Toward a Physical Interpretation of Substituent Effects: The Case of Fluorine and Trifluoromethyl Groups

Tomasz Siodła,*[,†] Wojciech P. Oziminski,[‡] Marcin Hoffmann, [†] Henryk Koroniak,[†] and Tadeusz M. Krygowski*[,§]

[†]Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, 61-614 Poznań, Poland.
[‡]National Medicines Institute, Chełmska 30/34, 00-725 Warsaw, Poland.
[§]Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland.

Supporting Information

Table of contents:

Table S1. Hammett's substituent constants and SESE values for ethene and benzene derivatives with fixed groups F and CF_3 (substituted in *trans* position 2 in ethene derivatives and in *meta* and *para* derivatives of benzene) (M06/cc-pVDZ level of theory)

	Hammett constants				SESE values					
	σ_p	σ_m	σ^+	σ^-	X-ethene-F	X-ethene-CF_3	*para*-X-(ben.)-F	*para*-X-(ben.)-CF_3	*meta*-X-(ben.)-F	*meta*-X-(ben.)-CF_3
Br	0.23	0.39	0.15	0.25	-3.7	-2.1	-0.8	-0.8	-0.7	-1.1
CF_3	0.54	0.43	0.61	0.65	-1.6	-2.5	-0.3	-1.4	-0.8	-1.3
CH_3	-0.17	-0.07	-0.31	-0.17	-1.0	1.0	-0.2	0.5	0.3	0.3
CHO	0.42	0.35	0.73	1.03	-0.6	-2.7	0.2	-1.5	-0.8	-1.1
Cl	**0.23**	0.37	0.11	0.19	-4.5	-2.1	-1.0	-0.8	-0.8	-1.2
CN	0.66	0.56	0.66	1.00	-1.1	-3.2	-0.4	-1.9	-1.2	-2.0
F	0.06	0.34	-0.07	-0.03	-7.0	-1.6	-1.3	-0.3	-0.5	-0.8
H	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0
NH_2	-0.66	-0.16	-1.30	-0.15	-5.5	2.9	-1.2	1.5	0.7	0.6
NMe_2	-0.83	-0.16	-1.70	-0.12	-5.3	3.2	-1.1	1.9	1.0	0.8
NO	0.91	0.62	0.41	1.63	-0.9	-3.9	0.2	-2.1	-1.3	-1.8
NO_2	0.78	0.71	0.44	1.27	-3.4	-4.6	-0.4	-2.2	-1.5	-2.2
OH	-0.37	0.12	-0.92	-0.37	-7.3	0.6	-1.3	0.7	0.1	0.2
BeH					4.3	0.7	0.6	-0.1	0.3	0.2
BF_2					2.4	-1.6	0.4	-1.1	-0.5	-0.9
BH_2					4.5	-1.6	0.9	-1.1	-0.5	-0.7
CFO					-0.3	-3.3	0.1	-1.8	-1.1	-1.6
Li					7.1	6.4	1.4	3.1	2.2	3.5

Table S2. SESE values for ethene and benzene derivatives with fixed groups F and CF_3 (substituted in *trans* position 2 in ethene derivatives and in *meta* and *para* derivatives of benzene) (MP2/cc-pVDZ level of theory).

	X-ethene-F	X-ethene-CF_3	*para*-X-(ben.)-F	*para*-X-(ben.)-CF_3	*meta*-X-(ben.)-F	*meta*-X-(ben.)-CF_3
Br	-3.8	-2.7	-1.0	-1.1	-1.0	-1.4
CF_3	-2.0	-3.3	-0.5	-1.8	-1.3	-1.6
CH_3	-0.9	1.0	-0.3	0.5	0.4	0.2
CHO	-1.4	-3.2	0.0	-1.7	-1.2	-1.0
Cl	-4.4	-2.6	-1.1	-1.0	-0.9	-1.4
CN	-1.8	-4.6	-0.7	-2.5	-1.8	-2.2
F	-7.0	-2.0	-1.6	-0.5	-0.6	-1.3
H	0.0	0.0	0.0	0.0	0.0	0.0
NH_2	-5.2	2.6	-1.4	1.6	0.9	0.1
NMe_2	-5.0	3.0	-0.8	2.1	1.4	0.6
NO	-2.2	-4.6	-0.2	-2.2	-1.8	-1.6
NO_2	-4.1	-6.3	-0.7	-3.1	-2.4	-2.5
OH	-7.2	0.4	-1.6	0.8	0.3	-0.4
BeH	3.8	0.5	0.6	-0.2	0.2	0.2
BF_2	2.0	-2.4	0.4	-1.6	-1.0	-0.9
BH_2	3.8	-1.6	0.9	-1.2	-0.7	-0.3
CFO	-1.2	-4.4	-0.1	-2.4	-1.8	-1.7
Li	6.8	7.0	1.7	3.5	2.6	3.7

Table S3. SESE values for ethene derivatives with fixed groups F and CF_3 (substituted in *trans* position 2 in ethene derivatives). M06/aug-cc-pVTZ, MP2/aug-cc-pVTZ and B3LYP/cc-pVDZ levels of theory.

	M06/aug-cc-pVTZ		MP2/aug-cc-pVTZ		B3LYP/cc-pVDZ	
	X-ethene-F	X-ethene-CF_3	X-ethene-F	X-ethene-CF_3	X-ethene-F	X-ethene-CF_3
BeH	4.2	0.6	3.8	0.6	4.4	0.5
BF_2	2.1	-1.7	1.9	-2.2	2.5	-1.6
BH_2	4.3	-1.5	3.7	-1.4	4.7	-1.6
Br	-3.7	-2.0	-3.9	-2.6	-3.9	-2.0
CF_3	-1.9	-2.8	-2.0	-3.1	-1.7	-2.4
CFO	-0.6	-3.6	-1.2	-4.4	-0.3	-3.1
CH_3	-1.1	0.8	-1.0	0.9	-1.1	0.8
CHO	-0.6	-3.0	-1.1	-3.3	-0.6	-2.5
Cl	-4.6	-2.1	-4.5	-2.5	-4.5	-2.0
CN	-1.4	-3.4	-1.9	-4.5	-1.2	-3.1
F	-7.3	-1.9	-7.3	-2.0	-7.1	-1.7
H	0.0	0.0	0.0	0.0	0.0	0.0
Li	7.4	6.4	6.7	6.7	7.2	5.9
NH_2	-5.9	2.4	-5.8	2.0	-5.5	2.8
NMe_2	-5.6	2.6	-5.5	2.3	-5.4	3.2
NO	-1.1	-4.1	-2.1	-4.3	-1.0	-3.8
NO_2	-3.8	-5.0	-4.2	-6.0	-3.4	-4.3
OH	-7.4	0.1	-7.5	0.0	-7.3	0.6

Table S4. The comparison of methods used for SESE calculations: The linear regression analysis with the *ab initio* MP2/aug-cc-pVTZ method as the reference. Regression and correlation coefficients.

	B3LYP/ cc-pVDZ	MP2/ cc-pVDZ	MP2/ aug-cc-pVTZ	M06/ cc-pVDZ	M06/ aug-cc-pVTZ
X-ethene-F					
R^2	0.993	0.998	1.000	0.993	0.995
a (slope)	1.035	0.973	1.000	1.020	1.042
b	0.500	0.057	0.000	0.483	0.351
X-ethene-CF_3					
R^2	0.976	0.996	1.000	0.982	0.992
a (slope)	0.857	1.066	1.000	0.912	0.913
b	0.344	0.119	0.000	0.406	0.193

The picture in Figure S1 shows dependences of SESE for 2-substituted 1- fluoro- and trifluoromethyl ethene derivatives in *trans* configuration again on σ_p and σ_m. Again it can be seen that SESE values for fluoro derivatives behave not so regularly as those for CF_3. In this case even relationships with σ_m do not work well (M06/cc-pVDZ).

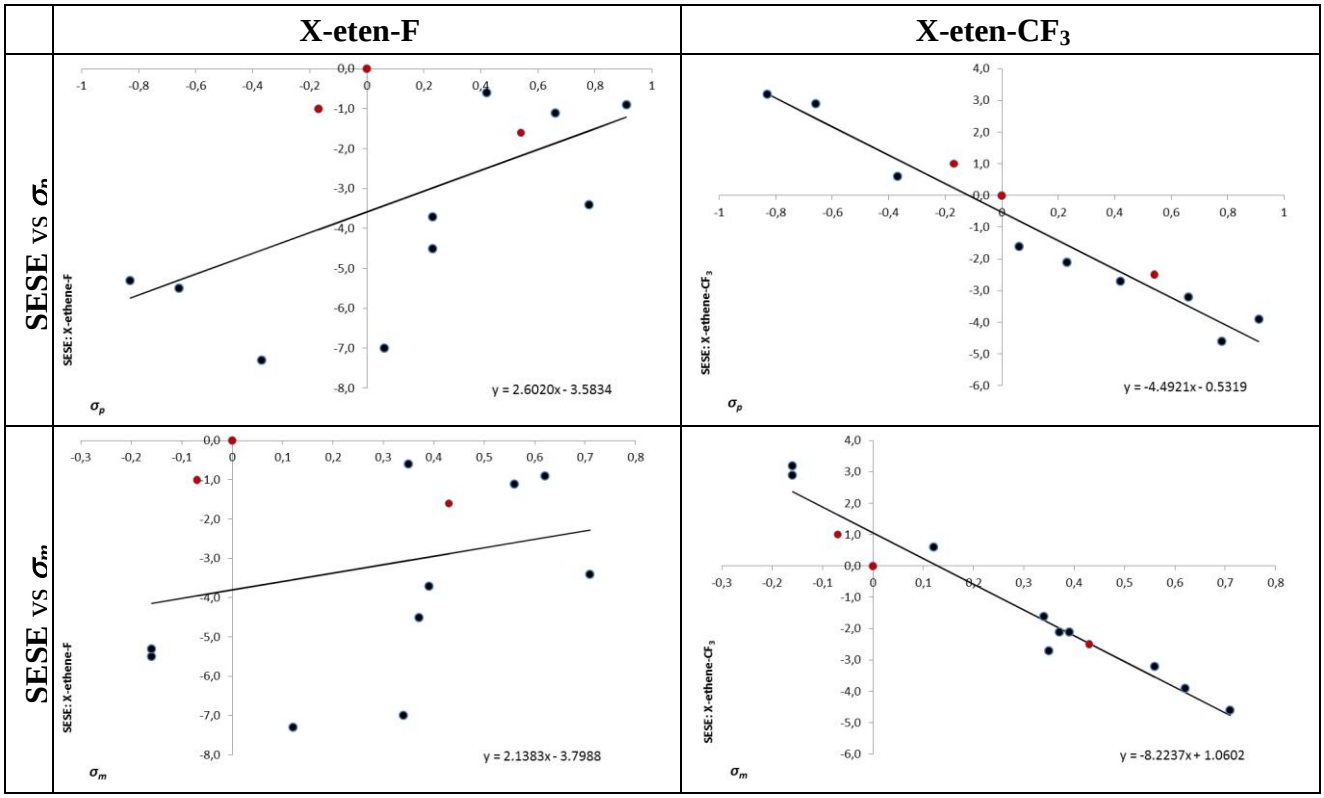

Figure S1. Dependences of SESE for *trans* substituted derivatives of fluoro- and trifluoromethyl ethene on the Hammett σ_p and σ_m. respectively.

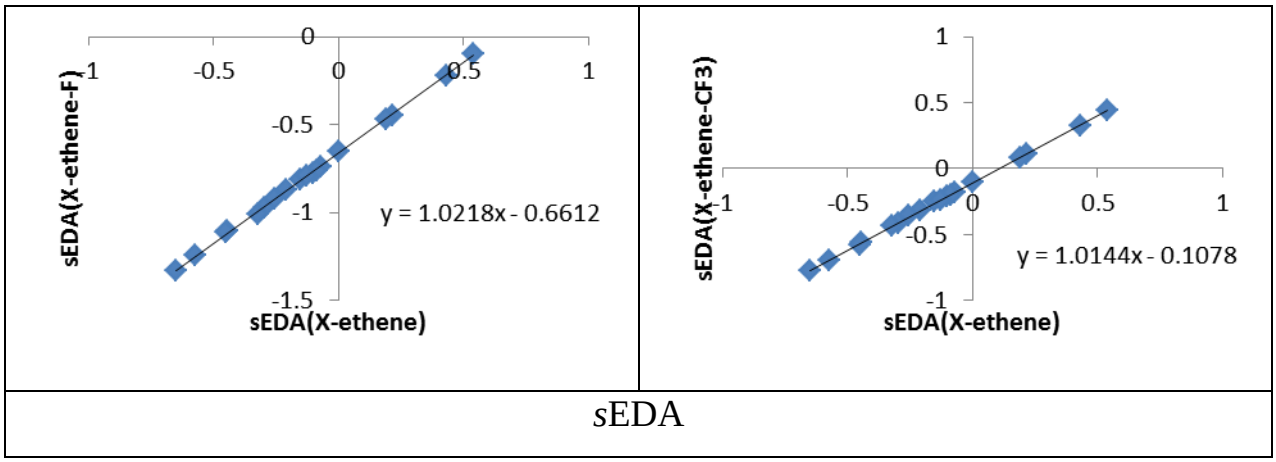

Figure S2. Dependences of *s*EDA of F-. CC=0.999 or CF_3-. CC=0.999 R-X on the data for H-R-X. where R stands for ethene moieties.

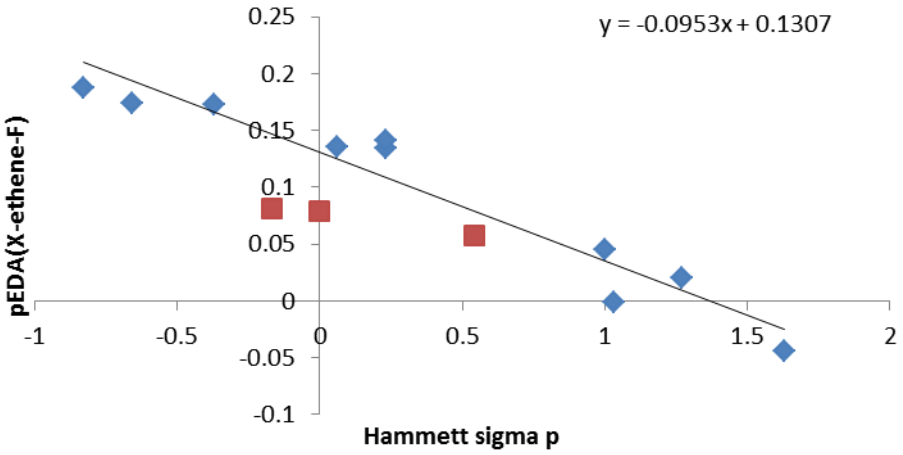

Figure S3. *p*EDA (F-ethene-X) vs Hammett σ_p (for electron withdrawing CHO. CN. NO. NO_2 - σ_p^-). Red squares not taken into correlation: H. CH_3. CF_3. cc-0.964.

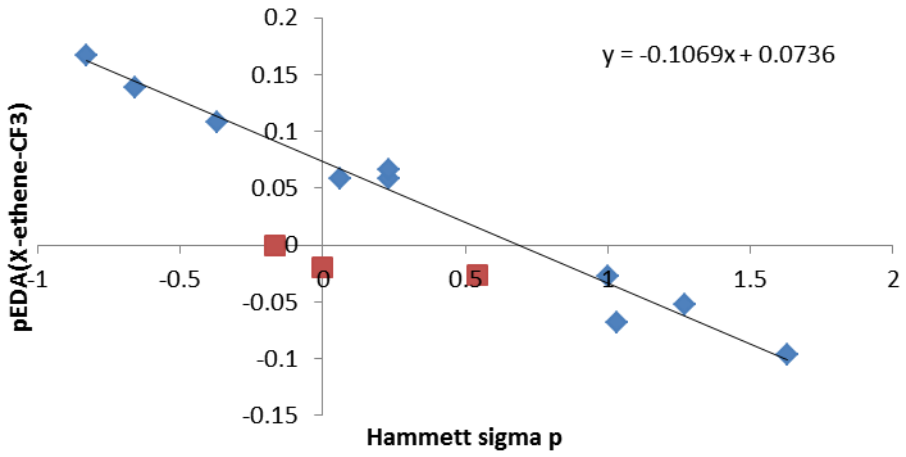

Figure S4. *p*EDA (CF_3-ethene-X) vs Hammett σ_p (for electron withdrawing CHO. CN. NO. NO_2 - σ_p^-). Red squares not taken into correlation: H. CH_3. CF_3. cc= -0.988

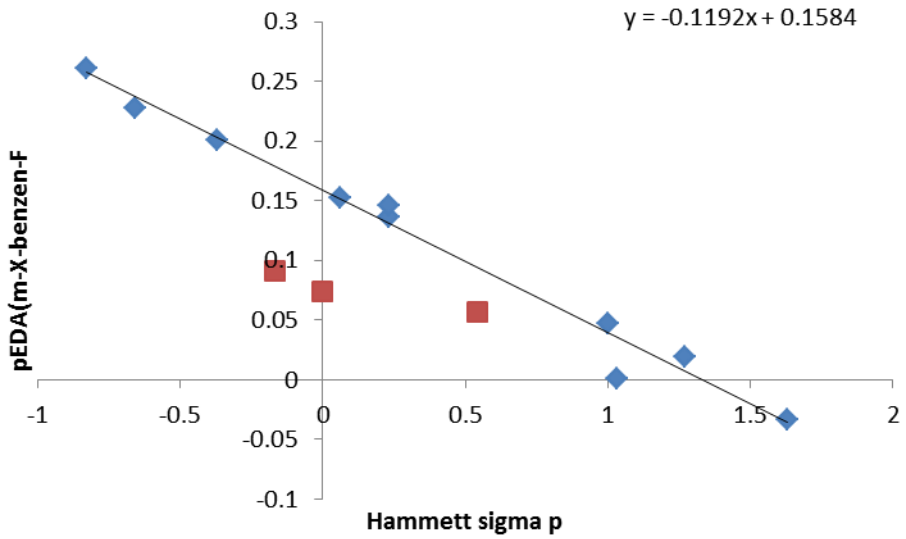

Figure S5. *p*EDA (*m*-X-benzen-F) Hammett σ_p (for electron withdrawing CHO. CN. NO. NO_2 - σ_p^-). Red squares excluded from regression: H. CH_3. CF_3. CC=-0.990

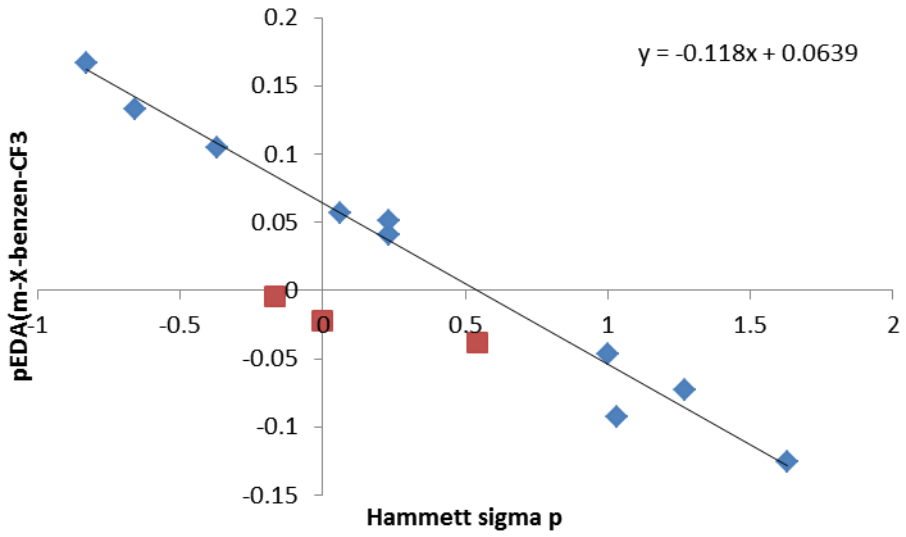

Figure S6. *p*EDA(*m*-X-benzen-CF_3) Hammett σ_p (for electron withdrawing CHO. CN. NO. NO_2 - σ_p^-). Red squares excluded from regression: H. CH_3. CF_3. CC=-0.990

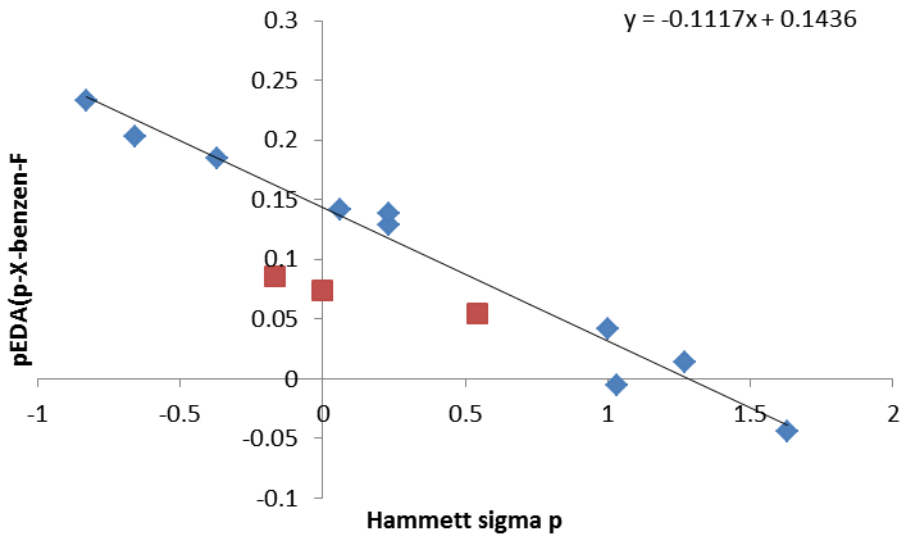

Figure S7. *p*EDA(p-X-benzen-F) Hammett σ_p (for electron withdrawing CHO. CN. NO. NO_2 - σ_p^-). Red squares excluded from regression: H. CH_3. CF_3. cc=-0.986

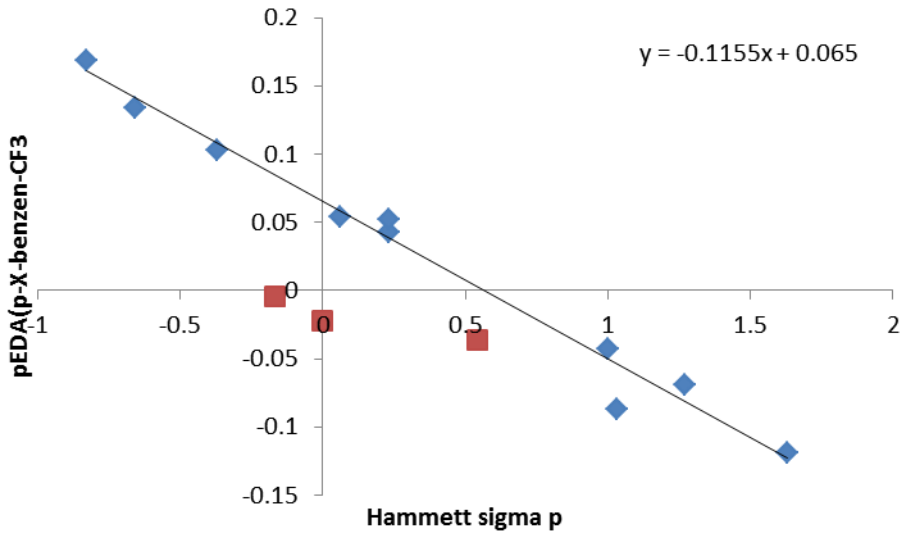

Figure S8. *p*EDA(p-X-benzen-CF_3) Hammett σ_p (for electron withdrawing CHO. CN. NO. NO_2 - σ_p^-). Red squares excluded from regression: H. CH_3. CF_3. cc=-0.990

Table S5. *s*EDA/*p*EDA data for substituted benzene derivatives (M06/cc-pVDZ)

	X-benzen		*m*-X-benzen-F		*m*-X-benzen-CF_3		*p*-X-benzen-F		*p*-X-benzen-CF_3	
	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA
BeH	0.415	-0.038	-0.224	0.038	0.301	-0.055	-0.224	0.037	0.301	-0.052
BF_2	0.215	-0.068	-0.428	0.011	0.099	-0.082	-0.427	0.009	0.098	-0.078
BH_2	0.195	-0.125	-0.447	-0.044	0.079	-0.135	-0.447	-0.049	0.077	-0.129
Br	-0.179	0.057	-0.818	0.136	-0.288	0.041	-0.817	0.129	-0.289	0.043
CFO	-0.070	-0.076	-0.714	0.005	-0.186	-0.087	-0.713	0.001	-0.187	-0.083
CHO	-0.090	-0.081	-0.733	0.000	-0.205	-0.092	-0.732	-0.006	-0.207	-0.087
Cl	-0.277	0.067	-0.917	0.146	-0.388	0.051	-0.916	0.138	-0.388	0.052
CN	-0.139	-0.034	-0.784	0.047	-0.255	-0.047	-0.782	0.042	-0.257	-0.043
F	-0.638	0.074	-1.282	0.152	-0.754	0.056	-1.278	0.142	-0.754	0.054
Li	0.518	-0.010	-0.112	0.059	0.411	-0.037	-0.112	0.057	0.412	-0.037
NH_2	-0.461	0.145	-1.103	0.227	-0.577	0.133	-1.094	0.203	-0.580	0.134
NMe_2	-0.482	0.177	-1.124	0.261	-0.596	0.167	-1.115	0.233	-0.602	0.169
NO	-0.280	-0.118	-0.925	-0.033	-0.395	-0.125	-0.923	-0.045	-0.398	-0.119
NO_2	-0.324	-0.062	-0.969	0.020	-0.439	-0.073	-0.968	0.014	-0.440	-0.069
OH	-0.577	0.122	-1.219	0.200	-0.692	0.104	-1.213	0.185	-0.693	0.103
H	0.000	0.000	-0.638	0.074	-0.111	-0.022	-0.638	0.074	-0.111	-0.022
CH_3	-0.215	0.016	-0.854	0.091	-0.326	-0.004	-0.852	0.086	-0.327	-0.004
CF_3	-0.111	-0.022	-0.754	0.056	-0.225	-0.038	-0.754	0.054	-0.226	-0.036

Table S6. sEDA/*p*EDA data for substituted ethene derivatives (M06/cc-pVDZ)

	X-ethene		X-ethene-F		X-ethene-CF_3	
	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA
BeH	0.434	-0.040	-0.219	0.041	0.328	-0.045
BF_2	0.216	-0.067	-0.445	0.015	0.108	-0.065
BH_2	0.191	-0.122	-0.468	-0.045	0.083	-0.109
Br	-0.154	0.066	-0.810	0.134	-0.250	0.058
CF_3	-0.100	-0.020	-0.774	0.058	-0.207	-0.026
CFO	-0.069	-0.066	-0.740	0.011	-0.179	-0.061
CH_3	-0.207	0.017	-0.869	0.082	-0.313	0.000
CHO	-0.089	-0.074	-0.761	-0.001	-0.200	-0.069
Cl	-0.257	0.076	-0.920	0.141	-0.358	0.067
CN	-0.125	-0.029	-0.794	0.046	-0.234	-0.027
F	-0.654	0.079	-1.332	0.136	-0.774	0.058
H	0.000	0.000	-0.654	0.079	-0.100	-0.020
Li	0.542	-0.016	-0.095	0.053	0.440	-0.040
NH_2	-0.444	0.146	-1.102	0.174	-0.562	0.139
NMe_2	-0.451	0.161	-1.108	0.187	-0.575	0.167
NO	-0.296	-0.109	-0.974	-0.044	-0.410	-0.097
NO_2	-0.324	-0.054	-1.006	0.020	-0.436	-0.052
OH	-0.573	0.131	-1.242	0.172	-0.691	0.108

Table S7. *s*EDA/*p*EDA data for substituted ethene derivatives (MP2/cc-pVDZ)

	X-ethene		X-ethene-F		X-ethene-CF_3	
	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA
BeH	1.203	-0.046	0.547	0.005	1.103	-0.052
BF_2	0.988	-0.069	0.329	-0.018	0.888	-0.069
BH_2	0.955	-0.107	0.295	-0.062	0.855	-0.098
Br	0.600	0.036	-0.054	0.078	0.515	0.024
CF_3	0.656	-0.032	-0.013	0.016	0.558	-0.041
CFO	0.683	-0.066	0.014	-0.019	0.582	-0.065
CH_3	0.558	-0.002	-0.102	0.037	0.462	-0.021
CHO	0.665	-0.067	-0.005	-0.023	0.562	-0.066
Cl	0.507	0.041	-0.153	0.080	0.417	0.028
CN	0.623	-0.041	-0.043	0.004	0.523	-0.043
F	0.095	0.037	-0.578	0.071	-0.013	0.016
H	0.749	-0.011	0.095	0.037	0.656	-0.032
Li	1.316	-0.026	0.671	0.018	1.219	-0.047
NH_2	0.320	0.081	-0.336	0.094	0.210	0.073
NMe_2	0.314	0.092	-0.342	0.105	0.199	0.093
NO	0.438	-0.079	-0.235	-0.042	0.335	-0.073
NO_2	0.398	-0.058	-0.278	-0.012	0.297	-0.059
OH	0.185	0.074	-0.481	0.097	0.075	0.052

Table S8. *s*EDA/*p*EDA data for substituted ethene derivatives (M06/aug-cc-pVTZ)

	X-ethene		X-ethene-F		X-ethene-CF_3	
	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA
BeH	1.135	-0.044	0.538	0.024	1.014	-0.047
BF_2	0.872	-0.070	0.277	0.001	0.751	-0.066
BH_2	0.867	-0.126	0.270	-0.061	0.743	-0.111
Br	0.563	0.060	-0.034	0.121	0.454	0.055
CF_3	0.585	-0.021	-0.018	0.051	0.468	-0.025
CFO	0.628	-0.070	0.026	0.001	0.507	-0.062
CH_3	0.500	0.011	-0.101	0.067	0.382	-0.003
CHO	0.618	-0.082	0.011	-0.018	0.494	-0.073
Cl	0.471	0.067	-0.133	0.126	0.359	0.062
CN	0.583	-0.033	-0.019	0.035	0.463	-0.030
F	0.105	0.066	-0.514	0.118	-0.018	0.051
H	0.699	-0.005	0.105	0.066	0.585	-0.021
Li	1.257	-0.014	0.673	0.042	1.144	-0.036
NH_2	0.305	0.138	-0.300	0.159	0.177	0.137
NMe_2	0.290	0.156	-0.314	0.174	0.158	0.165
NO	0.460	-0.119	-0.153	-0.062	0.336	-0.102
NO_2	0.426	-0.060	-0.190	0.009	0.306	-0.055
OH	0.189	0.114	-0.426	0.151	0.064	0.098

Table S9. *s*EDA/*p*EDA data for substituted ethene derivatives (MP2/aug-cc-pVTZ)

	X-ethene		X-ethene-F		X-ethene-CF_3	
	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA
BeH	1.099	-0.043	0.502	-0.004	0.991	-0.047
BF_2	0.842	-0.066	0.252	-0.024	0.735	-0.064
BH_2	0.828	-0.105	0.236	-0.071	0.719	-0.094
Br	0.513	0.036	-0.077	0.072	0.422	0.029
CF_3	0.538	-0.026	-0.059	0.016	0.435	-0.033
CFO	0.579	-0.065	-0.017	-0.024	0.473	-0.061
CH_3	0.459	-0.002	-0.137	0.030	0.355	-0.016
CHO	0.569	-0.072	-0.031	-0.036	0.460	-0.065
Cl	0.430	0.039	-0.167	0.074	0.335	0.031
CN	0.532	-0.041	-0.065	-0.002	0.426	-0.040
F	0.049	0.032	-0.565	0.062	-0.059	0.016
H	0.638	-0.010	0.049	0.032	0.538	-0.026
Li	1.221	-0.018	0.632	0.014	1.117	-0.038
NH_2	0.262	0.086	-0.337	0.091	0.148	0.084
NMe_2	0.252	0.095	-0.347	0.100	0.135	0.101
NO	0.391	-0.087	-0.214	-0.059	0.281	-0.075
NO_2	0.347	-0.059	-0.259	-0.019	0.243	-0.057
OH	0.141	0.067	-0.469	0.085	0.030	0.052

Table S10. *s*EDA/*p*EDA data for substituted ethene derivatives (B3LYP/cc-pVDZ)

	X-ethene		X-ethene-F		X-ethene-CF_3	
	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA
BeH	1.225	-0.051	0.587	0.034	1.116	-0.056
BF_2	1.009	-0.077	0.364	0.008	0.895	-0.075
BH_2	0.986	-0.137	0.342	-0.056	0.872	-0.124
Br	0.626	0.062	-0.011	0.132	0.526	0.053
CF_3	0.689	-0.026	0.034	0.055	0.576	-0.033
CFO	0.721	-0.073	0.067	0.007	0.605	-0.069
CH_3	0.589	0.012	-0.055	0.080	0.480	-0.007
CHO	0.704	-0.080	0.049	-0.004	0.587	-0.075
Cl	0.543	0.069	-0.100	0.136	0.438	0.058
CN	0.665	-0.031	0.014	0.046	0.550	-0.031
F	0.157	0.077	-0.502	0.136	0.034	0.055
H	0.794	-0.005	0.157	0.077	0.689	-0.026
Li	1.323	-0.025	0.705	0.049	1.222	-0.048
NH_2	0.355	0.143	-0.283	0.174	0.233	0.134
NMe_2	0.346	0.162	-0.292	0.190	0.218	0.163
NO	0.500	-0.114	-0.161	-0.045	0.382	-0.102
NO_2	0.469	-0.058	-0.195	0.019	0.352	-0.057
OH	0.233	0.128	-0.416	0.171	0.111	0.103

Table S11. *s*EDA/*p*EDA data for substituted ethene derivatives (B3LYP/6-31g(d.p))

	X-ethene		X-ethene-F		X-ethene-CF_3	
	*s*EDA	*p*EDA	*s*EDA	*p*EDA	*s*EDA	*p*EDA
BeH	1.260	-0.056	0.705	0.063	1.213	-0.038
BF_2	1.043	-0.077	0.395	0.010	0.912	-0.076
BH_2	1.016	-0.138	0.368	-0.055	0.883	-0.126
Br	0.674	0.062	0.034	0.134	0.556	0.053
CF_3	0.729	-0.024	0.073	0.059	0.599	-0.031
CFO	0.762	-0.073	0.106	0.010	0.628	-0.069
CH_3	0.628	0.011	-0.017	0.082	0.504	-0.007
CHO	0.748	-0.081	0.091	-0.002	0.614	-0.076
Cl	0.604	0.068	-0.042	0.139	0.483	0.058
CN	0.705	-0.031	0.050	0.049	0.573	-0.030
F	0.210	0.080	-0.448	0.141	0.073	0.059
H	0.851	-0.005	0.209	0.080	0.728	-0.024
Li	1.329	-0.032	0.719	0.048	1.222	-0.050
NH_2	0.415	0.141	-0.223	0.176	0.279	0.135
NMe_2	0.400	0.159	-0.237	0.191	0.260	0.161
NO	0.565	-0.119	-0.097	-0.046	0.429	-0.106
NO_2	0.527	-0.062	-0.140	0.018	0.392	-0.059
OH	0.291	0.126	-0.357	0.173	0.156	0.104

Table S12. The comparison of six methods used for *s*EDA/*p*EDA calculations: The linear regression analysis with the *ab initio* MP2/aug-cc-pVTZ method as the reference. Regression and correlation coefficients:

	B3LYP/ 6-31g(d.p)	B3LYP/ cc-pVDZ	MP2/ cc-pVDZ	MP2/ aug-cc-pVTZ	M06/ cc-pVDZ	M06/ aug-cc-pVTZ
X-ethene *s*EDA (6)						
R^2	0.994	0.996	0.996	1.000	0.996	0.999
a (slope)	0.995	1.034	1.070	1.000	1.050	0.981
b	0.173	0.107	0.049	0.000	0.106	0.058
X-ethene *p*EDA (2)						
R^2	0.989	0.991	0.995	1.000	0.993	0.995
a (slope)	1.472	1.467	0.996	1.000	1.428	1.399
b	0.017	0.018	0.000	0.000	0.018	0.017
X-ethene-F *s*EDA (6)						
R^2	0.995	0.998	0.997	1.000	0.998	0.999
a (slope)	1.029	1.038	1.068	1.000	1.057	0.989
b	0.128	0.079	0.026	0.000	0.070	0.042
X-ethene-F *p*EDA (2)						
R^2	0.984	0.991	0.995	1.000	0.992	0.994
a (slope)	1.411	1.413	0.972	1.000	1.380	1.371
b	0.045	0.041	0.008	0.000	0.039	0.030
X-ethene-CF_3 *s*EDA (6)						
R^2	0.994	0.996	0.996	1.000	0.996	0.999
a (slope)	1.037	1.047	1.077	1.000	1.062	0.986
b	0.135	0.097	0.059	0.000	0.102	0.040
X-ethene-CF_3 *p*EDA (2)						
R^2	0.989	0.993	0.996	1.000	0.994	0.995
a (slope)	1.469	1.468	0.982	1.000	1.440	1.426
b	0.018	0.017	-0.005	0.000	0.018	0.020

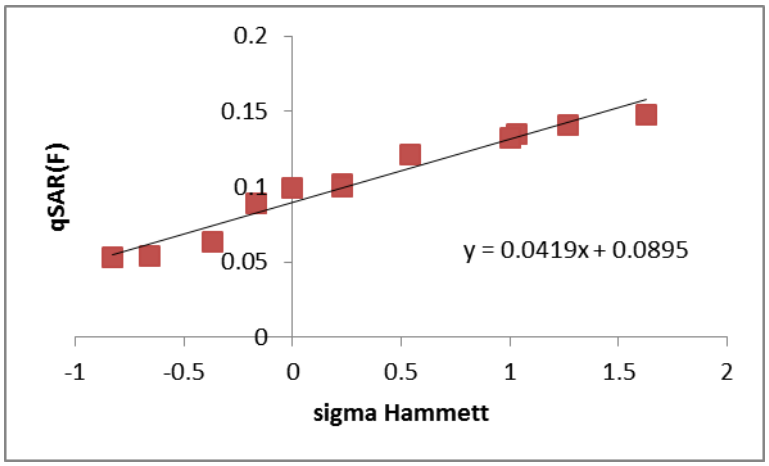

Figure S9. Dependence of *cSAR*(F) on Hammetts sigma. cc= -0.979

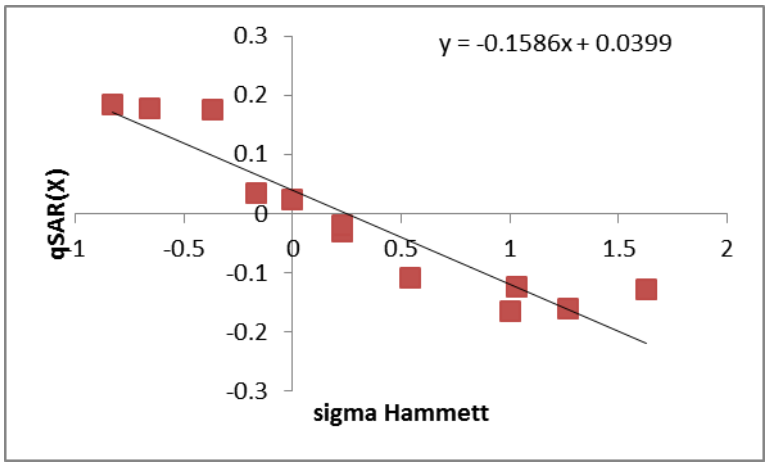

Figure S10. Dependence of *cSAR*(X) on Hammetts sigma.cc= -0.935

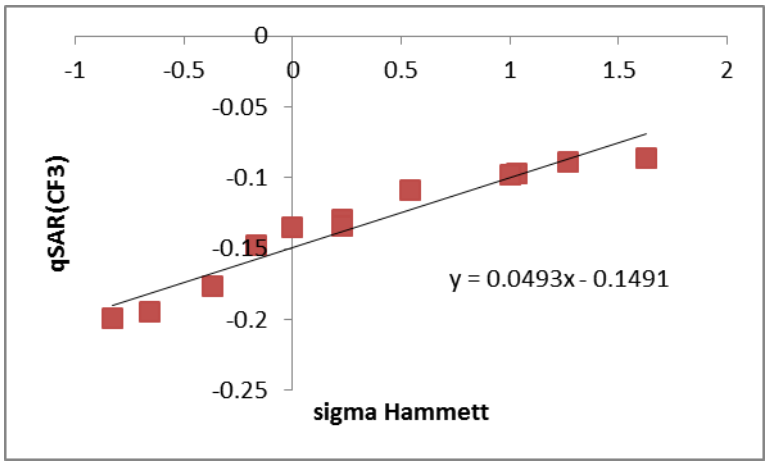

Figure S11. Dependence of *cSAR*(CF_3) on Hammetts sigma.cc= -0.965

Table S13. *cSAR* data for *p*-F-benzene-X and *p*-CF_3-benzene-X (M06/cc-pVDZ).

	cSAR(F)	*cSAR*(X)	*cSAR*(CF_3)	*cSAR*(X)
BeH	0.115	-0.050	-0.121	-0.001
BF_2	0.135	-0.168	-0.099	-0.119
BH_2	0.145	-0.197	-0.090	-0.141
Br	0.102	-0.073	-0.130	-0.030
CFO	0.141	-0.221	-0.090	-0.173
CHO	0.135	-0.174	-0.097	-0.123
Cl	0.100	-0.062	-0.134	-0.019
CN	0.132	-0.211	-0.098	-0.166
F	0.082	0.082	-0.152	0.121
Li	0.070	0.194	-0.176	0.245
NH_2	0.054	0.119	-0.195	0.178
NMe_2	0.053	0.123	-0.199	0.185
NO	0.148	-0.179	-0.086	-0.128
NO_2	0.141	-0.206	-0.089	-0.160
OH	0.063	0.129	-0.177	0.175
H	0.099	-0.017	-0.135	0.023
CH_3	0.089	-0.010	-0.148	0.034
CF_3	0.121	-0.152	-0.109	-0.109

Table S14. *cSAR* data for *p*-NH_2-benzene-X and *p*-NO-benzene-X

	NMe_2		NO	
	cSAR(X)	*cSAR*(NMe_2)	*cSAR*(X)	*cSAR*(NO)
Br	-0.107	0.148	-0.004	-0.156
CHO	-0.234	0.211	-0.101	-0.118
Cl	-0.095	0.144	0.005	-0.159
CN	-0.261	0.204	-0.144	-0.118
F	0.047	0.116	0.135	-0.176
NH_2	0.080	0.074	0.220	-0.242
NMe_2	0.074	0.077	0.236	-0.251
NO	-0.250	0.236	-0.105	-0.105
NO_2	-0.266	0.222	-0.138	-0.107
OH	0.093	0.086	0.196	-0.211
H	-0.045	0.136	0.042	-0.156
CH_3	-0.046	0.122	0.054	-0.173
CF_3	-0.198	0.182	-0.091	-0.126

Table S15. Data for regressions of Fig 11 (M06/cc-pVDZ) (bond lengths [Å])

	σ_p	σ_m	X-eten-F	X-eten-CF_3	*para*-X-(ben.)-F	*para*-X-(ben.)-CF_3	*meta*-X-(ben.)-F	*meta*-X-(ben.)-CF_3
Br	0.23	0.39	1.32938	1.49535	1.33545	1.49774	1.33480	1.49953
CF_3	0.54	0.43	1.32307	1.49363	1.33322	1.49978	1.33448	1.49970
CH_3	-0.17	-0.07	1.33692	1.49496	1.33899	1.49565	1.33839	1.49698
CHO	0.42	0.35	1.31975	1.49093	1.33243	1.50050	1.33547	1.49887
Cl	**0.23**	0.37	1.32946	1.49227	1.33556	1.49757	1.33458	1.49990
CN	0.66	0.56	1.31829	1.49389	1.33116	1.50055	1.33288	1.50090
F	0.06	0.34	1.33191	1.48611	1.33742	1.49637	1.33454	1.49955
H	0	0	1.33390	1.49207	1.33772	1.49749	1.33772	1.49749
NH_2	-0.66	-0.16	1.34425	1.48943	1.34242	1.49094	1.33846	1.49761
NMe_2	-0.83	-0.16	1.34599	1.49268	1.34272	1.49015	1.34003	1.49871
NO	0.91	0.62	1.31300	1.48372	1.33019	1.50169	1.33361	1.49972
NO_2	0.78	0.71	1.31460	1.49014	1.32968	1.50144	1.33243	1.50136
H	-0.37	0.12	1.34072	1.49115	1.34063	1.4934	1.33701	1.49799
BeH			1.33778	1.47590	1.33630	1.49792	1.33922	1.49780
BF_2			1.32281	1.47552	1.33303	1.50018	1.33618	1.49928
BH_2			1.32214	1.49129	1.33229	1.50047	1.33708	1.49868
CFO			1.31759	1.49266	1.33068	1.50108	1.33404	1.50043
Li			1.36620	1.47966	1.34562	1.49211	1.34806	1.49366

Coordinates of structures optimized using M06/cc-pVDZ method:

benzene

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.393115000
6	1.206314000	0.000000000	-0.696832000
1	-0.946992000	0.000000000	1.940004000
1	1.206190000	0.000000000	-1.790396000
6	1.206631000	0.000000000	2.089397000
6	2.412786000	0.000000000	-0.000275000
1	1.206756000	0.000000000	3.182994000
1	3.359807000	0.000000000	-0.547181000
6	2.413104000	0.000000000	1.392840000
1	3.360220000	0.000000000	1.939514000
1	-0.947145000	0.000000000	-0.546691000

benzene-BeH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.409410000
6	1.261437000	0.000000000	-0.628659000
1	-0.951362000	0.000000000	1.955055000
1	1.325446000	0.000000000	-1.723520000
6	1.180478000	0.000000000	2.147782000
6	2.448833000	0.000000000	0.098535000
1	1.144795000	0.000000000	3.240889000
1	3.411260000	0.000000000	-0.420975000
6	2.409045000	0.000000000	1.491048000
1	3.338851000	0.000000000	2.066541000
4	-1.423441000	0.000000000	-0.881021000
1	-2.558496000	0.000000000	-1.583549000

benzene-BF_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.402609000
6	1.229774000	0.000000000	-0.674600000
1	-0.954672000	-0.000046000	1.937016000
1	1.239234000	0.000058000	-1.768621000
6	1.195057000	0.000029000	2.112745000
6	2.427122000	-0.000042000	0.031676000
1	1.185559000	0.000087000	3.205686000
1	3.380808000	-0.000102000	-0.502269000

6	2.408368000	-0.000011000	1.425817000
1	3.349165000	-0.000019000	1.982793000
5	-1.325644000	-0.000019000	-0.785113000
9	-1.352427000	-0.000217000	-2.112529000
9	-2.502648000	0.000167000	-0.170807000

benzene-BH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.408485000
6	1.246653000	0.000000000	-0.655576000
1	-0.960414000	-0.000162000	1.934193000
1	1.264840000	0.000112000	-1.750299000
6	1.186638000	0.000090000	2.131144000
6	2.438571000	0.000157000	0.058348000
1	1.169306000	0.000165000	3.224098000
1	3.397856000	0.000208000	-0.465691000
6	2.405833000	0.000147000	1.453043000
1	3.341908000	0.000192000	2.018425000
5	-1.313704000	-0.000405000	-0.793920000
1	-1.293862000	-0.000478000	-2.001193000
1	-2.373625000	-0.000599000	-0.215664000

benzene-Br

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.391812000
6	1.188591000	0.000000000	-0.724149000
1	-0.945305000	0.000000000	1.939819000
1	1.164748000	0.000000000	-1.816553000
6	1.218358000	0.000000000	2.066638000
6	2.398786000	0.000000000	-0.034793000
1	1.226590000	0.000000000	3.159835000
1	3.336647000	0.000000000	-0.596545000
6	2.417394000	0.000000000	1.357914000
1	3.370212000	0.000000000	1.893137000
35	-1.657405000	0.000000000	-0.931008000

benzene-CF_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.395610000
6	1.198718000	0.000000000	-0.705856000
1	-0.952168000	0.003135000	1.932867000

1	1.186535000	0.001450000	-1.797176000
6	1.206011000	-0.001638000	2.084594000
6	2.405733000	-0.001354000	-0.010718000
1	1.209419000	-0.001106000	3.177175000
1	3.349191000	-0.000989000	-0.561802000
6	2.410215000	-0.002715000	1.380986000
1	3.358555000	-0.003907000	1.923961000
6	-1.321108000	-0.020842000	-0.704776000
9	-1.982089000	-1.162446000	-0.463987000
9	-2.116032000	0.973491000	-0.284605000
9	-1.200079000	0.096406000	-2.030290000

benzene-CFO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.398596000
6	1.208458000	0.000000000	-0.703751000
1	-0.958077000	-0.000087000	1.923192000
1	1.195844000	0.000033000	-1.795027000
6	1.203552000	-0.000303000	2.090353000
6	2.410731000	0.000042000	-0.006258000
1	1.206883000	-0.000551000	3.182817000
1	3.356986000	0.000143000	-0.552268000
6	2.408506000	-0.000241000	1.387398000
1	3.356125000	-0.000102000	1.931976000
6	-1.303887000	0.000028000	-0.684522000
8	-2.384207000	-0.000990000	-0.186567000
9	-1.174703000	0.001193000	-2.026174000

benzene-CH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.399208000
6	1.230593000	0.000000000	-0.660781000
1	-0.956929000	0.005085000	1.932258000
1	1.247455000	0.005110000	-1.755644000
6	1.192140000	-0.004824000	2.115516000
6	2.427836000	-0.004770000	0.051659000
1	1.169740000	-0.003714000	3.208841000
1	3.380054000	-0.003688000	-0.485965000
6	2.413273000	-0.008031000	1.443338000
1	3.351067000	-0.009871000	2.004667000
6	-1.291525000	-0.012600000	-0.761034000
1	-1.798422000	-0.989406000	-0.674248000
1	-1.993678000	0.745471000	-0.377305000

1 -1.133091000 0.182698000 -1.831819000

benzene-CHO

6 0.000000000 0.000000000 0.000000000
6 0.000000000 0.000000000 1.398961000
6 1.208436000 0.000000000 -0.699801000
1 -0.961519000 -0.000142000 1.918594000
1 1.193378000 0.000057000 -1.795002000
6 1.203625000 -0.000332000 2.089543000
6 2.415136000 0.000171000 -0.007608000
1 1.209970000 -0.000555000 3.182395000
1 3.362182000 0.000345000 -0.552533000
6 2.410132000 -0.000126000 1.385763000
1 3.357782000 -0.000059000 1.930884000
6 -1.278944000 0.000019000 -0.738229000
8 -2.370673000 0.000460000 -0.221445000
1 -1.159421000 -0.000085000 -1.856502000

benzene-Cl

6 0.000000000 0.000000000 0.000000000
6 0.000000000 0.000000000 1.391308000
6 1.186021000 0.000000000 -0.727387000
1 -0.947719000 0.000000000 1.933864000
1 1.153047000 0.000000000 -1.818924000
6 1.219200000 0.000000000 2.063577000
6 2.396505000 0.000000000 -0.039548000
1 1.228668000 0.000000000 3.156512000
1 3.333128000 0.000000000 -0.602872000
6 2.417505000 0.000000000 1.353291000
1 3.370662000 0.000000000 1.886857000
17 -1.527651000 0.000000000 -0.855161000

benzene-CN

6 0.000000000 0.000000000 0.000000000
6 0.000000000 0.000000000 1.400739000
6 1.211082000 0.000000000 -0.703810000
1 -0.951678000 0.000000000 1.936809000
1 1.196393000 0.000000000 -1.795985000
6 1.207004000 0.000000000 2.088681000
6 2.412346000 0.000000000 -0.005891000
1 1.208494000 0.000000000 3.181131000

1	3.357630000	0.000000000	-0.553512000
6	2.411715000	0.000000000	1.387844000
1	3.358765000	0.000000000	1.932833000
6	-1.242817000	0.000000000	-0.715191000
7	-2.251627000	0.000000000	-1.295720000

benzene-F

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.387058000
6	1.175665000	0.000000000	-0.736031000
1	-0.953426000	0.000000000	1.919501000
1	1.121033000	0.000000000	-1.826687000
6	1.221848000	0.000000000	2.054483000
6	2.389736000	0.000000000	-0.054562000
1	1.237266000	0.000000000	3.147337000
1	3.324216000	0.000000000	-0.621407000
6	2.417417000	0.000000000	1.338649000
1	3.372943000	0.000000000	1.867774000
9	-1.170273000	0.000000000	-0.648041000

benzene-Li

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.412818000
6	1.288955000	0.000000000	-0.578489000
1	-0.955546000	0.000000000	1.959777000
1	1.396706000	0.000000000	-1.674218000
6	1.164254000	0.000000000	2.183064000
6	2.468385000	0.000000000	0.168310000
1	1.101086000	0.000000000	3.277037000
1	3.440585000	0.000000000	-0.337255000
6	2.409972000	0.000000000	1.559953000
1	3.328553000	0.000000000	2.154542000
3	-1.663324000	0.000000000	-1.076654000

benzene-NH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.402268000
6	1.232747000	0.000000000	-0.668713000
1	-0.956028000	-0.001870000	1.936533000
1	1.246158000	-0.001928000	-1.763824000
6	1.197110000	-0.002136000	2.108306000

6	2.424063000	-0.002121000	0.046755000
1	1.171567000	-0.000626000	3.201688000
1	3.373034000	-0.000602000	-0.496921000
6	2.420111000	-0.003456000	1.440397000
1	3.358607000	-0.003997000	1.998919000
7	-1.194099000	-0.057438000	-0.710947000
1	-1.141015000	0.314119000	-1.654085000
1	-1.998016000	0.313884000	-0.214745000

benzene-NCH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.410012000
6	1.250065000	0.000000000	-0.652310000
1	-0.941536000	0.011242000	1.961396000
1	1.303304000	0.011214000	-1.742118000
6	1.193402000	-0.015955000	2.121607000
6	2.433010000	-0.015967000	0.076504000
1	1.154755000	-0.017745000	3.214757000
1	3.384303000	-0.017789000	-0.463414000
6	2.423286000	-0.025796000	1.468859000
1	3.357148000	-0.037084000	2.034853000
7	-1.183340000	-0.002703000	-0.717220000
6	-1.146465000	0.139497000	-2.149734000
1	-2.170701000	0.108808000	-2.543854000
1	-0.683848000	1.091864000	-2.477703000
1	-0.585381000	-0.683449000	-2.627633000
6	-2.436225000	0.139247000	-0.021620000
1	-2.600064000	-0.683831000	0.696816000
1	-2.512982000	1.091526000	0.540390000
1	-3.259550000	0.108573000	-0.747232000

benzene-NO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.393070000
6	1.193827000	0.000000000	-0.725092000
1	-0.965170000	-0.000029000	1.906883000
1	1.136103000	-0.000147000	-1.816292000
6	1.210402000	0.000409000	2.078336000
6	2.398094000	0.000395000	-0.039128000
1	1.226255000	0.000458000	3.170537000
1	3.343541000	0.000690000	-0.587315000
6	2.404538000	0.000574000	1.360184000
1	3.357526000	0.000831000	1.895805000

7	-1.303403000	-0.000271000	-0.618183000
8	-1.290903000	0.000538000	-1.824678000

benzene-NO_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.389509000
6	1.172425000	0.000000000	-0.745757000
1	-0.952014000	0.000046000	1.921479000
1	1.110334000	-0.000046000	-1.834549000
6	1.222350000	-0.000026000	2.051688000
6	2.387194000	0.000026000	-0.069770000
1	1.247096000	-0.000083000	3.143656000
1	3.321845000	0.000083000	-0.634956000
6	2.411926000	0.000000000	1.324333000
1	3.369670000	0.000000000	1.850208000
7	-1.294902000	0.000000000	-0.711001000
8	-1.264947000	-0.001025000	-1.925265000
8	-2.303384000	0.001025000	-0.034024000

benzene-OH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.396489000
6	1.210925000	0.000000000	-0.694496000
1	-0.960962000	0.000134000	1.916479000
1	1.206965000	-0.000045000	-1.790481000
6	1.205971000	0.000152000	2.085782000
6	2.413490000	0.000001000	0.007461000
1	1.197417000	0.000340000	3.179126000
1	3.356030000	0.000071000	-0.546523000
6	2.420583000	0.000199000	1.399093000
1	3.365626000	0.000349000	1.946452000
8	-1.203243000	-0.000632000	-0.626738000
1	-1.054034000	-0.000662000	-1.580710000

p-F-benzene-BeH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.409735000
6	1.263596000	0.000000000	-0.625042000
1	-0.949654000	0.000000000	1.957197000
1	1.333253000	0.000000000	-1.718982000
6	1.174183000	0.000000000	2.156212000

6	2.453295000	0.000000000	0.096451000
1	1.172202000	0.000000000	3.248576000
1	3.431541000	0.000000000	-0.389652000
6	2.385822000	0.000000000	1.481595000
4	-1.420934000	0.000000000	-0.882400000
1	-2.554472000	0.000000000	-1.586327000
9	3.521036000	0.000000000	2.186563000

p-F-benzene-BF_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.403458000
6	1.232540000	0.000000000	-0.671284000
1	-0.953666000	0.000087000	1.938749000
1	1.246539000	-0.000052000	-1.764806000
6	1.188223000	-0.000130000	2.121038000
6	2.431013000	0.000120000	0.029092000
1	1.213028000	-0.000455000	3.212606000
1	3.401510000	0.000465000	-0.471193000
6	2.385745000	-0.000022000	1.417312000
5	-1.322383000	-0.000056000	-0.786454000
9	-1.345460000	-0.000150000	-2.114103000
9	-2.500256000	-0.001632000	-0.173417000
9	3.531799000	-0.000077000	2.098137000

p-F-benzene-BH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.409568000
6	1.249758000	0.000000000	-0.651936000
1	-0.959246000	-0.000143000	1.936348000
1	1.273126000	0.000011000	-1.746057000
6	1.179485000	0.000188000	2.139677000
6	2.442600000	0.000152000	0.056140000
1	1.196320000	0.000268000	3.231565000
1	3.418480000	0.000099000	-0.433924000
6	2.382949000	0.000330000	1.444622000
5	-1.310173000	-0.000291000	-0.794419000
1	-1.288053000	-0.000596000	-2.001337000
1	-2.370226000	-0.000296000	-0.217019000
9	3.522227000	0.000185000	2.135301000

p-F-benzene-Br

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.392532000
6	1.192707000	0.000000000	-0.718746000
1	-0.944683000	0.000000000	1.940386000
1	1.174354000	0.000000000	-1.810640000
6	1.211600000	0.000000000	2.076917000
6	2.404243000	0.000000000	-0.034248000
1	1.251652000	0.000000000	3.167983000
1	3.359417000	0.000000000	-0.563089000
6	2.394719000	0.000000000	1.352829000
35	-1.652891000	0.000000000	-0.933754000
9	3.557456000	0.000000000	2.009685000

p-F-benzene-CF_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.396191000
6	1.201696000	0.000000000	-0.702030000
1	-0.950787000	0.002737000	1.935255000
1	1.194377000	0.001242000	-1.793139000
6	1.199360000	-0.001225000	2.093134000
6	2.409863000	-0.001008000	-0.012683000
1	1.236233000	-0.000532000	3.184071000
1	3.370566000	-0.000594000	-0.530956000
6	2.387728000	-0.002375000	1.373467000
6	-1.318791000	-0.020889000	-0.706743000
9	-1.983445000	-1.159755000	-0.463985000
9	-2.112746000	0.976352000	-0.292019000
9	-1.191810000	0.091716000	-2.032034000
9	3.542874000	-0.004075000	2.039127000

p-F-benzene-CFO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.399826000
6	1.211638000	0.000000000	-0.699918000
1	-0.957849000	-0.000072000	1.924421000
1	1.203889000	0.000237000	-1.790963000
6	1.196239000	-0.000150000	2.099234000
6	2.414615000	-0.000046000	-0.008436000
1	1.233153000	-0.000181000	3.190168000
1	3.378427000	-0.000103000	-0.520796000
6	2.385872000	-0.000175000	1.380043000

6	-1.300754000	-0.000123000	-0.685369000
8	-2.381840000	-0.000116000	-0.188984000
9	-1.168065000	-0.000606000	-2.026844000
9	3.538073000	-0.000220000	2.045742000

p-F-benzene-CH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.399055000
6	1.233378000	0.000000000	-0.656857000
1	-0.954849000	0.007330000	1.934525000
1	1.256950000	0.007281000	-1.751132000
6	1.186635000	-0.006101000	2.123979000
6	2.432581000	-0.006201000	0.050217000
1	1.196747000	-0.003555000	3.216152000
1	3.400870000	-0.003871000	-0.455030000
6	2.390235000	-0.010381000	1.434961000
6	-1.288168000	-0.019570000	-0.766925000
1	-1.716779000	-1.035613000	-0.808637000
1	-2.045994000	0.630028000	-0.301432000
1	-1.144995000	0.317107000	-1.804735000
9	3.537671000	-0.013534000	2.125079000

p-F-benzene-CHO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.400131000
6	1.210878000	0.000000000	-0.696443000
1	-0.961825000	-0.000419000	1.919127000
1	1.200732000	-0.000129000	-1.791262000
6	1.196373000	-0.000207000	2.098186000
6	2.418731000	0.000636000	-0.010634000
1	1.236142000	-0.000758000	3.189191000
1	3.382483000	0.000960000	-0.522985000
6	2.387093000	0.000690000	1.377745000
6	-1.278444000	0.000202000	-0.734523000
8	-2.368316000	0.000853000	-0.213298000
1	-1.161615000	0.000795000	-1.852740000
9	3.539959000	0.000442000	2.045776000

p-F-benzene-Cl

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.391842000

6	1.190120000	0.000000000	-0.721692000
1	-0.946853000	0.000000000	1.935464000
1	1.163996000	0.000000000	-1.813192000
6	1.212381000	0.000000000	2.073908000
6	2.401971000	0.000000000	-0.038686000
1	1.253981000	0.000000000	3.164879000
1	3.356396000	0.000000000	-0.568800000
6	2.394773000	0.000000000	1.348484000
17	-1.523969000	0.000000000	-0.858139000
9	3.558520000	0.000000000	2.003784000

p-F-benzene-CN

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.401527000
6	1.214768000	0.000000000	-0.699011000
1	-0.950560000	0.000000000	1.939009000
1	1.206537000	0.000000000	-1.790974000
6	1.199880000	0.000000000	2.098164000
6	2.417015000	0.000000000	-0.006468000
1	1.233340000	0.000000000	3.189079000
1	3.379249000	0.000000000	-0.521560000
6	2.389327000	0.000000000	1.381778000
6	-1.240121000	0.000000000	-0.717177000
7	-2.247734000	0.000000000	-1.299893000
9	3.541661000	0.000000000	2.048187000

p-F-benzene-F

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.387329000
6	1.179131000	0.000000000	-0.730979000
1	-0.952125000	0.000000000	1.921479000
1	1.131450000	0.000000000	-1.821661000
6	1.215811000	0.000000000	2.064096000
6	2.394943000	0.000000000	-0.054212000
1	1.263493000	0.000000000	3.154777000
1	3.347068000	0.000000000	-0.588363000
6	2.394943000	0.000000000	1.333116000
9	-1.168578000	0.000000000	-0.650475000
9	3.563521000	0.000000000	1.983592000

p-F-benzene-Li

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.412545000
6	1.289745000	0.000000000	-0.576057000
1	-0.953291000	0.000000000	1.961677000
1	1.402372000	0.000000000	-1.670418000
6	1.159489000	0.000000000	2.190957000
6	2.473342000	0.000000000	0.165184000
1	1.132019000	0.000000000	3.284621000
1	3.460726000	0.000000000	-0.305910000
6	2.385806000	0.000000000	1.547359000
3	-1.661230000	0.000000000	-1.077422000
9	3.514766000	0.000000000	2.279568000

p-F-benzene-NH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.401787000
6	1.233974000	0.000000000	-0.665335000
1	-0.954076000	-0.003072000	1.938271000
1	1.253143000	-0.003075000	-1.759740000
6	1.192360000	-0.000649000	2.116538000
6	2.428897000	-0.000651000	0.044888000
1	1.200793000	0.001236000	3.208776000
1	3.394343000	0.001233000	-0.465960000
6	2.396509000	-0.001512000	1.430495000
7	-1.195880000	-0.062128000	-0.713983000
1	-1.138978000	0.321874000	-1.652245000
1	-1.994896000	0.321558000	-0.218616000
9	3.549252000	0.000619000	2.118447000

p-F-benzene-NCH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.409508000
6	1.250712000	0.000000000	-0.649932000
1	-0.939875000	0.013033000	1.962776000
1	1.308281000	0.012948000	-1.739047000
6	1.188848000	-0.018814000	2.129290000
6	2.437591000	-0.018807000	0.073076000
1	1.184781000	-0.020907000	3.221683000
1	3.405067000	-0.020894000	-0.434203000
6	2.399295000	-0.030029000	1.457112000
7	-1.185189000	-0.004429000	-0.719798000

6	-1.142740000	0.180875000	-2.147241000
1	-2.164888000	0.150942000	-2.546836000
1	-0.686858000	1.146183000	-2.447735000
1	-0.574219000	-0.624660000	-2.644846000
6	-2.432263000	0.180196000	-0.023795000
1	-2.610987000	-0.625430000	0.710224000
1	-2.489223000	1.145480000	0.519275000
1	-3.258248000	0.149725000	-0.746416000
9	3.546893000	-0.044579000	2.154038000

p-F-benzene-NO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.394200000
6	1.198130000	0.000000000	-0.720560000
1	-0.964657000	-0.000008000	1.908431000
1	1.145972000	0.000165000	-1.811857000
6	1.202037000	-0.000187000	2.088530000
6	2.402208000	-0.000346000	-0.040178000
1	1.249731000	-0.000396000	3.178729000
1	3.365247000	-0.000268000	-0.554599000
6	2.381591000	-0.000493000	1.354481000
7	-1.298766000	0.000149000	-0.618460000
8	-1.286622000	0.000087000	-1.825878000
9	3.541331000	-0.000576000	2.005951000

p-F-benzene-NO_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.390840000
6	1.177006000	0.000000000	-0.741008000
1	-0.952322000	0.000585000	1.922107000
1	1.119218000	-0.000585000	-1.829962000
6	1.214405000	-0.000132000	2.061509000
6	2.391571000	0.000132000	-0.070628000
1	1.272568000	-0.000638000	3.151355000
1	3.344847000	0.000638000	-0.602052000
6	2.389657000	0.000000000	1.319344000
7	-1.289560000	0.000000000	-0.711974000
8	-1.256492000	-0.001546000	-1.926347000
8	-2.299612000	0.001546000	-0.037000000
9	3.553711000	0.000000000	1.962025000

p-F-benzene-OH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.396730000
6	1.212704000	0.000000000	-0.690425000
1	-0.959589000	0.000061000	1.918367000
1	1.216003000	0.000044000	-1.785757000
6	1.200599000	-0.000018000	2.094623000
6	2.418168000	-0.000014000	0.006763000
1	1.225403000	0.000013000	3.186479000
1	3.377972000	0.000018000	-0.513974000
6	2.397362000	-0.000060000	1.391217000
8	-1.204437000	-0.000012000	-0.626647000
1	-1.057673000	-0.000169000	-1.580719000
9	3.555590000	-0.000065000	2.066352000

p-CF_3-benzene-BeH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.410212000
6	1.258136000	0.000000000	-0.630290000
1	-0.948861000	-0.001166000	1.958263000
1	1.323147000	-0.000782000	-1.724262000
6	1.177882000	0.001243000	2.145564000
6	2.449031000	0.001260000	0.091942000
1	1.156925000	0.000225000	3.239002000
1	3.412009000	0.001477000	-0.422382000
6	2.405086000	0.002774000	1.481712000
4	-1.426364000	0.001799000	-0.886917000
1	-2.557841000	0.005069000	-1.591660000
6	3.655960000	0.025142000	2.305479000
9	3.746951000	1.158587000	3.015816000
9	3.676317000	-0.981283000	3.190449000
9	4.763409000	-0.070658000	1.564424000

p-CF_3-benzene-BF_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.403315000
6	1.226362000	0.000000000	-0.676070000
1	-0.952468000	-0.001716000	1.940313000
1	1.236537000	-0.001376000	-1.769547000
6	1.192745000	0.001749000	2.110758000
6	2.427298000	0.001892000	0.025216000
1	1.198106000	0.000185000	3.203804000

1	3.382308000	0.002000000	-0.502748000
6	2.404182000	0.003988000	1.416702000
5	-1.330012000	0.001685000	-0.786328000
9	-1.352631000	0.003958000	-2.111477000
9	-2.502034000	0.002000000	-0.167421000
6	3.672697000	0.028037000	2.217222000
9	3.775503000	1.165178000	2.917204000
9	3.704537000	-0.974135000	3.104602000
9	4.763480000	-0.073838000	1.454554000

p-CF_3-benzene-BH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.408804000
6	1.242991000	0.000000000	-0.657068000
1	-0.957982000	-0.001500000	1.937511000
1	1.262289000	-0.001154000	-1.751156000
6	1.184617000	0.001396000	2.128821000
6	2.438756000	0.001546000	0.052117000
1	1.181850000	-0.000318000	3.221971000
1	3.398913000	0.001530000	-0.466570000
6	2.402117000	0.003385000	1.443959000
5	-1.318564000	0.001157000	-0.795424000
1	-1.296459000	0.002479000	-2.001138000
1	-2.374932000	0.001525000	-0.213775000
6	3.663680000	0.027131000	2.255938000
9	3.761116000	1.165539000	2.954771000
9	3.686167000	-0.973709000	3.145186000
9	4.761861000	-0.077243000	1.504251000

p-CF_3-benzene-Br

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.391122000
6	1.190851000	0.000000000	-0.725024000
1	-0.944316000	0.000835000	1.939283000
1	1.167591000	0.001270000	-1.816566000
6	1.215487000	-0.001042000	2.069550000
6	2.397111000	-0.000966000	-0.038353000
1	1.231410000	-0.000922000	3.160776000
1	3.342038000	0.000455000	-0.588022000
6	2.409900000	-0.001953000	1.356906000
35	-1.651151000	0.000800000	-0.930579000
6	3.736452000	-0.022412000	2.051944000
9	4.404231000	-1.153483000	1.786462000

9	4.517289000	0.986193000	1.641942000
9	3.620891000	0.072020000	3.379182000

p-CF_3-benzene-CF_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.393792000
6	1.198484000	0.000000000	-0.708693000
1	-0.950328000	0.004996000	1.933136000
1	1.186907000	0.003749000	-1.799555000
6	1.204206000	-0.004001000	2.085680000
6	2.402691000	-0.003629000	-0.016805000
1	1.215794000	-0.003420000	3.176548000
1	3.353036000	-0.001557000	-0.556139000
6	2.402682000	-0.007607000	1.376981000
6	-1.323184000	-0.020046000	-0.705782000
9	-1.976145000	-1.164916000	-0.467914000
9	-2.116218000	0.970166000	-0.278426000
9	-1.199189000	0.103998000	-2.028849000
6	3.725753000	-0.035881000	2.082694000
9	4.373331000	-1.183122000	1.841556000
9	4.523431000	0.951811000	1.658161000
9	3.602333000	0.084966000	3.406111000

p-CF_3-benzene-CFO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.396569000
6	1.207440000	0.000000000	-0.706378000
1	-0.956962000	0.001208000	1.922500000
1	1.196746000	0.001496000	-1.797096000
6	1.202544000	-0.001816000	2.091023000
6	2.407918000	-0.001504000	-0.012177000
1	1.214612000	-0.002017000	3.181966000
1	3.360580000	0.000143000	-0.547391000
6	2.401676000	-0.003561000	1.383210000
6	-1.307554000	-0.000519000	-0.684615000
8	-2.383662000	-0.001496000	-0.180162000
9	-1.178988000	-0.000360000	-2.023609000
6	3.724631000	-0.025913000	2.092112000
9	4.386986000	-1.158928000	1.829048000
9	4.506065000	0.981960000	1.686655000
9	3.596427000	0.068307000	3.416647000

p-CF_3-benzene-CH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.395465000
6	1.233892000	0.000000000	-0.664326000
1	-0.954703000	0.002938000	1.930110000
1	1.251749000	0.002585000	-1.758777000
6	1.191854000	-0.001976000	2.115758000
6	2.425679000	-0.001674000	0.043202000
1	1.176716000	-0.001010000	3.207155000
1	3.384466000	-0.000998000	-0.482477000
6	2.405873000	-0.002639000	1.439658000
6	-1.278338000	-0.009812000	-0.779673000
1	-1.415453000	-0.969766000	-1.305410000
1	-2.152371000	0.141888000	-0.129736000
1	-1.283790000	0.777986000	-1.549931000
6	3.711807000	0.016566000	2.168452000
9	4.501884000	-0.998898000	1.789162000
9	4.396427000	1.142017000	1.914202000
9	3.563773000	-0.066959000	3.494450000

p-CF_3-benzene-CHO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.397221000
6	1.207095000	0.000000000	-0.702671000
1	-0.961438000	0.001415000	1.916786000
1	1.193640000	0.002386000	-1.797193000
6	1.202582000	0.000048000	2.090246000
6	2.412012000	-0.000688000	-0.014349000
1	1.216768000	0.002819000	3.181500000
1	3.365593000	0.001803000	-0.547799000
6	2.403505000	-0.001274000	1.381072000
6	-1.283126000	0.001250000	-0.738245000
8	-2.369613000	-0.000610000	-0.213660000
1	-1.167454000	0.004076000	-1.855835000
6	3.724688000	-0.026092000	2.091954000
9	4.349690000	-1.195422000	1.904200000
9	4.542478000	0.926344000	1.626794000
9	3.600765000	0.155542000	3.408308000

p-CF_3-benzene-Cl

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.390444000

6	1.188359000	0.000000000	-0.727983000
1	-0.946596000	0.000868000	1.934238000
1	1.157351000	0.001297000	-1.819233000
6	1.216120000	-0.001382000	2.066920000
6	2.394987000	-0.001065000	-0.042811000
1	1.233107000	-0.001739000	3.158026000
1	3.339476000	0.000430000	-0.593118000
6	2.409663000	-0.002407000	1.352608000
17	-1.521477000	0.000550000	-0.854494000
6	3.736813000	-0.025379000	2.046054000
9	4.398882000	-1.161140000	1.785607000
9	4.522222000	0.977135000	1.629704000
9	3.623749000	0.076345000	3.372951000

p-CF_3-benzene-CN

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.398833000
6	1.210929000	0.000000000	-0.706311000
1	-0.950071000	0.001293000	1.936907000
1	1.197192000	0.001650000	-1.798042000
6	1.205555000	-0.001628000	2.089760000
6	2.409666000	-0.001390000	-0.011425000
1	1.215052000	-0.001511000	3.180631000
1	3.361648000	0.000588000	-0.547779000
6	2.404766000	-0.003267000	1.384389000
6	-1.243073000	0.000365000	-0.714655000
7	-2.251628000	0.000239000	-1.294746000
6	3.727180000	-0.026520000	2.093143000
9	4.384150000	-1.164885000	1.839899000
9	4.513801000	0.973820000	1.679175000
9	3.598812000	0.079444000	3.416840000

p-CF_3-benzene-Li

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.411340000
6	1.289470000	0.000000000	-0.581050000
1	-0.953329000	0.000340000	1.959796000
1	1.398011000	0.001000000	-1.675420000
6	1.161504000	-0.000881000	2.184326000
6	2.465938000	-0.001351000	0.161533000
1	1.106968000	-0.001180000	3.276104000
1	3.443563000	-0.002025000	-0.332269000
6	2.402361000	-0.001930000	1.555614000

3	-1.672654000	-0.004720000	-1.077102000
6	3.678622000	-0.020730000	2.328400000
9	4.388844000	-1.137380000	2.088728000
9	4.481386000	1.005249000	1.995670000
9	3.489690000	0.044016000	3.652995000

p-CF_3-benzene-NH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.403357000
6	1.235177000	0.000000000	-0.671112000
1	-0.954397000	0.001740000	1.938861000
1	1.250354000	0.001916000	-1.765358000
6	1.193163000	-0.004233000	2.110671000
6	2.421751000	-0.003083000	0.041199000
1	1.176446000	-0.001557000	3.202318000
1	3.378431000	0.002584000	-0.488263000
6	2.412543000	-0.006193000	1.437673000
7	-1.185258000	-0.051558000	-0.707767000
1	-1.145125000	0.280677000	-1.664812000
1	-2.010150000	0.272416000	-0.215287000
6	3.713032000	-0.039431000	2.166040000
9	4.338106000	-1.220205000	2.022982000
9	4.566342000	0.888981000	1.703889000
9	3.569895000	0.169990000	3.480258000

p-CF_3-benzene-NCH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.410781000
6	1.252230000	0.000000000	-0.655529000
1	-0.940430000	0.002998000	1.962856000
1	1.304448000	0.002963000	-1.744837000
6	1.190029000	-0.004312000	2.123470000
6	2.430643000	-0.003396000	0.069195000
1	1.161322000	-0.004798000	3.214897000
1	3.388297000	-0.002788000	-0.459105000
6	2.415865000	-0.006228000	1.464968000
7	-1.175467000	-0.000173000	-0.714798000
6	-1.139794000	0.043460000	-2.155511000
1	-2.165673000	0.029850000	-2.544487000
1	-0.645298000	0.956644000	-2.537677000
1	-0.608790000	-0.827026000	-2.582319000
6	-2.437608000	0.050668000	-0.019892000
1	-2.572789000	-0.814609000	0.654485000

1	-2.546512000	0.968598000	0.588415000
1	-3.255673000	0.033228000	-0.750946000
6	3.712594000	0.009211000	2.198991000
9	4.504462000	-1.014623000	1.837630000
9	4.415985000	1.126054000	1.944346000
9	3.555115000	-0.061988000	3.526520000

p-CF_3-benzene-NO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.394493000
6	1.189391000	0.000000000	-0.725501000
1	-0.959906000	0.001483000	1.915731000
1	1.129399000	0.002450000	-1.816813000
6	1.210611000	-0.000140000	2.070503000
6	2.401610000	-0.000865000	-0.050381000
1	1.239119000	0.002633000	3.161464000
1	3.349838000	0.001580000	-0.592850000
6	2.404310000	-0.001615000	1.345258000
7	-1.208600000	0.001321000	-0.798332000
8	-2.230416000	0.000381000	-0.160772000
6	3.733143000	-0.027012000	2.044272000
9	4.351982000	-1.198043000	1.852415000
9	4.546332000	0.923023000	1.568574000
9	3.621193000	0.157884000	3.360963000

p-CF_3-benzene-NO_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.387341000
6	1.171655000	0.000000000	-0.748472000
1	-0.950398000	0.001185000	1.921732000
1	1.110262000	0.001707000	-1.837108000
6	1.221051000	-0.001716000	2.052662000
6	2.384198000	-0.001649000	-0.075606000
1	1.253988000	-0.001531000	3.142976000
1	3.325757000	0.000157000	-0.629858000
6	2.404736000	-0.003634000	1.320552000
7	-1.297611000	-0.000135000	-0.711283000
8	-1.264835000	0.001243000	-1.924397000
8	-2.302856000	-0.001993000	-0.031570000
6	3.741713000	-0.027337000	2.003379000
9	4.390880000	-1.166775000	1.737617000
9	4.519727000	0.971953000	1.572421000
9	3.639657000	0.080098000	3.328985000

p-CF_3-benzene-OH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.396415000
6	1.212490000	0.000000000	-0.696984000
1	-0.959382000	0.001422000	1.918074000
1	1.210477000	0.001981000	-1.792148000
6	1.203017000	-0.001837000	2.087545000
6	2.410823000	-0.001673000	0.000932000
1	1.203327000	-0.002089000	3.179035000
1	3.360758000	-0.000666000	-0.540175000
6	2.412799000	-0.002970000	1.395513000
8	-1.198173000	0.000718000	-0.624432000
1	-1.055053000	-0.000594000	-1.579795000
6	3.726781000	-0.026860000	2.104816000
9	4.399980000	-1.161826000	1.857353000
9	4.524618000	0.974922000	1.702924000
9	3.596591000	0.074714000	3.431639000

m-F-benzene-BeH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.409116000
6	1.254006000	0.000000000	-0.638465000
1	-0.949153000	0.000000000	1.956670000
1	1.352283000	0.000000000	-1.729292000
6	1.183239000	0.000000000	2.144095000
6	2.423747000	0.000000000	0.105025000
1	1.153259000	0.000000000	3.236914000
6	2.412919000	0.000000000	1.491781000
4	-1.438790000	0.000000000	-0.862187000
1	-2.591231000	0.000000000	-1.533381000
9	3.601584000	0.000000000	-0.532310000
1	3.360975000	0.000000000	2.034271000

m-F-benzene-BF_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.401711000
6	1.222332000	0.000000000	-0.685312000
1	-0.952830000	0.000000000	1.937133000
1	1.262191000	0.000009000	-1.777470000
6	1.198793000	-0.000034000	2.107655000

6	2.403506000	0.000044000	0.035792000
1	1.195321000	-0.000044000	3.200195000
6	2.412350000	0.000028000	1.424382000
5	-1.325599000	-0.000015000	-0.790063000
9	-1.342902000	0.000197000	-2.116318000
9	-2.501628000	-0.000234000	-0.176952000
9	3.569566000	0.000072000	-0.616653000
1	3.370837000	0.000046000	1.947926000

m-F-benzene-BH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.407587000
6	1.239587000	0.000000000	-0.665874000
1	-0.958275000	0.000030000	1.935294000
1	1.290321000	-0.000025000	-1.758224000
6	1.189638000	0.000044000	2.127700000
6	2.414303000	-0.000053000	0.064505000
1	1.177995000	0.000024000	3.220121000
6	2.408902000	-0.000025000	1.453645000
5	-1.320169000	-0.000023000	-0.789584000
1	-1.306929000	0.000004000	-1.995606000
1	-2.372275000	-0.000055000	-0.199101000
9	3.588273000	0.000081000	-0.575482000
1	3.363339000	-0.000036000	1.985234000

m-F-benzene-Br

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.392332000
6	1.184275000	0.000000000	-0.730463000
1	-0.944318000	0.000000000	1.939213000
1	1.194007000	0.000000000	-1.821572000
6	1.220582000	0.000000000	2.062966000
6	2.379243000	0.000000000	-0.025093000
6	2.422619000	0.000000000	1.361453000
35	-1.652439000	0.000000000	-0.931173000
1	3.389369000	0.000000000	1.867615000
9	3.524597000	0.000000000	-0.710544000
1	1.232660000	0.000000000	3.155537000

m-F-benzene-CF_3

6	0.000000000	0.000000000	0.000000000

6	0.000000000	0.000000000	1.395248000
6	1.192863000	0.000000000	-0.714326000
1	-0.948848000	0.000289000	1.936431000
1	1.213274000	0.000471000	-1.804750000
6	1.209437000	-0.000405000	2.080049000
6	2.384314000	-0.000804000	-0.003741000
6	2.414997000	-0.001046000	1.381978000
6	-1.320302000	-0.016174000	-0.710778000
9	-1.999779000	-1.138889000	-0.442121000
9	-2.096007000	1.003283000	-0.321106000
9	-1.187863000	0.063060000	-2.036995000
1	3.379978000	-0.001670000	1.892510000
9	3.535442000	-0.001136000	-0.678820000
1	1.218157000	-0.000024000	3.172185000

m-F-benzene-CFO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.397959000
6	1.201678000	0.000000000	-0.712951000
1	-0.955949000	0.000000000	1.924943000
1	1.221149000	0.000000000	-1.803275000
6	1.207181000	0.000000000	2.085933000
6	2.388493000	0.000000000	0.000067000
1	1.215989000	0.000000000	3.177810000
6	2.412580000	0.000000000	1.387998000
6	-1.305440000	0.000000000	-0.686211000
8	-2.383611000	0.000000000	-0.185244000
9	-1.175383000	0.000000000	-2.025440000
1	3.376874000	0.000000000	1.900373000
9	3.543929000	0.000000000	-0.666738000

m-F-benzene-CH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.399180000
6	1.226436000	0.000000000	-0.668012000
1	-0.954159000	0.007160000	1.934878000
1	1.280797000	0.007027000	-1.760087000
6	1.195027000	-0.006336000	2.112304000
6	2.405956000	-0.005669000	0.061255000
1	1.177138000	-0.004341000	3.205044000
6	2.418112000	-0.009571000	1.447266000
6	-1.287583000	-0.023928000	-0.766221000
1	-1.658313000	-1.056394000	-0.885859000

1	-2.075287000	0.543078000	-0.246872000
1	-1.168657000	0.398591000	-1.775108000
9	3.570175000	-0.003403000	-0.598955000
1	3.372830000	-0.010203000	1.976600000

m-F-benzene-CHO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.398163000
6	1.202224000	0.000000000	-0.709694000
1	-0.960192000	0.000000000	1.918550000
1	1.218996000	0.000000000	-1.803402000
6	1.207065000	0.000000000	2.084822000
6	2.392581000	0.000000000	-0.001421000
1	1.218594000	0.000000000	3.177377000
6	2.414856000	0.000000000	1.386337000
6	-1.279474000	0.000000000	-0.741879000
8	-2.369069000	0.000000000	-0.223333000
1	-1.158708000	0.000000000	-1.859577000
9	3.549597000	0.000000000	-0.668359000
1	3.378586000	0.000000000	1.899726000

m-F-benzene-Cl

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.391764000
6	1.182630000	0.000000000	-0.731968000
1	-0.945936000	0.000000000	1.935737000
1	1.185740000	0.000000000	-1.822858000
6	1.221481000	0.000000000	2.060274000
6	2.377873000	0.000000000	-0.028014000
1	1.234490000	0.000000000	3.152720000
6	2.423419000	0.000000000	1.358393000
17	-1.520377000	0.000000000	-0.859535000
1	3.391251000	0.000000000	1.862593000
9	3.521381000	0.000000000	-0.716113000

m-F-benzene-CN

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.400170000
6	1.204920000	0.000000000	-0.712131000
1	-0.950063000	0.000000000	1.937152000
1	1.223406000	0.000000000	-1.803165000

6	1.209866000	0.000000000	2.084809000
6	2.391046000	0.000000000	0.001685000
1	1.215885000	0.000000000	3.176792000
6	2.415941000	0.000000000	1.389758000
6	-1.243017000	0.000000000	-0.714854000
7	-2.252910000	0.000000000	-1.292745000
1	3.379545000	0.000000000	1.902827000
9	3.544799000	0.000000000	-0.665710000

m-F-benzene-F

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.387514000
6	1.171854000	0.000000000	-0.742300000
1	-0.950357000	0.000000000	1.923528000
1	1.151245000	0.000000000	-1.832616000
6	1.224608000	0.000000000	2.049985000
6	2.370913000	0.000000000	-0.044788000
1	1.245261000	0.000000000	3.142058000
6	2.423323000	0.000000000	1.341721000
9	-1.165545000	0.000000000	-0.650009000
9	3.511081000	0.000000000	-0.738364000
1	3.393235000	0.000000000	1.841487000

m-F-benzene-Li

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.413694000
6	1.281952000	0.000000000	-0.588145000
1	-0.954351000	0.000000000	1.960393000
1	1.426883000	0.000000000	-1.677850000
6	1.165905000	0.000000000	2.180321000
6	2.441159000	0.000000000	0.175372000
1	1.108745000	0.000000000	3.274126000
6	2.413684000	0.000000000	1.560629000
3	-1.658997000	0.000000000	-1.089198000
9	3.637461000	0.000000000	-0.446019000
1	3.350784000	0.000000000	2.122218000

m-F-benzene-NH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.404131000
6	1.228176000	0.000000000	-0.675297000
1	-0.953457000	-0.002166000	1.941010000

1	1.278755000	-0.003472000	-1.767316000
6	1.199267000	-0.002473000	2.105382000
6	2.403305000	-0.002145000	0.057503000
1	1.179740000	-0.001193000	3.198206000
6	2.425267000	-0.003368000	1.444148000
7	-1.191244000	-0.055636000	-0.706653000
1	-1.149682000	0.302827000	-1.654628000
1	-2.002447000	0.290065000	-0.205174000
9	3.563573000	0.000173000	-0.609772000
1	3.380201000	-0.003478000	1.971385000

m-F-benzene-NCH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.411978000
6	1.246182000	0.000000000	-0.658470000
1	-0.939845000	0.011195000	1.964777000
1	1.338606000	0.006537000	-1.744763000
6	1.196144000	-0.013888000	2.117643000
6	2.412885000	-0.013699000	0.085903000
1	1.163203000	-0.015525000	3.210407000
6	2.429390000	-0.022156000	1.471619000
7	-1.176606000	-0.001681000	-0.718438000
6	-1.134214000	0.104853000	-2.154720000
1	-2.157933000	0.096351000	-2.549878000
1	-0.644695000	1.037212000	-2.497121000
1	-0.593311000	-0.742413000	-2.613751000
6	-2.438283000	0.082179000	-0.028106000
1	-2.571941000	-0.753588000	0.681851000
1	-2.554607000	1.025300000	0.540849000
1	-3.255421000	0.026324000	-0.758980000
9	3.578097000	-0.016787000	-0.575885000
1	3.379278000	-0.031428000	2.007491000

m-F-benzene-NO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.395568000
6	1.184524000	0.000000000	-0.732681000
1	-0.960052000	0.000000000	1.915517000
1	1.151467000	0.000000000	-1.824412000
6	1.215061000	0.000000000	2.064952000
6	2.382958000	0.000000000	-0.038361000
1	1.242749000	0.000000000	3.157057000
6	2.414990000	0.000000000	1.349595000

7	-1.206639000	0.000000000	-0.798091000
8	-2.229311000	0.000000000	-0.160924000
9	3.533199000	0.000000000	-0.713231000
1	3.383481000	0.000000000	1.854329000

m-F-benzene-NO_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.388708000
6	1.166370000	0.000000000	-0.753551000
1	-0.948344000	0.000098000	1.925132000
1	1.135690000	-0.000073000	-1.842773000
6	1.226193000	-0.000106000	2.046389000
6	2.366758000	0.000030000	-0.063252000
1	1.256159000	-0.000215000	3.137817000
6	2.416672000	-0.000058000	1.324972000
7	-1.294987000	-0.000022000	-0.715858000
8	-1.259688000	-0.001077000	-1.929100000
8	-2.303222000	0.000963000	-0.040112000
9	3.507278000	0.000058000	-0.752153000
1	3.390587000	-0.000123000	1.818276000

m-F-benzene-OH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.397686000
6	1.206702000	0.000000000	-0.700725000
1	-0.958573000	0.000845000	1.920247000
1	1.241411000	0.000648000	-1.794010000
6	1.208388000	-0.000696000	2.082329000
6	2.393768000	-0.001134000	0.018376000
1	1.204932000	-0.000996000	3.174966000
6	2.426066000	-0.001716000	1.403049000
8	-1.200756000	0.001628000	-0.624373000
1	-1.058473000	0.001085000	-1.579426000
9	3.544332000	-0.001169000	-0.662659000
1	3.386945000	-0.002548000	1.919606000

m-CF_3-benzene-BeH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.410046000
6	1.257423000	0.000000000	-0.626297000
1	-0.951487000	-0.000006000	1.954194000

1	1.332762000	0.000000000	-1.720404000
6	1.178081000	-0.000006000	2.149924000
6	2.444013000	-0.000021000	0.108063000
1	1.142166000	-0.000013000	3.242245000
6	2.408930000	-0.000020000	1.498541000
4	-1.417050000	-0.000118000	-0.900217000
1	-2.541219000	-0.000244000	-1.616632000
6	3.743314000	0.000025000	-0.637066000
9	4.802967000	-0.000782000	0.177698000
9	3.851349000	-1.073309000	-1.433021000
9	3.852042000	1.074165000	-1.431790000
1	3.341378000	-0.000054000	2.066324000

m-CF_3-benzene-BF_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.403454000
6	1.226082000	0.000000000	-0.672443000
1	-0.955231000	0.000110000	1.936017000
1	1.247030000	-0.000153000	-1.766574000
6	1.192638000	-0.000137000	2.115247000
6	2.422182000	0.000042000	0.040913000
1	1.183211000	-0.000339000	3.207380000
6	2.408261000	-0.000031000	1.433245000
5	-1.325634000	0.000206000	-0.792018000
9	-1.342418000	-0.000206000	-2.117104000
9	-2.500141000	0.000744000	-0.176831000
6	3.711217000	0.000036000	-0.724735000
9	3.805493000	1.073823000	-1.519150000
9	4.779652000	0.000219000	0.077289000
9	3.805656000	-1.074000000	-1.518964000
1	3.350443000	-0.000108000	1.984710000

m-CF_3-benzene-BH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.408825000
6	1.242763000	0.000000000	-0.653470000
1	-0.960486000	-0.000003000	1.933640000
1	1.272387000	0.000047000	-1.748283000
6	1.184599000	0.000023000	2.133535000
6	2.433347000	-0.000004000	0.068055000
1	1.167330000	0.000043000	3.225827000
6	2.405826000	0.000030000	1.461136000

5	-1.315832000	0.000035000	-0.797542000
1	-1.291807000	0.000093000	-2.002986000
1	-2.372006000	0.000011000	-0.215076000
6	3.728684000	-0.000114000	-0.685696000
9	3.829572000	1.072788000	-1.480995000
9	4.791005000	0.001253000	0.125317000
9	3.830673000	-1.074600000	-1.478737000
1	3.345463000	0.000078000	2.017520000

m-CF_3-benzene-Br

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.394146000
6	1.187943000	0.000000000	-0.718230000
1	-0.946416000	0.000317000	1.938586000
1	1.178914000	-0.000533000	-1.810701000
6	1.213207000	0.000254000	2.073367000
6	2.395862000	0.001074000	-0.019279000
6	2.416077000	0.001505000	1.371068000
35	-1.654331000	0.002262000	-0.926081000
6	3.665431000	-0.005809000	-0.817237000
9	3.768936000	-1.118598000	-1.555131000
9	3.708958000	1.024895000	-1.670539000
9	4.751895000	0.066020000	-0.044306000
1	3.370309000	0.003575000	1.900085000
1	1.219294000	0.000358000	3.165546000

m-CF_3-benzene-CF_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.396995000
6	1.196126000	0.000000000	-0.702752000
1	-0.951202000	0.000006000	1.935504000
1	1.196181000	-0.000006000	-1.794784000
6	1.202662000	-0.000018000	2.088545000
6	2.401525000	-0.000026000	0.000346000
1	1.205703000	-0.000024000	3.180333000
6	2.409666000	-0.000037000	1.389892000
6	-1.321586000	0.000028000	-0.708947000
9	-2.048594000	-1.073928000	-0.375365000
9	-2.048615000	1.073918000	-0.375277000
9	-1.188463000	0.000087000	-2.036339000
6	3.677913000	-0.000066000	-0.786942000
9	3.757259000	-1.074044000	-1.582094000
9	3.757269000	1.073803000	-1.582206000

9	4.758054000	-0.000039000	-0.002268000
1	3.359897000	-0.000071000	1.926606000

m-CF_3-benzene-CFO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.399934000
6	1.205409000	0.000000000	-0.700115000
1	-0.959428000	-0.000017000	1.922008000
1	1.209911000	-0.000024000	-1.791765000
6	1.200996000	0.000003000	2.093401000
6	2.406809000	0.000030000	0.004268000
1	1.203591000	-0.000028000	3.185142000
6	2.408755000	0.000028000	1.396052000
6	-1.305451000	-0.000027000	-0.687255000
8	-2.381841000	-0.000051000	-0.183031000
9	-1.176190000	0.000000000	-2.025284000
6	3.687275000	0.000120000	-0.777843000
9	3.769410000	-1.073623000	-1.572475000
9	3.769698000	1.074372000	-1.571736000
9	4.763302000	-0.000300000	0.012292000
1	3.356806000	0.000021000	1.936942000

m-CF_3-benzene-CH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.401229000
6	1.228792000	0.000000000	-0.655244000
1	-0.957568000	0.003658000	1.932380000
1	1.265613000	0.006904000	-1.749218000
6	1.187797000	-0.000966000	2.121106000
6	2.423357000	-0.001167000	0.066393000
1	1.163837000	0.001799000	3.213577000
6	2.412715000	-0.001203000	1.456008000
6	-1.290606000	-0.002261000	-0.760154000
1	-1.849807000	-0.938009000	-0.593928000
1	-1.946693000	0.822250000	-0.437501000
1	-1.124533000	0.100222000	-1.842335000
6	3.708372000	-0.024406000	-0.701167000
9	3.882561000	-1.197678000	-1.327150000
9	3.729849000	0.919229000	-1.653122000
9	4.775842000	0.170191000	0.079552000
1	3.352482000	0.002569000	2.010693000

m-CF_3-benzene-CHO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.399870000
6	1.204530000	0.000000000	-0.697829000
1	-0.963402000	0.002258000	1.915841000
1	1.202707000	0.004527000	-1.792961000
6	1.201601000	-0.000507000	2.091840000
6	2.410010000	-0.000999000	0.000837000
1	1.209257000	0.001792000	3.184043000
6	2.409953000	-0.000880000	1.392896000
6	-1.283131000	0.004871000	-0.736722000
8	-2.368012000	0.006079000	-0.208427000
1	-1.170587000	0.006974000	-1.854401000
6	3.689910000	-0.032944000	-0.778550000
9	3.883439000	-1.232497000	-1.342258000
9	3.676348000	0.861308000	-1.774966000
9	4.755481000	0.226819000	-0.017215000
1	3.359291000	0.001187000	1.931946000

m-CF_3-benzene-Cl

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.393692000
6	1.185485000	0.000000000	-0.720890000
1	-0.948548000	0.000007000	1.934449000
1	1.167628000	0.000013000	-1.813087000
6	1.214941000	0.000000000	2.068954000
6	2.394446000	-0.000004000	-0.025335000
1	1.224275000	0.000002000	3.161180000
6	2.417525000	-0.000011000	1.365166000
17	-1.522507000	-0.000011000	-0.854560000
6	3.659103000	-0.000012000	-0.831769000
9	3.725654000	-1.073862000	-1.629273000
9	3.725802000	1.073960000	-1.629065000
9	4.751707000	-0.000125000	-0.064820000
1	3.372139000	-0.000020000	1.893679000

m-CF_3-benzene-CN

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.402251000
6	1.208154000	0.000000000	-0.699953000
1	-0.951956000	-0.000017000	1.937353000
1	1.206562000	0.000015000	-1.792591000

6	1.204259000	-0.000010000	2.091688000
6	2.408531000	-0.000032000	0.004555000
1	1.206181000	0.000014000	3.183476000
6	2.412094000	-0.000016000	1.396200000
6	-1.243175000	0.000027000	-0.714152000
7	-2.254738000	0.000033000	-1.288785000
6	3.685216000	-0.000024000	-0.784601000
9	3.760471000	-1.073939000	-1.579345000
9	3.760610000	1.074121000	-1.579044000
9	4.764889000	-0.000208000	-0.000508000
1	3.361603000	0.000010000	1.934680000

m-CF_3-benzene-Li

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.413797000
6	1.286231000	0.000000000	-0.572419000
1	-0.956299000	0.000039000	1.957347000
1	1.407705000	0.000068000	-1.665977000
6	1.160393000	-0.000021000	2.186778000
6	2.465112000	-0.000056000	0.181737000
1	1.095835000	0.000004000	3.279565000
6	2.409571000	-0.000068000	1.571859000
3	-1.618748000	-0.001061000	-1.152381000
6	3.772151000	-0.000103000	-0.541212000
9	3.902397000	-1.073535000	-1.341215000
9	3.902671000	1.073475000	-1.340906000
9	4.828523000	-0.000349000	0.282566000
1	3.328138000	-0.000114000	2.162512000

m-CF_3-benzene-NH_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.404911000
6	1.232180000	0.000000000	-0.662854000
1	-0.956579000	-0.001126000	1.937232000
1	1.266379000	0.003146000	-1.756878000
6	1.192354000	0.000393000	2.114006000
6	2.420304000	0.000162000	0.062226000
1	1.165417000	0.004332000	3.206562000
6	2.419786000	0.000783000	1.453276000
7	-1.189549000	-0.051642000	-0.707871000
1	-1.142418000	0.287651000	-1.662657000
1	-2.002349000	0.304097000	-0.216234000
6	3.702850000	-0.021237000	-0.710731000

9	3.873244000	-1.191176000	-1.344058000
9	3.722781000	0.927639000	-1.659020000
9	4.774217000	0.168246000	0.065308000
1	3.360320000	0.006543000	2.005040000

m-CF_3-benzene-NCH_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.411151000
6	1.249883000	0.000000000	-0.649980000
1	-0.941705000	0.017052000	1.961976000
1	1.313487000	0.019164000	-1.738035000
6	1.190885000	-0.019926000	2.124347000
6	2.429788000	-0.020799000	0.084437000
1	1.152649000	-0.019032000	3.216623000
6	2.422370000	-0.032069000	1.476704000
7	-1.175582000	0.002196000	-0.721243000
6	-1.130302000	0.131171000	-2.156524000
1	-2.152043000	0.096962000	-2.555775000
1	-0.666811000	1.081124000	-2.487311000
1	-0.565964000	-0.695525000	-2.623069000
6	-2.435155000	0.131403000	-0.033013000
1	-2.589805000	-0.688405000	0.690654000
1	-2.527204000	1.087609000	0.518779000
1	-3.252737000	0.082228000	-0.763581000
6	3.734895000	-0.089609000	-0.649114000
9	4.087342000	-1.359976000	-0.899391000
9	3.687440000	0.535489000	-1.834083000
9	4.736901000	0.458349000	0.048710000
1	3.357715000	-0.042235000	2.037847000

m-CF_3-benzene-NO

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.397117000
6	1.187330000	0.000000000	-0.721033000
1	-0.962956000	0.002636000	1.913313000
1	1.139641000	0.004936000	-1.813615000
6	1.209458000	-0.000950000	2.072496000
6	2.399760000	-0.002261000	-0.035222000
1	1.231901000	0.001561000	3.164519000
6	2.410499000	-0.001953000	1.357131000
7	-1.207893000	0.005355000	-0.796707000
8	-2.228816000	0.003473000	-0.157202000
6	3.674329000	-0.033898000	-0.824923000

9	3.867178000	-1.235894000	-1.381460000
9	3.649109000	0.855023000	-1.823895000
9	4.743213000	0.233705000	-0.070496000
1	3.364373000	0.000206000	1.888018000

m-CF_3-benzene-NO_2

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.390401000
6	1.169159000	0.000000000	-0.743035000
1	-0.951508000	0.000444000	1.923034000
1	1.117472000	-0.000082000	-1.833369000
6	1.220577000	-0.000152000	2.053244000
6	2.383425000	0.000004000	-0.061817000
1	1.245847000	-0.000411000	3.144562000
6	2.412711000	-0.000192000	1.330487000
7	-1.292990000	-0.000127000	-0.718618000
8	-1.252333000	-0.000241000	-1.931313000
8	-2.302504000	-0.000200000	-0.045086000
6	3.646554000	-0.000124000	-0.873351000
9	3.709212000	-1.074361000	-1.667460000
9	3.708945000	1.073741000	-1.668070000
9	4.738724000	0.000168000	-0.106109000
1	3.371513000	-0.000187000	1.851839000

m-CF_3-benzene-OH

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.399269000
6	1.208572000	0.000000000	-0.690495000
1	-0.961589000	-0.000043000	1.917495000
1	1.219401000	-0.000020000	-1.786022000
6	1.201600000	0.000045000	2.090888000
6	2.409310000	0.000050000	0.020561000
1	1.192884000	0.000083000	3.183464000
6	2.419737000	0.000080000	1.409414000
8	-1.201829000	0.000013000	-0.620498000
1	-1.064357000	0.000201000	-1.576594000
6	3.683510000	0.000172000	-0.767084000
9	3.763310000	-1.073263000	-1.567000000
9	3.763502000	1.074092000	-1.566327000
9	4.768285000	-0.000180000	0.010887000
1	3.367402000	0.000148000	1.948959000

ethene

1	-0.930374000	0.000862000	-0.576674000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.328954000
1	0.930374000	0.000000000	1.905628000
1	0.930374000	0.000000000	-0.576674000
1	-0.930374000	0.000862000	1.905628000

ethene-BeH

1	-0.930121000	0.000127000	-0.585055000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.344361000
1	0.998319000	0.000000000	1.808995000
1	0.917620000	-0.000821000	-0.604960000
4	-1.424202000	0.000693000	2.210582000
1	-2.585006000	0.001069000	2.871188000

ethene-BF_2

1	-0.940714000	-0.000183000	-0.561809000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.338182000
1	0.953639000	0.000000000	1.877213000
1	0.920719000	0.000334000	-0.592462000
5	-1.323663000	-0.000244000	2.126498000
9	-2.498794000	-0.000125000	1.505859000
9	-1.356246000	-0.000447000	3.452709000

ethene-BH_2

1	-0.945625000	0.000252000	-0.555502000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.344732000
1	0.970814000	0.000000000	1.856703000
1	0.916753000	-0.000632000	-0.601398000
5	-1.328517000	0.000907000	2.118881000
1	-2.361217000	-0.000109000	1.489531000
1	-1.370835000	0.002435000	3.323744000

ethene-Br

1	-0.924783000	0.001647000	-0.582243000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.326344000
1	0.902990000	0.000000000	1.942072000
1	0.950504000	0.000820000	-0.540704000
35	-1.587805000	0.000520000	2.353010000

ethene-CF_3

1	-0.934312000	-0.000226000	-0.566845000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.327363000
1	0.920021000	0.000000000	1.919023000
1	0.935249000	-0.000250000	-0.563649000
6	-1.246217000	-0.000625000	2.144340000
9	-1.296632000	1.075105000	2.941787000
9	-2.355402000	-0.001441000	1.401118000
9	-1.295326000	-1.076040000	2.942335000

ethene-CFO

1	-0.936653000	0.000119000	-0.562697000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.333654000
1	0.920733000	0.000000000	1.922062000
1	0.933878000	0.000018000	-0.566729000
6	-1.226279000	0.000078000	2.140829000
8	-1.301708000	0.000658000	3.327020000
9	-2.341067000	-0.000436000	1.383434000

ethene-CH_3

1	-0.937711000	-0.000250000	-0.567496000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.332193000
1	0.963442000	0.000000000	1.859615000
1	0.929232000	0.000045000	-0.575932000
6	-1.221527000	-0.000182000	2.185657000
1	-1.250480000	0.882203000	2.847764000
1	-2.138512000	-0.000097000	1.575985000
1	-1.250434000	-0.882801000	2.847454000

ethene-CHO

1	-0.945779000	0.001320000	-0.554380000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.334983000
1	0.919674000	0.000000000	1.929290000
1	0.920280000	0.000413000	-0.588555000
6	-1.267820000	0.001125000	2.083107000
8	-1.351887000	0.001868000	3.286881000
1	-2.180472000	0.001899000	1.423522000

ethene-Cl

1	-0.926550000	-0.000142000	-0.578525000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.326200000
1	0.901478000	0.000000000	1.943549000
1	0.951643000	0.000498000	-0.536630000
17	-1.462869000	-0.001748000	2.273312000

ethene-CN

1	-0.932819000	-0.000473000	-0.569477000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.335663000
1	0.934156000	0.000000000	1.905837000
1	0.937834000	0.000178000	-0.559086000
6	-1.204502000	-0.001275000	2.104443000
7	-2.176989000	-0.002241000	2.743801000

ethene-F

1	-0.936899000	0.000329000	-0.560817000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.323538000
1	0.895026000	0.000000000	1.953613000
1	0.947168000	0.000251000	-0.539091000
9	-1.124746000	-0.000218000	2.040645000

ethene-Li

1	-0.933435000	-0.000086000	-0.592671000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.349123000
1	1.030750000	0.000000000	1.758578000
1	0.907214000	-0.000007000	-0.631444000
3	-1.730384000	0.000985000	2.269432000

ethene-NH_2

1	-0.933660000	-0.002357000	-0.572524000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.338310000
1	0.950879000	0.000000000	1.885316000
1	0.939066000	-0.022099000	-0.553908000
7	-1.111504000	-0.078942000	2.165027000
1	-1.990045000	0.139377000	1.702272000
1	-1.025567000	0.423928000	3.042453000

ethene-NCH_3

1	-0.914378000	0.019371000	-0.597366000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.342639000
1	0.954792000	0.000000000	1.883826000
1	0.949807000	-0.043938000	-0.534635000
7	-1.095338000	-0.036610000	2.184862000
6	-2.397363000	0.062613000	1.579976000
1	-3.171562000	-0.068949000	2.350625000
1	-2.564289000	1.039638000	1.077570000
1	-2.527247000	-0.729902000	0.825483000
6	-0.960940000	0.589973000	3.477931000
1	-1.712874000	0.184726000	4.174377000
1	0.035064000	0.376703000	3.895298000
1	-1.086979000	1.692652000	3.444485000

ethene-NO

1	-0.961455000	0.000089000	-0.522093000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.334049000
1	0.886304000	0.000000000	1.982069000
1	0.919240000	0.000342000	-0.588627000

7	-1.278719000	-0.000888000	1.974545000
8	-1.209908000	-0.000888000	3.180658000

ethene-NO_2

1	-0.947934000	0.000624000	-0.542809000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.324136000
1	0.861108000	0.000000000	1.992019000
1	0.939279000	-0.000445000	-0.555173000
7	-1.269615000	0.000652000	2.066495000
8	-1.165687000	0.001130000	3.277343000
8	-2.308941000	0.000782000	1.440149000

ethene-OH

1	-0.932478000	-0.000009000	-0.575026000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.333513000
1	0.925409000	0.000000000	1.918902000
1	0.942287000	-0.000003000	-0.548243000
8	-1.076768000	-0.000017000	2.148413000
1	-1.872929000	-0.000049000	1.598205000

F-ethene-BeH

1	-0.884878000	0.000000000	-0.649563000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.332738000
1	1.010133000	0.000000000	1.770542000
4	-1.394544000	0.000000000	2.230345000
1	-2.521928000	0.000000000	2.943918000
9	1.116930000	0.000000000	-0.736297000

F-ethene-BF_2

1	-0.903201000	-0.000009000	-0.620700000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.333403000
1	0.962386000	0.000000000	1.852442000
5	-1.335141000	-0.000021000	2.083410000
9	-1.400556000	0.001203000	3.407112000
9	-2.495048000	0.001276000	1.430941000

9	1.108604000	-0.000029000	-0.721675000

F-ethene-BH_2

1	-0.907823000	0.000000000	-0.616325000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.339757000
1	0.974845000	0.000000000	1.839565000
5	-1.349590000	0.000000000	2.050255000
1	-1.437728000	0.000000000	3.250807000
1	-2.355816000	0.000000000	1.379270000
9	1.102379000	0.000000000	-0.729947000

F-ethene-Br

1	-0.897426000	0.000000000	-0.625839000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.327947000
1	0.920981000	0.000000000	1.914671000
35	-1.608301000	0.000000000	2.299798000
9	1.138034000	0.000000000	-0.687121000

F-ethene-CF_3

1	-0.899846000	0.000001000	-0.620433000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.326117000
1	0.931461000	0.000000000	1.895473000
6	-1.262013000	0.000011000	2.106335000
9	-1.341115000	-1.074142000	2.901182000
9	-1.341167000	1.074236000	2.901077000
9	-2.348440000	-0.000054000	1.323785000
9	1.123205000	0.000004000	-0.699239000

F-ethene-CFO

1	-0.900364000	0.000000000	-0.620540000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.333914000
1	0.935652000	0.000000000	1.895408000
6	-1.235182000	0.000000000	2.107992000
8	-1.346188000	0.000000000	3.290136000
9	-2.331043000	0.000000000	1.314164000

9	1.120358000	0.000000000	-0.693422000

F-ethene-CH_3

1	-0.899690000	0.000045000	-0.625537000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.326770000
1	0.972278000	0.000000000	1.832805000
6	-1.246090000	0.000035000	2.141150000
1	-1.300980000	-0.884028000	2.798310000
1	-1.300934000	0.884086000	2.798334000
1	-2.143822000	0.000066000	1.503113000
9	1.127934000	0.000081000	-0.717720000

F-ethene-CHO

1	-0.912315000	0.000000000	-0.608385000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.333145000
1	0.928380000	0.000000000	1.910121000
6	-1.281845000	0.000000000	2.039507000
8	-1.402049000	0.000000000	3.240639000
1	-2.177657000	0.000000000	1.358087000
9	1.103386000	0.000000000	-0.724080000

F-ethene-Cl

1	-0.899441000	0.000000000	-0.621796000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.328262000
1	0.916374000	0.000000000	1.921616000
17	-1.485935000	0.000000000	2.218315000
9	1.139810000	0.000000000	-0.684318000

F-ethene-CN

1	-0.899929000	0.000000000	-0.622400000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.334575000
1	0.944976000	0.000000000	1.884441000
6	-1.222448000	0.000000000	2.060275000
7	-2.218092000	0.000000000	2.663450000
9	1.124796000	0.000000000	-0.687548000

F-ethene-F

1	-0.906053000	0.000000000	-0.611009000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.326294000
1	0.905849000	0.000000000	1.937589000
9	-1.146050000	0.000000000	2.004988000
9	1.145871000	0.000000000	-0.678907000

F-ethene-Li

1	-0.879509000	0.000000000	-0.663410000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.331009000
1	1.038557000	0.000000000	1.717192000
3	-1.658056000	0.000000000	2.356046000
9	1.121044000	0.000000000	-0.780874000

F-ethene-NH_2

1	-0.893345000	-0.003582000	-0.632241000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.332997000
1	0.965135000	0.000000000	1.850773000
7	-1.130076000	-0.097406000	2.146723000
1	-1.095018000	0.532305000	2.945118000
1	-1.998466000	0.057825000	1.638659000
9	1.151342000	-0.029664000	-0.693205000

F-ethene-NCH_3

1	-0.871271000	0.013034000	-0.657959000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.337676000
1	0.970747000	0.000000000	1.846595000
7	-1.110152000	-0.043234000	2.169371000
9	1.167301000	-0.050521000	-0.668235000
6	-1.007393000	0.748472000	3.375405000
1	-1.792320000	0.446329000	4.086558000
1	-0.030520000	0.575822000	3.852789000
1	-1.109761000	1.838787000	3.189000000
6	-2.392428000	0.027353000	1.518295000

1	-2.544917000	0.985692000	0.973432000
1	-2.492827000	-0.795972000	0.792073000
1	-3.191879000	-0.076050000	2.266978000

F-ethene-NO

1	-0.930469000	-0.000038000	-0.576420000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.337261000
1	0.895232000	0.000000000	1.969259000
7	-1.292442000	-0.000025000	1.913684000
8	-1.288348000	0.000007000	3.124084000
9	1.097982000	-0.000054000	-0.719998000

F-ethene-NO_2

1	-0.915731000	-0.000003000	-0.596812000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.330514000
1	0.882090000	0.000000000	1.967708000
7	-1.271222000	-0.000003000	2.031635000
8	-1.205131000	-0.000022000	3.244018000
8	-2.295181000	-0.000019000	1.373359000
9	1.121381000	-0.000002000	-0.686069000

F-ethene-OH

1	-0.896990000	0.000000000	-0.628691000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.331619000
1	0.939750000	0.000000000	1.890303000
8	-1.092300000	0.000000000	2.129585000
1	-1.886334000	0.000000000	1.577854000
9	1.150717000	0.000000000	-0.688022000

CF_3-ethene-BeH

1	-0.914644000	-0.000076000	-0.607183000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.339959000
1	1.005458000	0.000000000	1.788089000
4	-1.399254000	0.000315000	2.260262000
1	-2.520917000	0.000775000	2.978724000

6	1.232785000	0.001137000	-0.846355000
9	2.359552000	-0.005296000	-0.131900000
9	1.264911000	1.081501000	-1.639738000
9	1.259471000	-1.071073000	-1.650890000

CF_3-ethene-BF_2

1	-0.927498000	0.000214000	-0.583255000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.334940000
1	0.959878000	0.000000000	1.861441000
5	-1.329120000	0.001516000	2.126274000
9	-1.352080000	0.005957000	3.447730000
9	-2.497391000	-0.001234000	1.500912000
6	1.239945000	0.002754000	-0.832749000
9	1.266666000	-1.063944000	-1.639351000
9	2.353841000	-0.012637000	-0.101233000
9	1.278932000	1.089771000	-1.611589000

CF_3-ethene-BH_2

1	-0.933415000	-0.000001000	-0.575197000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.340724000
1	0.972970000	0.000000000	1.845489000
5	-1.337661000	-0.000015000	2.114449000
1	-1.375444000	-0.000037000	3.316554000
1	-2.364507000	-0.000004000	1.480276000
6	1.229176000	0.000006000	-0.850896000
9	1.247831000	1.077252000	-1.644834000
9	1.247798000	-1.077185000	-1.644906000
9	2.356282000	-0.000029000	-0.140470000

CF_3-ethene-Br

1	-0.919095000	-0.000068000	-0.591833000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.328089000
1	0.915792000	0.000000000	1.924115000
35	-1.578190000	-0.000021000	2.344039000
6	1.265927000	0.001063000	-0.787590000
9	1.331855000	-1.070372000	-1.586211000
9	2.354985000	-0.004347000	-0.014668000
9	1.336015000	1.079403000	-1.576567000

CF_3-ethene-CF_3

1	-0.925539000	0.000000000	-0.581268000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.325953000
1	0.925537000	0.000000000	1.907223000
6	-1.253012000	0.001175000	2.136408000
9	-1.297046000	-1.070653000	2.933267000
9	-1.302515000	1.081705000	2.921222000
9	-2.354108000	-0.005687000	1.383946000
6	1.253011000	-0.001162000	-0.810457000
9	2.354108000	0.005684000	-0.057983000
9	1.297046000	1.070709000	-1.607272000
9	1.302525000	-1.081647000	-1.595307000

CF_3-ethene-CFO

1	-0.927803000	0.000163000	-0.578166000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.331637000
1	0.926509000	0.000000000	1.910019000
6	-1.232000000	0.000847000	2.135255000
8	-1.301799000	0.002930000	3.319728000
9	-2.339754000	-0.000786000	1.373405000
6	1.253412000	0.001554000	-0.812811000
9	2.353879000	-0.007010000	-0.062342000
9	1.298713000	1.083906000	-1.593996000
9	1.292207000	-1.069562000	-1.609572000

CF_3-ethene-CH_3

1	-0.926696000	-0.000001000	-0.583601000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.331620000
1	0.966538000	0.000000000	1.848943000
6	-1.222157000	0.000026000	2.176822000
6	1.238053000	0.000507000	-0.822038000
1	-2.140120000	-0.000235000	1.570696000
1	-1.241699000	-0.881567000	2.838748000
1	-1.241914000	0.881974000	2.838273000
9	1.286950000	-1.072568000	-1.626304000
9	2.355785000	-0.002490000	-0.087690000
9	1.289515000	1.077225000	-1.621255000

CF_3-ethene-CHO

1	-0.935550000	0.000008000	-0.571178000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.332969000
1	0.924664000	0.000000000	1.917901000
6	-1.275173000	-0.000037000	2.075592000
8	-1.352081000	-0.000446000	3.277674000
1	-2.186580000	-0.000085000	1.417705000
6	1.235649000	-0.000160000	-0.836319000
9	2.350523000	0.001325000	-0.107174000
9	1.264058000	1.075364000	-1.630144000
9	1.265386000	-1.077408000	-1.627755000

CF_3-ethene-Cl

1	-0.921748000	-0.000068000	-0.586694000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.328268000
1	0.912230000	0.000000000	1.928856000
17	-1.454917000	-0.000064000	2.260531000
6	1.265820000	0.000792000	-0.784919000
9	2.354281000	-0.003275000	-0.009900000
9	1.337365000	1.078158000	-1.575201000
9	1.334221000	-1.071448000	-1.582379000

CF_3-ethene-CN

1	-0.922521000	-0.000013000	-0.586239000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.334390000
1	0.942089000	0.000000000	1.891099000
6	-1.204949000	0.000025000	2.097922000
7	-2.178448000	0.000128000	2.734595000
6	1.261810000	0.000149000	-0.797447000
9	2.350933000	-0.000565000	-0.027747000
9	1.317840000	1.076979000	-1.585324000
9	1.317316000	-1.075728000	-1.586639000

CF_3-ethene-Li

1	-0.916464000	0.000053000	-0.614074000

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.345317000
1	1.036032000	0.000000000	1.737184000
3	-1.672038000	-0.000086000	2.394166000
6	1.203842000	-0.000133000	-0.879942000
9	1.222573000	1.074823000	-1.696235000
9	1.222937000	-1.075705000	-1.695426000
9	2.363697000	0.000304000	-0.214007000

CF_3-ethene-NH_2

1	-0.924454000	0.000087000	-0.584684000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.342907000
1	0.955397000	0.000000000	1.876946000
7	-1.102000000	-0.059293000	2.150786000
1	-1.007195000	0.294188000	3.094204000
1	-2.000480000	0.138403000	1.723607000
6	1.244924000	-0.020869000	-0.792463000
9	1.340670000	-1.119442000	-1.563610000
9	2.349954000	0.016300000	-0.030402000
9	1.318285000	1.023285000	-1.638403000

CF_3-ethene-NCH_3

1	-0.908114000	0.028620000	-0.605106000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.348354000
1	0.959758000	0.000000000	1.876254000
7	-1.089226000	-0.025147000	2.165752000
6	-0.960724000	0.377419000	3.546066000
1	-1.650954000	-0.203920000	4.178594000
1	0.063953000	0.184746000	3.895351000
1	-1.178618000	1.452341000	3.700333000
6	-2.402383000	0.039785000	1.576169000
1	-2.595065000	1.011526000	1.079416000
1	-2.521279000	-0.755447000	0.822208000
1	-3.161821000	-0.110954000	2.356214000
6	1.254799000	-0.052526000	-0.774529000
9	2.351396000	-0.056573000	0.002337000
9	1.329072000	-1.147801000	-1.554560000
9	1.374245000	0.994550000	-1.612115000

CF_3-ethene-NO

1	-0.953323000	-0.000005000	-0.537492000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.332401000
1	0.888501000	0.000000000	1.975504000
7	-1.290355000	-0.000006000	1.963899000
8	-1.222734000	-0.000003000	3.167190000
6	1.233970000	0.000014000	-0.837413000
9	1.260326000	-1.077020000	-1.626492000
9	2.347559000	-0.000119000	-0.105585000
9	1.260447000	1.077204000	-1.626274000

CF_3-ethene-NO_2

1	-0.942736000	-0.000119000	-0.553856000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.323569000
1	0.867986000	0.000000000	1.981885000
7	-1.274995000	-0.000399000	2.055317000
8	-1.177333000	-0.001669000	3.264878000
8	-2.305144000	0.000491000	1.415321000
6	1.258576000	-0.000597000	-0.802518000
9	2.350834000	0.003332000	-0.038974000
9	1.307844000	-1.080052000	-1.584575000
9	1.304822000	1.073880000	-1.591522000

CF_3-ethene-OH

1	-0.924843000	0.000034000	-0.585321000
6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.336656000
1	0.929874000	0.000000000	1.911326000
8	-1.073608000	0.000170000	2.136050000
1	-1.875709000	0.000067000	1.593348000
6	1.249522000	-0.000815000	-0.792513000
9	1.325450000	1.069373000	-1.599808000
9	2.348206000	0.003655000	-0.025499000
9	1.329246000	-1.076346000	-1.592351000

Benzene-3xF

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.386161000

6	1.176973000	0.000000000	-0.735933000
1	-0.948407000	0.000000000	1.924995000
1	1.163095000	0.000000000	-1.826631000
6	1.221457000	0.000000000	2.055741000
6	2.381092000	0.000000000	-0.051811000
1	1.272073000	0.000000000	3.146219000
6	2.406698000	0.000000000	1.340296000
9	-1.163175000	0.000000000	-0.654361000
9	3.527949000	0.000000000	-0.722742000
9	3.581017000	0.000000000	1.968980000

Benzene-3xCF_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.385760000
6	1.205247000	0.000000000	-0.699170000
1	-0.940822000	0.000010000	1.937696000
1	1.197390000	-0.003311000	-1.790521000
6	1.212658000	0.001467000	2.067922000
6	2.419712000	0.001324000	-0.024535000
1	1.218434000	0.004284000	3.158062000
6	2.424302000	0.004262000	1.383384000
6	3.689038000	-0.030562000	2.212815000
9	4.220879000	-1.253539000	2.237408000
9	4.614354000	0.813540000	1.760773000
9	3.436450000	0.309722000	3.482364000
6	3.676713000	0.043492000	-0.864604000
9	3.415954000	-0.291532000	-2.133166000
9	4.205382000	1.268178000	-0.885931000
9	4.608521000	-0.799067000	-0.421361000
6	-1.277576000	-0.001905000	-0.788854000
9	-1.363015000	-1.089849000	-1.560931000
9	-2.355398000	0.023910000	-0.003396000
9	-1.340618000	1.058272000	-1.601164000

Benzene-6xF

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.390021000
6	1.203911000	0.000000000	-0.695404000
6	1.203911000	0.000000000	2.085424000
6	2.407822000	0.000000000	-0.000001000
6	2.407822000	0.000000000	1.390020000
9	-1.145830000	0.000000000	-0.660616000
9	3.553652000	0.000000000	-0.660617000

9	3.553652000	0.000000000	2.050636000
9	-1.145830000	0.000000000	2.050637000
9	1.203911000	0.000000000	3.408027000
9	1.203911000	0.000000000	-2.018007000

Fulvene

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.467798000
6	1.407924000	0.000000000	-0.415973000
6	2.168357000	0.000000000	0.702408000
6	1.288093000	0.000000000	1.880080000
6	-1.074348000	0.000000000	-0.804645000
1	3.258428000	0.000000000	0.744814000
1	1.637303000	0.000000000	2.913603000
1	-0.898880000	0.000000000	2.084143000
1	1.743622000	0.000000000	-1.452900000
1	-0.968690000	0.000000000	-1.893089000
1	-2.089170000	0.000000000	-0.396944000

Fulvene-3xF

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.459691000
6	1.381163000	0.000000000	-0.481672000
6	2.147883000	0.000000000	0.627977000
6	1.301854000	0.000000000	1.815962000
6	-1.075870000	0.000000000	-0.798547000
1	-0.874883000	0.000000000	2.103777000
1	1.705447000	0.000000000	-1.519418000
1	-1.036134000	0.000000000	-1.891655000
9	-2.307873000	0.000000000	-0.313316000
9	1.824609000	0.000000000	3.028754000
9	3.465635000	0.000000000	0.721343000

Fulvene-3xCF_3

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.467066000
6	1.403416000	0.000000000	-0.422475000
6	2.169765000	0.002114000	0.687360000
6	1.287094000	0.001660000	1.873378000
6	-1.049426000	-0.007763000	-0.837291000
1	-0.883456000	-0.002368000	2.101278000

1	1.749020000	-0.005926000	-1.454612000
1	-0.900993000	-0.029522000	-1.920080000
6	3.661522000	-0.030079000	0.692619000
9	4.145623000	0.121954000	-0.543696000
9	4.167526000	0.945173000	1.452164000
9	4.126812000	-1.187675000	1.166888000
6	1.725653000	0.039986000	3.300356000
9	2.142482000	1.259217000	3.652837000
9	0.723053000	-0.290218000	4.117349000
9	2.734521000	-0.806071000	3.524299000
6	-2.477416000	-0.037659000	-0.386102000
9	-2.834963000	-1.269413000	-0.011127000
9	-2.699145000	0.771818000	0.654384000
9	-3.287155000	0.339157000	-1.375272000

Fulvene-6xF

6	0.000000000	0.000000000	0.000000000
6	0.000000000	0.000000000	1.456694000
6	1.393613000	0.000000000	-0.423611000
6	2.158011000	0.000000000	0.688452000
6	1.286391000	0.000000000	1.864447000
6	-1.073552000	0.000000000	-0.796139000
9	-2.298813000	0.000000000	-0.366272000
9	1.761572000	0.000000000	3.093791000
9	3.472481000	0.000000000	0.785279000
9	1.768564000	0.000000000	-1.692305000
9	-1.018543000	0.000000000	-2.093167000
9	-1.104651000	0.000000000	2.184565000