2.9010800	0.1619930	0.8656600
S	2.0304380	-0.0286680	-0.7287060
H	3.9415580	0.3820950	0.6091970
H	2.4840560	0.9933020	1.4434810
H	2.8571500	-0.7630680	1.4497780
C	0.3536890	-0.3830860	-0.2369910
C	-0.5793050	-0.5849860	-1.2719650
C	-0.0744930	-0.4692610	1.0966030
C	-1.9104210	-0.8666710	-0.9720370
H	-0.2600730	-0.5208950	-2.3096560
C	-1.4136230	-0.7526900	1.3849350
H	0.6229740	-0.3181750	1.9131210
C	-2.3380060	-0.9527300	0.3585300
H	-2.6176940	-1.0198220	-1.7835710
H	-1.7293080	-0.8160240	2.4236750
H	-3.3768190	-1.1725720	0.5889310
N	-1.7099310	2.7035060	0.0477570
H	-1.4982840	1.7071650	0.0513300
H	-0.9253960	3.1528280	0.5165150
H	-1.6491870	2.9939050	-0.9262250

17

NH3...C6H5SH

C	0.7350550	-0.3231800	0.0180690
C	0.0336340	-0.4457960	1.2284270
C	0.0701530	-0.5622290	-1.1938440
S	2.4602010	0.1372630	0.0929670
C	-1.3155070	-0.8033250	1.2189940
H	0.5392640	-0.2627930	2.1733980
C	-1.2799480	-0.9193820	-1.1911670
H	0.6040550	-0.4699950	-2.1362150

17
OH2...C6H5CCH
C 0.7876970 -0.3671440 0.0002480
C 0.0847080 -0.4977800 -1.2152610
C 0.0846460 -0.4950900 1.2160070
C 2.1919410 -0.1088930 -0.0000020
C -1.2866680 -0.7499810 -1.2097700
H 0.6244820 -0.3995530 -2.1524910
C -1.2867310 -0.7473020 1.2110030
H 0.6243710 -0.3947890 2.1530450
C 3.3838640 0.1103100 -0.0002140
C -1.9765710 -0.8755140 0.0007390
H -1.8187280 -0.8488780 -2.1524950
H -1.8188390 -0.8441130 2.1539170
H 4.4329760 0.3032490 -0.0004000
H -3.0456060 -1.0721170 0.0009290
O -1.1950920 2.6201010 -0.0031090
H -1.0203420 1.6698950 -0.0020530
H -0.3148990 3.0138660 0.0079190
18
OH2...C6H5CF3
C 1.6632180 -0.0116560 -0.0000170
C 0.1886220 -0.3475460 0.0005490
F 2.0304170 0.7063450 -1.0963630
F 2.4322880 -1.1423600 0.0028310
F 2.0301150 0.7117070 1.0927860
C -0.4905860 -0.5052260 -1.2127100
C -0.4909030 -0.4993670 1.2144140
C -1.8516350 -0.8152450 -1.2089610
H 0.0429020 -0.3859960 -2.1501720
C -1.8519480 -0.8094010 1.2118630
H 0.0423640 -0.3756070 2.1514160
C -2.5335890 -0.9676260 0.0017290
H -2.3782550 -0.9375050 -2.1514670
H -2.3788630 -0.9271210 2.1547800
H -3.5932820 -1.2090090 0.0021670
O -1.9045320 2.5599050 -0.0067140
H -1.6900470 1.6182990 -0.0044130
H -1.0430270 2.9928640 0.0169060
19
OH2...C6H5CH2OH
C 2.0944130 -0.1178830 -0.6157370
C 0.6544470 -0.3749610 -0.2233430
O 2.8895650 0.2019770 0.5298640
H 2.1196930 0.7082660 -1.3473580
H 2.4888540 -1.0158440 -1.1222060
C 0.2088470 -0.2974940 1.1004680
C -0.2625900 -0.7031620 -1.2329740
H 3.7885220 0.3540100 0.2201240
C -1.1340890 -0.5450060 1.4070250
H 0.9127370 -0.0441910 1.8860440
C -1.6012660 -0.9499220 -0.9276500
H 0.0759250 -0.7656130 -2.2662330
C -2.0425540 -0.8712780 0.3981160
H -1.4684530 -0.4817250 2.4398310
H -2.2994220 -1.2031180 -1.7218040
H -3.0849840 -1.0629350 0.6396660
O -1.3772300 2.5570050 -0.3284200
H -1.1764220 1.6191620 -0.2059470
H -0.9583760 2.9783680 0.4308970
18
OH2...C6H5CH3
C -2.5438840 0.1858770 -0.0017490
C -1.0930720 -0.2382350 0.0011080
H -2.7820340 0.7863070 0.8835020
H -3.2079540 -0.6900370 0.0052610
H -2.7825060 0.7725720 -0.8959990
C -0.4027430 -0.4305710 1.2066000
C -0.4038500 -0.4491820 -1.2019430
C 0.9385770 -0.8226540 1.2121050
H -0.9234670 -0.2709340 2.1488830
C 0.9374430 -0.8413050 -1.2027240
H -0.9255010 -0.3041020 -2.1460640
C 1.6141850 -1.0296450 0.0059090
H 1.4557200 -0.9664030 2.1578400
H 1.4536350 -0.9996300 -2.1466440
H 2.6575400 -1.3346480 0.0078020
O 1.1877410 2.5207910 -0.0213000
H 0.9164040 1.5926450 -0.0140040
H 0.3563020 3.0021940 0.0539840
17
OH2...C6H5CHO

C	0.7410100	-0.3559270	-0.1815620
C	0.2454370	-0.3579100	1.1343240
C	-0.1212990	-0.6284850	-1.2542390
C	2.1693710	-0.0689470	-0.4599990
C	-1.0997680	-0.6305510	1.3669690
H	0.9316170	-0.1441280	1.9491010
C	-1.4700020	-0.9017490	-1.0199210
H	0.2740460	-0.6240740	-2.2686340
O	3.0130820	0.1810020	0.3805040
H	2.4336120	-0.0986190	-1.5455700
C	-1.9575620	-0.9024010	0.2909140
H	-1.4876230	-0.6332560	2.3824150
H	-2.1383540	-1.1129340	-1.8504810
H	-3.0074560	-1.1147990	0.4773640
O	-1.3067160	2.5866400	-0.2013250
H	-1.1029790	1.6456710	-0.1260140
H	-0.5969160	3.0168280	0.2894790

16

OH2...C6H5CN

C	-0.8057310	-0.3544700	0.0005280
C	-0.1172740	-0.4957020	-1.2189200
C	-0.1171040	-0.4896780	1.2205640
C	-2.2107610	-0.0724200	-0.0000700
C	1.2496440	-0.7700840	-1.2110960
H	-0.6576230	-0.3895540	-2.1545350
C	1.2498130	-0.7640960	1.2139050
H	-0.6573230	-0.3789100	2.1557180
N	-3.3508920	0.1564530	-0.0005560
C	1.9338800	-0.9044290	0.0016960
H	1.7815170	-0.8791920	-2.1522230
H	1.7818160	-0.8685540	2.1554850
H	2.9994420	-1.1183330	0.0021500
O	1.2174650	2.6178070	-0.0069520
H	1.0274570	1.6712890	-0.0046020
H	0.3464340	3.0309060	0.0178770

20

OH2...C6H5COCH3

C	-2.7367960	-0.2353520	-1.0395040
C	-1.9081730	0.0084690	0.2164940
H	-3.7728500	0.0491880	-0.8442180
H	-2.3416220	0.3498770	-1.8798300
H	-2.6893100	-1.2923280	-1.3316550
C	-0.4406800	-0.3177350	0.1700390
O	-2.4260030	0.4561730	1.2292700
C	0.3393170	-0.0990570	1.3198720
C	0.1760010	-0.8332420	-0.9831620
C	1.7014550	-0.3890220	1.3151600
H	-0.1473520	0.2994620	2.2050660
C	1.5416080	-1.1239680	-0.9879540
H	-0.4090210	-1.0089480	-1.8805930
C	2.3061030	-0.9023260	0.1609250
H	2.2961220	-0.2166690	2.2086650
H	2.0081120	-1.5222560	-1.8852460
H	3.3695310	-1.1284290	0.1580670
O	1.5856730	2.4515140	-0.8564310
H	1.3954730	1.5531550	-0.5565550
H	1.1405420	3.0088630	-0.2076340

21

OH2...C6H5COOCH3

C	-3.6205360	0.1582320	-0.5602010
O	-2.2047010	-0.0769410	-0.7493920
H	-3.7811920	1.1101550	-0.0434030
H	-4.0633870	-0.6493980	0.0319690
H	-4.0448170	0.1831930	-1.5660120
C	-1.4750830	-0.1447180	0.4000900
C	-0.0231370	-0.3889100	0.1355560
O	-1.9632740	-0.0190180	1.5067540
C	0.8368330	-0.4794180	1.2424110
C	0.5015180	-0.5285710	-1.1605220
C	2.1997470	-0.7059480	1.0568680
H	0.4176020	-0.3695480	2.2377130
C	1.8663420	-0.7552170	-1.3416220
H	-0.1587940	-0.4594020	-2.0179930
C	2.7174470	-0.8443300	-0.2353960
H	2.8588940	-0.7747610	1.9182870
H	2.2665800	-0.8624490	-2.3464480
H	3.7803570	-1.0209970	-0.3801050
O	1.8713740	2.6351310	-0.1897610
H	1.7185270	1.6820940	-0.1489370
H	1.3602480	2.9810160	0.5510160

18

OH2...C6H5COOH

C	-0.4508320	-0.3442210	0.0833960
C	-1.9095350	-0.0353150	0.1324870
C	0.2754500	-0.2747450	1.2840430
C	0.2081020	-0.6966390	-1.1067960
O	-2.5184970	-0.1331880	-1.0916020
O	-2.5242620	0.2737290	1.1345700
C	1.6406150	-0.5535910	1.2943530
H	-0.2482120	-0.0010710	2.1948060
C	1.5750030	-0.9748910	-1.0912700
H	-0.3496280	-0.7512160	-2.0355230
H	-3.4518280	0.0864990	-0.9392750
C	2.2929650	-0.9041470	0.1069490
H	2.1971800	-0.4982040	2.2262090
H	2.0807300	-1.2470520	-2.0139690
H	3.3581670	-1.1216060	0.1156310
O	1.5778360	2.5570900	-0.4847860
H	1.3863080	1.6256880	-0.3150330
H	0.9560570	3.0272070	0.0827260
15			
OH2...C6H5F			
C	1.1191430	-0.1223260	0.0000260
C	0.4993410	-0.3773510	-1.2201930
C	0.4992500	-0.3765460	1.2203670
F	2.3769280	0.3943490	-0.0000970
C	-0.7940150	-0.9086350	-1.2100610
H	1.0241350	-0.1620950	-2.1457790
C	-0.7941050	-0.9078370	1.2104890
H	1.0239740	-0.1606800	2.1458510
C	-1.4422790	-1.1745130	0.0002780
H	-1.2937380	-1.1142380	-2.1530250
H	-1.2938990	-1.1128180	2.1535510
H	-2.4471090	-1.5872790	0.0003760
O	-1.4075090	2.4115820	-0.0009040
H	-1.0403750	1.5178390	-0.0005950
H	-0.6292860	2.9807270	0.0022800
15			
OH2...C6H5H			
C	-0.6032580	0.2189240	-1.3868630
C	-0.5048500	1.3243220	-0.5353140
C	-0.7178560	-1.0683330	-0.8515500
H	-0.5906740	0.3602830	-2.4648640
C	-0.5210400	1.1424620	0.8515500
H	-0.4157730	2.3249000	-0.9514090
C	-0.7340450	-1.2501930	0.5353140
H	-0.7943480	-1.9275530	-1.5134540
C	-0.6356370	-0.1447950	1.3868640
H	-0.4445470	2.0016820	1.5134540
H	-0.8231220	-2.2507710	0.9514100
H	-0.6482220	-0.2861540	2.4648640
O	2.6669540	-0.2555070	0.0000000
H	1.7040430	-0.1697840	0.0000000
H	2.9771240	0.6571310	0.0000010
23			
OH2...C6H5NCH32			
C	-2.5336860	-1.2498200	-0.1230590
N	-1.7837520	-0.0352510	0.1689860
H	-2.5788180	-1.4685370	-1.2041020
H	-3.5527260	-1.1401180	0.2568780
H	-2.0796250	-2.1128480	0.3792270
C	-2.5450330	1.1974560	0.3228340
C	-0.4513180	0.0425740	-0.2250370
H	-2.5974310	1.7815390	-0.6130290
H	-2.0956080	1.8334070	1.0953400
H	-3.5612070	0.9517970	0.6420530
C	0.2494350	1.2745080	-0.2193320
C	0.2611990	-1.1070500	-0.6487100
C	1.5842560	1.3425440	-0.6158350
H	-0.2450940	2.1861410	0.0950550
C	1.5958990	-1.0195980	-1.0417050
H	-0.2241620	-2.0757080	-0.6732900
C	2.2752210	0.2013920	-1.0313960
H	2.0869470	2.3069280	-0.5973250
H	2.1078220	-1.9248740	-1.3602800
H	3.3151790	0.2619480	-1.3389610
O	1.8663500	-0.4307410	2.4636040
H	1.5872030	-0.2677330	1.5518290
H	2.7771460	-0.7313000	2.3683110
17			
OH2...C6H5NH2			
N	-2.4319790	0.3691480	-0.0000240
C	-1.1243200	-0.1302640	-0.0000150
H	-2.9596400	0.1612390	-0.8361440

H	-2.9596550	0.1612580	0.8360940
C	-0.4535000	-0.3864610	-1.2103310
C	-0.4535690	-0.3864280	1.2103160
C	0.8494550	-0.8840750	-1.2048950
H	-0.9615860	-0.1924190	-2.1531710
C	0.8493900	-0.8840440	1.2049240
H	-0.9616880	-0.1923680	2.1531360
C	1.5132160	-1.1375710	0.0000320
H	1.3488840	-1.0748160	-2.1518890
H	1.3488070	-1.0747740	2.1519250
H	2.5279280	-1.5251010	0.0000780
O	1.3697410	2.4364810	-0.0000030
H	1.0247110	1.5330560	0.0000000
H	0.5741330	2.9810930	-0.0000250
20			
OH2...C6H5NHCH3			
C	3.0583420	0.1989270	0.3710350
N	1.9866090	0.2024360	-0.6125960
H	2.8684330	0.9545930	1.1436120
H	3.1774090	-0.7777070	0.8712860
H	3.9941220	0.4580870	-0.1327550
C	0.7026330	-0.2133480	-0.2784080
H	2.2720030	-0.0601220	-1.5435630
C	0.2781880	-0.3380950	1.0600340
C	-0.2175460	-0.5244090	-1.3040440
C	-1.0219110	-0.7595900	1.3511960
H	0.9610550	-0.1067400	1.8710990
C	-1.5088910	-0.9429070	-0.9996310
H	0.0971160	-0.4324040	-2.3424180
C	-1.9261610	-1.0653780	0.3323800
H	-1.3257660	-0.8480430	2.3917570
H	-2.1965200	-1.1758040	-1.8093840
H	-2.9344780	-1.3938190	0.5673510
O	-1.6354470	2.4827420	-0.0053780
H	-1.3352720	1.5634210	0.0041290
H	-2.5887180	2.4083550	0.1147190
18			
OH2...C6H5NHOH			
N	1.9605400	0.3335890	0.5538950
C	0.6837630	-0.2042970	0.2604700
O	2.9815270	-0.0956000	-0.3762700
H	2.2823650	0.0134830	1.4639380
C	-0.2075160	-0.4237890	1.3256020
C	0.2552600	-0.4285410	-1.0559120
H	3.2886460	0.7446220	-0.7408520
C	-1.5136050	-0.8403270	1.0718550
H	0.1267760	-0.2603700	2.3486340
C	-1.0517120	-0.8574600	-1.2952870
H	0.9506450	-0.2807360	-1.8746620
C	-1.9459940	-1.0609850	-0.2402540
H	-2.1916240	-1.0047470	1.9056980
H	-1.3712910	-1.0345920	-2.3194000
H	-2.9616040	-1.3935030	-0.4353290
O	-1.6089990	2.4959720	-0.1939520
H	-1.3210890	1.5749630	-0.1336570
H	-0.8280020	2.9951760	0.0712940
17			
OH2...C6H5NO2			
N	1.9258300	-0.0375530	0.0006810
C	0.4655400	-0.3487420	0.0111110
O	2.4828340	0.1214870	1.0857450
O	2.4844010	0.0411360	-1.0923490
C	-0.1974510	-0.4448260	1.2359910
C	-0.1956950	-0.5348510	-1.2043120
C	-1.5619240	-0.7358970	1.2376130
H	0.3532950	-0.2931990	2.1569830
C	-1.5601800	-0.8253220	-1.1864430
H	0.3563810	-0.4514660	-2.1331800
C	-2.2431880	-0.9259730	0.0304570
H	-2.0922530	-0.8140490	2.1824660
H	-2.0891550	-0.9729080	-2.1237300
H	-3.3060380	-1.1524670	0.0380480
O	-1.5737610	2.6055080	-0.0993410
H	-1.3724680	1.6620920	-0.0643920
H	-0.7209810	3.0334940	0.0400930
16			
OH2...C6H5NO			
C	0.7572910	-0.3338060	-0.2127350
C	-0.1076640	-0.5476090	-1.2945810
C	0.2956800	-0.4199510	1.1119770
N	2.1272750	-0.0257460	-0.5795920
C	-1.4483220	-0.8508300	-1.0549590

H	0.2921120	-0.4709590	-2.3027170
C	-1.0408840	-0.7223560	1.3433290
H	0.9970590	-0.2475490	1.9234030
O	2.8921010	0.1629560	0.3531240
C	-1.9121380	-0.9375960	0.2618100
H	-2.1291940	-1.0188120	-1.8848690
H	-1.4166550	-0.7933750	2.3609470
H	-2.9561700	-1.1736750	0.4519680
O	-1.3153320	2.5959640	-0.0216890
H	-1.1000440	1.6550170	-0.0078590
H	-0.4559690	3.0311100	-0.0642540
19			
OH2...C6H5OCF3			
C	-2.0895410	0.0055180	0.0356980
O	-1.0299990	-0.1918050	0.8590530
F	-3.1693220	0.1794610	0.8128670
F	-1.9527070	1.1048320	-0.7524170
F	-2.3257960	-1.0494940	-0.7886040
C	0.2663700	-0.4078630	0.3560520
C	1.2297210	-0.5913890	1.3497320
C	0.6045170	-0.4436830	-0.9977790
C	2.5562000	-0.8149300	0.9817930
H	0.9299250	-0.5569860	2.3925400
C	1.9404050	-0.6691710	-1.3468080
H	-0.1415180	-0.3015260	-1.7691540
C	2.9182760	-0.8549570	-0.3682390
H	3.3061310	-0.9577910	1.7549910
H	2.2088130	-0.6979740	-2.3993540
H	3.9516810	-1.0291300	-0.6536000
O	2.1486140	2.6188590	0.0503700
H	1.9837950	1.6671450	0.0343840
H	1.2869960	3.0054820	-0.1445030
16			
OH2...C6H5OH			
C	-1.1378840	-0.1167320	0.0383240
C	-0.4510730	-0.2882470	1.2476720
C	-0.5265010	-0.4703050	-1.1722280
O	-2.4085640	0.4025300	0.0998540
C	0.8418430	-0.8121170	1.2360570
H	-0.9395320	-0.0091060	2.1767750
C	0.7691950	-0.9940480	-1.1696040
H	-1.0648490	-0.3349210	-2.1094120
H	-2.7608380	0.4662280	-0.7967940
C	1.4605940	-1.1681080	0.0318970
H	1.3699620	-0.9430040	2.1773440
H	1.2355590	-1.2655460	-2.1134040
H	2.4675770	-1.5753750	0.0313580
O	1.3890650	2.3992500	-0.2317500
H	1.0278090	1.5059260	-0.1532820
H	1.0832620	2.8389030	0.5698790
19			
OH2...C6H5OCH3			
C	-2.9354580	0.1617900	-0.3381890
O	-1.9514380	0.0167170	0.6876020
H	-3.8663870	0.4164020	0.1745660
H	-2.6627360	0.9659370	-1.0374810
H	-3.0631190	-0.7754740	-0.8996830
C	-0.6783070	-0.3068610	0.2975840
C	0.2606170	-0.4406390	1.3350890
C	-0.2786810	-0.5040430	-1.0331450
C	1.5811310	-0.7675670	1.0404160
H	-0.0667700	-0.2843340	2.3591460
C	1.0540250	-0.8324790	-1.3114570
H	-0.9869160	-0.4057130	-1.8483400
C	1.9891260	-0.9662990	-0.2855930
H	2.2979830	-0.8681830	1.8517540
H	1.3542870	-0.9833490	-2.3456430
H	3.0207690	-1.2213400	-0.5111350
O	1.3891500	2.5582900	-0.2456390
H	1.1731330	1.6187520	-0.1712940
H	1.3433490	2.8738330	0.6641820
19			
OH2...C6H5SCH3			
C	2.8955900	0.3675150	0.8160280
S	2.0416420	-0.2099890	-0.6918290
H	3.9417130	0.5065610	0.5277510
H	2.4821570	1.3211760	1.1602150
H	2.8331550	-0.3805010	1.6131700
C	0.3548650	-0.4140710	-0.1514400
C	-0.5682140	-0.8612220	-1.1160090
C	-0.0901800	-0.1582280	1.1545920
C	-1.9062190	-1.0462890	-0.7744460

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H       -0.2358950       -1.0630370       -2.1317130
C       -1.4360830       -0.3478260        1.4852520
H        0.5993680        0.1869580        1.9170610
C       -2.3506310       -0.7911000        0.5286350
H       -2.6056580       -1.3921300       -1.5317170
H       -1.7648570       -0.1450460        2.5018330
H       -3.3947770       -0.9364620        0.7916490
O       -1.6431420        2.5177610       -0.6429570
H       -1.4541700        1.6016040       -0.3990930
H       -1.3169330        3.0259200        0.1080910
16
OH2...C6H5SH
C       -0.7151470       -0.3247320       -0.0081080
C       -0.0191450       -0.4572100       -1.2205540
C       -0.0317740       -0.5004240        1.2043710
S       -2.4575020        0.0659170       -0.0811650
C        1.3429630       -0.7616710       -1.2126140
H       -0.5390550       -0.3231070       -2.1659810
C        1.3311820       -0.8048460        1.2001870
H       -0.5613400       -0.4000340        2.1483530
H       -2.6651240        0.0870190        1.2506560
C        2.0262610       -0.9372510       -0.0051970
H        1.8705900       -0.8616040       -2.1578990
H        1.8485660       -0.9384120        2.1471140
H        3.0865750       -1.1741600       -0.0040110
O        1.3728860        2.5790270        0.0539560
H        1.1622060        1.6360150        0.0360530
H        0.5284830        3.0041970       -0.1358020
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16
FH...C6H5CCH
C -0.4800890 0.7229370 0.0000000
C -0.4800890 0.0081270 1.2156350
C -0.4800890 0.0081270 -1.2156350
C -0.4800890 2.1507310 0.0000000
C -0.4800890 -1.3862480 1.2103870
H -0.4800890 0.5569280 2.1527690
C -0.4800890 -1.3862480 -1.2103870
H -0.4800890 0.5569280 -2.1527690
C -0.4800890 3.3626420 0.0000000
C -0.4800890 -2.0876890 0.0000000
H -0.4800890 -1.9272550 2.1532070
H -0.4800890 -1.9272550 -2.1532070
H -0.4800890 4.4293480 0.0000000
H -0.4800890 -3.1746520 0.0000000
F 2.6853490 -0.6868320 0.0000000
H 1.7566860 -0.6868320 0.0000000
17
FH...C6H5CF3
C -1.6701780 -0.0026130 -0.0000430
C -0.1934700 -0.3290900 0.0000280
F -2.0418340 0.7157010 1.0945950
F -2.4320190 -1.1382050 -0.0000410
F -2.0418010 0.7157280 -1.0945600
C 0.4868610 -0.4794750 1.2135840
C 0.4868800 -0.4795320 -1.2135470
C 1.8498600 -0.7808130 1.2104240
H -0.0472760 -0.3613660 2.1508190
C 1.8498760 -0.7808680 -1.2104070
H -0.0472670 -0.3614600 -2.1507820
C 2.5326420 -0.9317910 0.0000250
H 2.3773510 -0.8974120 2.1531610
H 2.3774300 -0.8975230 -2.1530990
H 3.5938530 -1.1664090 0.0000450
F 1.8532320 2.4656440 -0.0000490
H 1.6528840 1.5594410 -0.0000290
18
FH...C6H5CH2OH
C 2.0928480 -0.0677500 -0.6229170
C 0.6510570 -0.3387950 -0.2469700
O 2.8964570 0.1425280 0.5419760
H 2.1264090 0.8176040 -1.2812880
H 2.4733970 -0.9240900 -1.2062620
C 0.2114660 -0.3691790 1.0807620
C -0.2740300 -0.5674440 -1.2765150
H 3.7962000 0.3088580 0.2420190
C -1.1334980 -0.6246030 1.3715350
H 0.9215930 -0.1932020 1.8817030
C -1.6147280 -0.8220690 -0.9869270
H 0.0597700 -0.5455890 -2.3129600
C -2.0499840 -0.8515020 0.3428330
H -1.4631360 -0.6456460 2.4075790
H -2.3191520 -0.9972790 -1.7964330
H -3.0939680 -1.0496100 0.5721580
F -1.3153040 2.4847720 -0.0852380
H -1.1338220 1.5738290 -0.0459980
17
FH...C6H5CH3
C -2.5535080 0.1847140 -0.0000160
C -1.0974310 -0.2209640 0.0001400
H -2.7995260 0.7752030 0.8897590
H -3.2064090 -0.6995840 -0.0000480
H -2.7992870 0.7752380 -0.8897950
C -0.4050800 -0.4138510 1.2043830
C -0.4052250 -0.4138290 -1.2042320
C 0.9411070 -0.7889130 1.2073900
H -0.9280720 -0.2681330 2.1476650
C 0.9409360 -0.7888830 -1.2075110
H -0.9283920 -0.2680760 -2.1474100
C 1.6196510 -0.9779700 -0.0001010
H 1.4597480 -0.9334040 2.1521910
H 1.4593810 -0.9333340 -2.1524210
H 2.6667920 -1.2697150 -0.0001520
F 1.1082570 2.4235510 -0.0000110
H 0.8587520 1.5280190 -0.0000040
16
FH...C6H5CHO
C 0.7456810 -0.3254410 -0.1943750
C 0.2527340 -0.3936960 1.1207280
C -0.1202170 -0.5369600 -1.2778800
C 2.1749970 -0.0317690 -0.4606640

C	-1.0934430	-0.6710870	1.3418480
H	0.9416760	-0.2264510	1.9440120
C	-1.4698920	-0.8150430	-1.0551140
H	0.2731180	-0.4815330	-2.2915520
O	3.0217120	0.1694220	0.3898440
H	2.4369060	-0.0059660	-1.5468990
C	-1.9548290	-0.8817470	0.2549970
H	-1.4792770	-0.7249040	2.3566420
H	-2.1410230	-0.9789620	-1.8940640
H	-3.0054690	-1.0981080	0.4324670
F	-1.2600850	2.5002570	-0.0521110
H	-1.0690480	1.5926870	-0.0276070
15			
FH...C6H5CN			
C	-0.4825070	0.7348190	0.0000000
C	-0.4825070	0.0325410	-1.2197460
C	-0.4825070	0.0325410	1.2197460
C	-0.4825070	2.1678790	0.0000000
C	-0.4825070	-1.3616470	-1.2125040
H	-0.4825070	0.5836030	-2.1551330
C	-0.4825070	-1.3616470	1.2125040
H	-0.4825070	0.5836030	2.1551330
N	-0.4825070	3.3307560	0.0000000
C	-0.4825070	-2.0594470	0.0000000
H	-0.4825070	-1.9041970	-2.1538610
H	-0.4825070	-1.9041970	2.1538610
H	-0.4825070	-3.1462670	0.0000000
F	2.6982820	-0.6638070	0.0000000
H	1.7708350	-0.6638070	0.0000000
19			
FH...C6H5COCH3			
C	2.7349140	-1.0643250	-0.0983200
C	1.9112720	0.2159370	-0.0199700
H	3.7745910	-0.8351220	0.1446760
H	2.3453710	-1.8149320	0.6014290
H	2.6743960	-1.4988610	-1.1044610
C	0.4399330	0.1298180	-0.3197120
O	2.4360190	1.2789700	0.2782020
C	-0.3355570	1.3013090	-0.2522290
C	-0.1846900	-1.0813080	-0.6645870
C	-1.7010510	1.2611780	-0.5230350
H	0.1572410	2.2313110	0.0151330
C	-1.5536630	-1.1216120	-0.9360960
H	0.3967550	-1.9962580	-0.7219650
C	-2.3136160	0.0492920	-0.8657250
H	-2.2921860	2.1718100	-0.4683260
H	-2.0263130	-2.0636300	-1.2017980
H	-3.3796600	0.0188130	-1.0769860
F	-1.5296610	-0.4752830	2.4561740
H	-1.3566490	-0.3090820	1.5591610
20			
FH...C6H5COOCH3			
C	3.6235730	-0.5794200	-0.0762950
O	2.2055990	-0.6621900	-0.3559220
H	3.7922090	-0.4711910	1.0002250
H	4.0630510	0.2788520	-0.5952130
H	4.0446750	-1.5167930	-0.4454840
C	1.4793620	0.4243850	0.0316090
C	0.0249700	0.2756460	-0.2852140
O	1.9720340	1.3960140	0.5720250
C	-0.8319060	1.3317730	0.0658260
C	-0.5048830	-0.8652290	-0.9115070
C	-2.1968900	1.2489970	-0.2048080
H	-0.4086660	2.2068680	0.5490730
C	-1.8717640	-0.9438610	-1.1805150
H	0.1530260	-1.6830320	-1.1842830
C	-2.7197690	0.1111410	-0.8284980
H	-2.8536190	2.0703030	0.0698150
H	-2.2760260	-1.8287690	-1.6651530
H	-3.7842930	0.0465790	-1.0395640
F	-1.8308570	-1.1384460	2.2748700
H	-1.6898650	-0.7479990	1.4443390
17			
FH...C6H5COOH			
C	0.4534520	-0.3359240	0.0199540
C	1.9146950	-0.0683680	-0.1172750
C	-0.2695490	-0.6437780	-1.1446740
C	-0.2109620	-0.2902800	1.2574600
O	2.5201000	0.2207470	1.0780090
O	2.5341330	-0.0955160	-1.1628030
C	-1.6368830	-0.9021960	-1.0728590
H	0.2583380	-0.6750490	-2.0928130

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C       -1.5800150       -0.5497680        1.3241310
H        0.3442240       -0.0529130        2.1585700
H        3.4555050        0.3747010        0.8685110
C       -2.2946920       -0.8557110        0.1614450
H       -2.1908900       -1.1397900       -1.9771890
H       -2.0899810       -0.5134210        2.2832010
H       -3.3615830       -1.0574380        0.2168390
F       -1.5283010        2.4840380       -0.3476290
H       -1.3510540        1.5818830       -0.2191910
14
FH...C6H5F
C       -0.5124000        1.0043260        0.0000000
C       -0.5124000        0.3342190        1.2202800
C       -0.5124000        0.3342190       -1.2202800
F       -0.5124000        2.3640970        0.0000000
C       -0.5124000       -1.0640070        1.2102750
H       -0.5124000        0.9015270        2.1458150
C       -0.5124000       -1.0640070       -1.2102750
H       -0.5124000        0.9015270       -2.1458150
C       -0.5124000       -1.7647860        0.0000000
H       -0.5124000       -1.6042880        2.1532880
H       -0.5124000       -1.6042880       -2.1532880
H       -0.5124000       -2.8510910        0.0000000
F        2.6548630       -0.3700060        0.0000000
H        1.7262230       -0.3700060        0.0000000
14
FH...C6H5H
C        0.0000000        1.3988300       -0.5895920
C       -1.2114220        0.6994150       -0.5895920
C        1.2114220        0.6994150       -0.5895920
H        0.0000000        2.4861320       -0.5895920
C       -1.2114220       -0.6994150       -0.5895920
H       -2.1530540        1.2430660       -0.5895920
C        1.2114220       -0.6994150       -0.5895920
H        2.1530540        1.2430660       -0.5895920
C        0.0000000       -1.3988300       -0.5895920
H       -2.1530540       -1.2430660       -0.5895920
H        2.1530540       -1.2430660       -0.5895920
H        0.0000000       -2.4861320       -0.5895920
F        0.0000000        0.0000000        2.5691900
H        0.0000000        0.0000000        1.6401350
22
FH...C6H5NCH32
C        2.5247900        1.2434060        0.0479760
N        1.7713450       -0.0005560        0.1359980
H        2.5405800        1.6559560       -0.9757830
H        3.5533120        1.0612770        0.3701550
H        2.0944110        2.0021210        0.7131120
C        2.5241740       -1.2441670        0.0387170
C        0.4272540        0.0012600       -0.2247050
H        2.5432730       -1.6474540       -0.9892590
H        2.0910230       -2.0085730        0.6954090
H        3.5516860       -1.0658150        0.3662370
C       -0.2855670       -1.2076290       -0.4227440
C       -0.2855580        1.2123170       -0.4092490
C       -1.6320170       -1.1957250       -0.7840230
H        0.2085990       -2.1637000       -0.2954550
C       -1.6319830        1.2044920       -0.7706310
H        0.2087370        2.1668390       -0.2712740
C       -2.3231370        0.0054180       -0.9628010
H       -2.1437680       -2.1448530       -0.9266530
H       -2.1437220        2.1551590       -0.9026650
H       -3.3721930        0.0070250       -1.2443260
F       -1.7680240       -0.0135330        2.4331870
H       -1.5268700       -0.0085220        1.5345920
16
FH...C6H5NH2
N       -2.4463780        0.3388630       -0.0000250
C       -1.1268070       -0.1281650       -0.0000150
H       -2.9687550        0.1180080       -0.8361440
H       -2.9687690        0.1180330        0.8360940
C       -0.4498750       -0.3677550       -1.2103300
C       -0.4499450       -0.3677140        1.2103170
C        0.8649490       -0.8331020       -1.2048920
H       -0.9625900       -0.1862990       -2.1531700
C        0.8648830       -0.8330630        1.2049270
H       -0.9626930       -0.1862340        2.1531370
C        1.5347570       -1.0701550        0.0000360
H        1.3689280       -1.0114790       -2.1518860
H        1.3688500       -1.0114220        2.1519280
H        2.5587120       -1.4325570        0.0000830
F        1.2573450        2.3696250       -0.0000130
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H        0.9470870        1.4930020       -0.0000070
19
FH...C6H5NHCH3
C        3.0449590        0.0905180        0.3686340
N        1.9723810        0.1535920       -0.6120570
H        2.8864130        0.8393210        1.1548460
H        3.1263580       -0.8987260        0.8513500
H        3.9892950        0.3214770       -0.1329020
C        0.6736330       -0.2171400       -0.2819610
H        2.2454840       -0.1035270       -1.5482140
C        0.2470730       -0.3486810        1.0551570
C       -0.2599870       -0.4735690       -1.3105610
C       -1.0680900       -0.7237230        1.3421740
H        0.9400270       -0.1587500        1.8684230
C       -1.5662600       -0.8461960       -1.0102650
H        0.0561400       -0.3757130       -2.3479550
C       -1.9855720       -0.9756330        0.3204450
H       -1.3732730       -0.8184950        2.3817900
H       -2.2640290       -1.0375030       -1.8222330
H       -3.0056170       -1.2682070        0.5521730
F       -1.5175640        2.4286410        0.0432500
H       -1.2639270        1.5337570        0.0361270
17
FH...C6H5NHOH
N        1.9706740        0.3287560        0.5598870
C        0.6878190       -0.1903240        0.2591930
O        2.9858750       -0.0957130       -0.3787390
H        2.2900880       -0.0100590        1.4639870
C       -0.2045310       -0.4180750        1.3216920
C        0.2553770       -0.3877670       -1.0601900
H        3.3016250        0.7471620       -0.7295670
C       -1.5153390       -0.8161820        1.0627490
H        0.1327050       -0.2754950        2.3468710
C       -1.0564320       -0.7984860       -1.3049700
H        0.9513580       -0.2337210       -1.8772810
C       -1.9516230       -1.0100700       -0.2522960
H       -2.1941180       -0.9872820        1.8946280
H       -1.3791050       -0.9549150       -2.3314810
H       -2.9709940       -1.3282920       -0.4515560
F       -1.5372210        2.4121790       -0.1404680
H       -1.2699050        1.5228300       -0.0977560
16
FH...C6H5NO2
N        0.4174940        1.8881230        0.0000000
C        0.4174940        0.3950070        0.0000000
O        0.4174940        2.4584490        1.0897880
O        0.4174940        2.4584490       -1.0897880
C        0.4174940       -0.2819890        1.2209820
C        0.4174940       -0.2819890       -1.2209820
C        0.4174940       -1.6771400        1.2128530
H        0.4174940        0.2818170        2.1465410
C        0.4174940       -1.6771400       -1.2128530
H        0.4174940        0.2818170       -2.1465410
C        0.4174940       -2.3746090        0.0000000
H        0.4174940       -2.2186980        2.1545630
H        0.4174940       -2.2186980       -2.1545630
H        0.4174940       -3.4613510        0.0000000
F       -2.7647040       -0.9829770        0.0000000
H       -1.8372820       -0.9829770        0.0000000
15
FH...C6H5NO
C        0.7654130       -0.3125790       -0.2101800
C       -0.0997610       -0.5358500       -1.2899370
C        0.3032910       -0.3836940        1.1152450
N        2.1361740       -0.0114890       -0.5799080
C       -1.4411560       -0.8335100       -1.0474800
H        0.3004280       -0.4707470       -2.2987210
C       -1.0340050       -0.6806360        1.3494250
H        1.0048620       -0.2043100        1.9249910
O        2.9011990        0.1853320        0.3509650
C       -1.9054820       -0.9053250        0.2700090
H       -2.1222040       -1.0087150       -1.8757500
H       -1.4101790       -0.7400610        2.3676370
H       -2.9500880       -1.1370370        0.4623730
F       -1.2720260        2.4972600       -0.0474260
H       -1.0671980        1.5928570       -0.0245370
18
FH...C6H5OCF3
C       -2.0965930        0.0143810        0.0349980
O       -1.0355620       -0.1609120        0.8614150
F       -3.1766260        0.1993650        0.8092620
F       -1.9654460        1.0977540       -0.7758300
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F	-2.3285040	-1.0585700	-0.7670830
C	0.2614460	-0.3813140	0.3619580
C	1.2263430	-0.5397300	1.3584540
C	0.5988020	-0.4436020	-0.9911110
C	2.5535910	-0.7646750	0.9941610
H	0.9271250	-0.4851240	2.4005650
C	1.9354810	-0.6700580	-1.3364650
H	-0.1484320	-0.3209290	-1.7646670
C	2.9148980	-0.8309810	-0.3550420
H	3.3047260	-0.8879980	1.7695520
H	2.2032790	-0.7194140	-2.3884030
H	3.9489030	-1.0062210	-0.6375610
F	2.1074420	2.5171440	-0.0073390
H	1.9532960	1.6016190	-0.0036250
15			
FH...C6H5OH			
C	1.1265200	-0.1657320	-0.0252990
C	0.4414500	-0.3927000	-1.2264700
C	0.4815670	-0.3762890	1.2010540
O	2.4292840	0.2627440	-0.1105220
C	-0.8833280	-0.8284840	-1.1909380
H	0.9561450	-0.2246190	-2.1680550
C	-0.8458400	-0.8129570	1.2223460
H	1.0187160	-0.1983430	2.1317880
H	2.7764220	0.3781300	0.7829620
C	-1.5357310	-1.0415000	0.0291360
H	-1.4099340	-1.0029670	-2.1259790
H	-1.3381240	-0.9736460	2.1782740
H	-2.5674000	-1.3808780	0.0482710
F	-1.1868410	2.3889310	-0.0023220
H	-0.8963600	1.5059680	-0.0011530
18			
FH...C6H5OCH3			
C	2.9328210	0.1569160	0.3310410
O	1.9529550	-0.0849810	-0.6803620
H	3.8730700	0.3288450	-0.1988130
H	2.6740870	1.0432420	0.9289710
H	3.0344910	-0.7108860	0.9993390
C	0.6698580	-0.3320530	-0.2676920
C	-0.2645770	-0.5651180	-1.2916080
C	0.2563080	-0.3632390	1.0729880
C	-1.5944470	-0.8256010	-0.9736990
H	0.0736250	-0.5370320	-2.3236630
C	-1.0856690	-0.6268590	1.3747070
H	0.9608670	-0.1861860	1.8780090
C	-2.0163650	-0.8586900	0.3623950
H	-2.3077000	-1.0042800	-1.7747060
H	-1.3966990	-0.6489730	2.4164510
H	-3.0552760	-1.0623700	0.6060790
F	-1.3054650	2.4855360	-0.0774070
H	-1.1184960	1.5755370	-0.0409010
18			
FH...C6H5SCH3			
C	2.9035230	0.3061350	0.8323330
S	2.0380350	-0.1756690	-0.7023220
H	3.9507030	0.4468940	0.5487600
H	2.5039090	1.2447600	1.2300160
H	2.8329780	-0.4838950	1.5871420
C	0.3500180	-0.3867230	-0.1685230
C	-0.5814600	-0.7674880	-1.1532970
C	-0.0882270	-0.1975260	1.1510920
C	-1.9209820	-0.9532340	-0.8181090
H	-0.2544670	-0.9172830	-2.1796780
C	-1.4357350	-0.3870880	1.4751700
H	0.6078520	0.0957330	1.9292060
C	-2.3586100	-0.7645360	0.4985220
H	-2.6269470	-1.2473030	-1.5910370
H	-1.7591690	-0.2364260	2.5024680
H	-3.4039620	-0.9102310	0.7565150
F	-1.5840920	2.4615910	-0.4634200
H	-1.4137750	1.5668860	-0.2785810
15			
FH...C6H5SH			
C	-0.7226380	-0.3028800	-0.0036510
C	-0.0271330	-0.4587160	-1.2136020
C	-0.0378330	-0.4509460	1.2117040
S	-2.4662340	0.0808440	-0.0835060
C	1.3359060	-0.7587980	-1.2003570
H	-0.5481520	-0.3461140	-2.1612220
C	1.3260450	-0.7512390	1.2128270
H	-0.5670040	-0.3323310	2.1537920
H	-2.6729330	0.1293270	1.2477430

C	2.0206310	-0.9068580	0.0099360
H	1.8631340	-0.8769880	-2.1437550
H	1.8445360	-0.8632810	2.1619370
H	3.0816660	-1.1404630	0.0152510
F	1.3288380	2.4820210	-0.0040820
H	1.1290810	1.5747710	-0.0020560