Supporting Information for

Energetics of electron pairs in Electrophilic Aromatic Substitutions

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ELF basin populations

Table S1. *bij* basin populations (*nij*) for the complete set of Ph-X systems. All data in au.

X	*n12*	*n23*	*n34*	Average
H	2.79	2.79	2.79	2.79
O^-	2.49	3.29	2.64	2.80
NH_2	2.73	2.96	2.81	2.83
SH	2.75	2.89	2.78	2.82
CH_3	2.83	2.80	2.79	2.81
F	2.86	2.86	2.81	2.84
Br	2.85	2.84	2.79	2.83
NO_2	2.86	2.81	2.75	2.81
CN	2.74	2.84	2.76	2.78
CF_3	2.82	2.80	2.77	2.80
NH_3^+	2.92	2.79	2.75	2.80
BH_2	2.55	2.84	2.73	2.70
Li	2.59	2.81	2.79	2.73
Et	2.82	2.81	2.79	2.81
Pr	2.82	2.81	2.79	2.81
CHF_2	2.82	2.80	2.78	2.80
CH_2Cl	2.80	2.81	2.78	2.80
Cl	2.86	2.84	2.79	2.83
SiH_3	2.66	2.81	2.77	2.75
SiH_2Me	2.66	2.82	2.77	2.75

CCH	2.72	2.87	2.77	2.79
AlH_2	2.55	2.82	2.75	2.71
Ph	2.78	2.83	2.78	2.79
BF2	2.62	2.82	2.75	2.73
BMe_2	2.59	2.82	2.74	2.72
CC-F	2.73	2.86	2.77	2.79
CC-Cl	2.72	2.87	2.77	2.78
CC-Me	2.72	2.87	2.77	2.79

ELF basin populations with respect to benzene

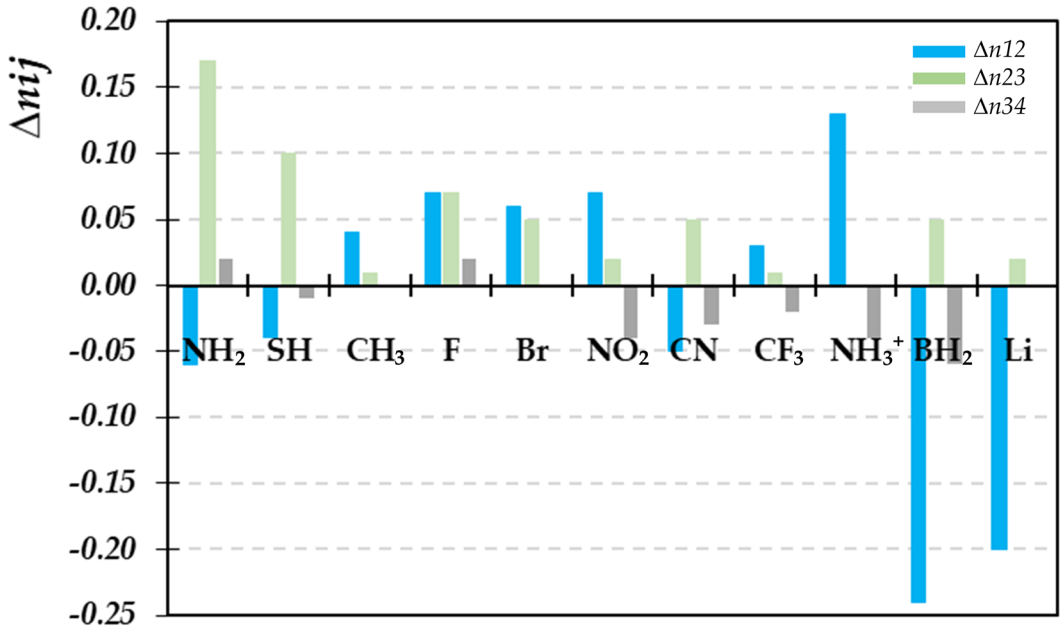

Figure S1. *bij* basin populations with respect to benzene (Δ*nij*) for the selected set of Ph-X systems commented in the main text. All data in au. We have excluded X = O^- for visual purposes (Δ*n12* = -0.30, Δ*n23* = 0.50, Δ*n34* = -0.15).

Delocalization Indices with respect to benzene

Table S2. Vicinal delocalization indices, ΔDI(a), in the aromatic ring basins for the full set of molecules. All data in au $\times 10^{-3}$, referred to the DI of adjacent carbon bonds in benzene, equal to 0.555 au.

X	ΔDI(*i*)	ΔDI(*o*)	ΔDI(*m*)	ΔDI(*p*)
O^-	-147.1	57.7	-4.6	-111.9
NH_2	-34.3	38.2	-3.1	22.0
SH	-8.2	9.9	-3.0	7.2
CH_3	1.6	7.8	-2.5	3.5
F	21.6	31.9	-4.1	13.7
Br	22.2	9.6	-1.5	0.6
NO_2	37.9	-13.6	2.9	-20.3
CN	-11.3	-16.8	3.7	-16.1
CF_3	17.8	-9.3	-0.5	-8.9
NH_3^+	76.2	7.4	-15.0	-18.2

BH_2	-148.1	-48.4	12.0	-32.4
Li	-140.7	-16.6	3.5	1.4
Et	-4.5	6.6	-2.2	3.8
Pr	-5.0	5.9	-2.6	3.6
CHF_2	13.9	-5.3	-1.9	-5.3
CH_2Cl	-2.0	-5.3	-0.3	-5.6
Cl	30.3	11.7	-1.3	1.5
SiH_3	-80.6	-21.9	2.3	-9.9
SiH_2Me	-87.1	-21.4	2.7	-7.8
CCH	-23.5	-8.9	4.5	-9.6
AlH_2	-145.3	-38.8	6.3	-18.9
Ph	-16.4	-2.5	-1.0	-3.8
BF_2	-103.6	-34.8	6.8	-22.2
BMe_2	-129.3	-37.1	8.5	-22.4
CC-F	-19.9	-6.5	3.6	-8.2
CC-Cl	-24.9	-8.9	4.2	-10.1
CC-Me	-25.4	-6.2	4.2	-7.2

Kinetic energy

Table S3. *bij* basin kinetic energies (*tij*) for the full set of systems. Notation as in Table 2 in the main text. All data in au.

X	***t12***	***t23***	***t34***	**Average**
H	3.254	3.254	3.254	3.254
O^-	2.985	3.678	3.112	3.259
NH_2	3.259	3.407	3.275	3.314
SH	3.274	3.354	3.255	3.294
CH_3	3.305	3.27	3.255	3.277
F	3.470	3.322	3.27	3.354
Br	3.368	3.309	3.251	3.309
NO_2	3.412	3.292	3.219	3.307
CN	3.225	3.328	3.221	3.258
CF_3	3.330	3.260	3.245	3.279
NH_3^+	3.464	3.265	3.214	3.314
BH_2	3.011	3.304	3.190	3.168
Li	3.007	3.280	3.243	3.177
Et	3.293	3.283	3.255	3.277
Pr	3.294	3.279	3.257	3.277
CHF_2	3.312	3.257	3.248	3.272
CH_2Cl	3.294	3.268	3.251	3.271
Cl	3.387	3.312	3.251	3.317
SiH_3	3.111	3.276	3.235	3.208
SiH_2Me	3.097	3.274	3.248	3.206
CCH	3.212	3.344	3.228	3.261
AlH_2	2.993	3.297	3.213	3.168

Ph	3.263	3.290	3.246	3.266
BF2	3.081	3.294	3.208	3.194
BMe_2	3.050	3.294	3.218	3.187
CC-F	3.224	3.344	3.229	3.266
CC-Cl	3.208	3.349	3.226	3.261
CC-Me	3.212	3.349	3.230	3.264

Kinetic energy relative to benzene

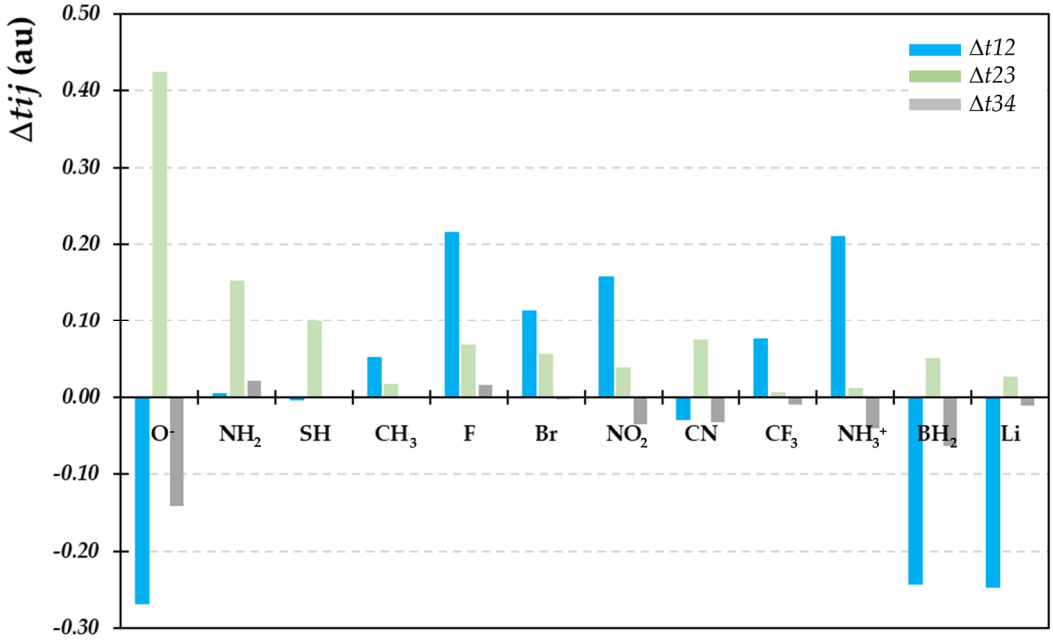

Figure S2. *bij* basin kinetic energies relative to benzene (Δ*tij*) for the selected set of Ph-X systems commented in the main text. All data in au.

Exchange-correlation energies relative to benzene

Table S4. Vicinal exchange-correlation energies relative to benzene (ΔV_{xc}) for the full set of molecules. See the main text for a description. All data in kcal/mol, referred to the vicinal V_{xc} value in benzene, equal to -100.4 kcal/mol.

X	ΔVxc(*i*)	ΔVxc(*o*)	ΔVxc(*m*)	ΔVxc(*p*)
O^-	21.3	-11.9	-0.534	18.2
NH_2	2.49	-6.87	0.687	-3.78
SH	-1.25	-2.17	0.799	-1.26
CH_3	-0.963	-1.05	0.159	-0.729
F	-1.37	-3.05	4.25	-0.346
Br	-6.43	-1.83	0.492	-0.066
NO_2	-9.41	2.32	-0.110	2.99
CN	-0.878	2.52	-0.201	2.37
CF_3	-4.81	1.46	0.343	1.28
NH_3^+	-16.6	-1.29	3.05	3.56
BH_2	22.6	6.80	-1.59	4.32

Li	22.7	1.46	-0.985	-0.859
Et	-0.025	-0.986	0.177	-0.884
Pr	0.031	-0.876	0.289	-0.816
CHF_2	-3.70	0.898	0.429	0.658
CH_2Cl	-1.39	0.945	0.176	0.632
Cl	-7.78	-2.11	0.447	-0.196
SiH_3	12.3	2.79	-0.230	1.23
SiH_2Me	13.5	2.69	-0.340	0.763
CCH	1.29	1.20	-0.434	1.19
AlH_2	22.6	4.84	-0.887	2.44
Ph	1.28	0.499	0.167	0.379
BF_2	15.3	4.70	-0.850	3.05
BMe_2	20.0	5.22	-1.27	2.74
CC-F	0.779	0.85	-0.332	0.983
CC-Cl	1.47	1.15	-0.350	1.28
CC-Me	1.65	0.835	-0.400	0.769

Cartesian Coordinates

Table S5. xyz coordinates (in bohr) for the optimized geometries of all the molecules considered in this work (Ph-X).

X = H

6 0.000179 -1.396578 -0.000093
6 1.209602 -0.698085 -0.000040
6 1.209464 0.698416 0.000043
6 -0.000179 1.396706 0.000085
6 -1.209643 0.698106 0.000043
6 -1.209423 -0.698395 -0.000040
1 2.150994 -1.241780 -0.000070
1 2.150932 1.241840 0.000080
1 -0.000318 2.483668 0.000154
1 -2.151250 1.241290 0.000079
1 -2.150676 -1.242331 -0.000070
1 0.000318 -2.483711 -0.000157

X = O^-

6 -1.084352 0.000000 -0.000037
6 -0.286381 1.213131 0.000001
6 1.102020 1.201106 -0.000005
6 1.830814 0.000000 -0.000004
6 1.102020 -1.201106 0.000016
6 -0.286381 -1.213131 -0.000002
1 -0.832838 2.156953 0.000025
1 1.642376 2.152193 0.000000
1 2.919897 0.000000 -0.000002
1 1.642376 -2.152193 0.000026
1 -0.832838 -2.156953 0.000006
8 -2.350677 0.000000 0.000017

X = NH2

6 0.938719 -0.000041 -0.010145
6 0.221274 1.208272 -0.005203
6 -1.171806 1.202652 0.003385
6 -1.881669 0.000007 0.008366
6 -1.171860 -1.202617 0.003359
6 0.221261 -1.208281 -0.005196
1 0.763329 2.151748 -0.013398
1 -1.705683 2.149782 0.008807
1 -2.967630 0.000051 0.016695
1 -1.705716 -2.149760 0.008745
1 0.763246 -2.151800 -0.013300
7 2.337402 -0.000002 -0.078895
1 2.777543 0.834924 0.288615
1 2.777583 -0.834877 0.288702

X = SH

6 0.506804 -0.000198 -0.000039
6 -0.201602 -1.209423 -0.000071
6 -1.595546 -1.201760 -0.000025
6 -2.298111 0.004804 0.000035
6 -1.591283 1.207831 0.000025
6 -0.196050 1.211041 0.000002
1 0.335869 -2.153977 -0.000204
1 -2.133216 -2.146231 -0.000031
1 -3.384249 0.007202 0.000075
1 -2.124816 2.154754 0.000040

1 0.340605 2.156090 0.000067
16 2.293903 -0.083608 0.000105
1 2.518082 1.246117 -0.001195

X = CH_3

6 -0.914018 0.000032 -0.011139
6 -0.194225 -1.202283 -0.008864
6 1.201268 -1.205486 0.002163
6 1.905062 -0.000022 0.008406
6 1.201323 1.205456 0.002163
6 -0.194186 1.202305 -0.008866
1 -0.734317 -2.146857 -0.017698
1 1.738955 -2.150290 0.001414
1 2.991880 -0.000046 0.013688
1 1.739042 2.150242 0.001414
1 -0.734244 2.146894 -0.017695
6 -2.425683 0.000014 0.009226
1 -2.834054 -0.885153 -0.490551
1 -2.810495 -0.001926 1.038152
1 -2.834020 0.887038 -0.487252

X = F

6 0.931557 0.000004 -0.000024
6 0.260449 1.217592 0.000058
6 -1.135579 1.208706 -0.000057
6 -1.835846 -0.000001 -0.000003
6 -1.135572 -1.208711 0.000073
6 0.260449 -1.217590 -0.000064
9 2.282496 -0.000001 0.000012
1 0.828684 2.142022 0.000081
1 -1.675344 2.151646 -0.000065
1 -2.921909 -0.000008 -0.000012
1 -1.675343 -2.151648 0.000092
1 0.828699 -2.142011 -0.000097

X = Br

6 -0.104266 0.000001 0.000015
6 -0.785169 1.215825 0.000010
6 -2.181348 1.207844 -0.000008
6 -2.881397 -0.000001 -0.000005
6 -2.181346 -1.207846 0.000004
6 -0.785169 -1.215823 -0.000004
35 1.810984 0.000000 -0.000002
1 -0.233202 2.149453 0.000024
1 -2.719130 2.152011 -0.000021
1 -3.967620 -0.000002 -0.000009
1 -2.719128 -2.152013 0.000016
1 -0.233194 -2.149448 -0.000003

X = NO_2

6 -0.244824 0.000021 -0.000016
6 0.427781 -1.220751 -0.000127
6 1.820975 -1.212340 -0.000094
6 2.516514 0.000006 0.000029
6 1.821086 1.212335 0.000129
6 0.427817 1.220783 0.000120
1 -0.140231 -2.142803 -0.000246
1 2.363133 -2.153181 -0.000162
1 3.602876 -0.000087 0.000047
1 2.363225 2.153189 0.000213
1 -0.140051 2.142894 0.000218
7 -1.717857 0.000057 -0.000037
8 -2.290143 1.089788 0.000377
8 -2.289863 -1.089881 -0.000383

X = CN

6 -0.610440 0.000167 -0.000007
6 0.091612 -1.217354 0.000044
6 1.483864 -1.210952 0.000058
6 2.180727 0.000007 0.000021
6 1.484080 1.210834 -0.000031
6 0.091589 1.217347 -0.000044
1 -0.459219 -2.152459 0.000071
1 2.025879 -2.152105 0.000098
1 3.267140 -0.000079 0.000032
1 2.026021 2.152028 -0.000060
1 -0.458775 2.152736 -0.000083
6 -2.045059 -0.000270 -0.000019
7 -3.208470 0.000172 -0.000028

X = CF_3

6 0.049324 -0.000005 -0.034500
6 0.745085 -1.212050 -0.022342
6 2.139180 -1.209396 0.002219
6 2.836988 -0.000010 0.015397
6 2.139171 1.209395 0.002207
6 0.745097 1.212052 -0.022363
1 0.197322 -2.148566 -0.039928
1 2.679848 -2.151562 0.007656
1 3.923421 0.000011 0.033065
1 2.679873 2.151542 0.007634
1 0.197315 2.148561 -0.039964
6 -1.455010 0.000019 -0.002045
9 -1.973233 1.090073 -0.611276
9 -1.928708 0.000034 1.266983
9 -1.973258 -1.090109 -0.611253

X = NH_3^+

6 -0.826535 0.000793 -0.007992
6 -0.167492 1.223782 -0.004316
6 1.228945 1.212273 0.001264
6 1.920560 -0.000549 0.004533
6 1.226424 -1.213321 0.001314
6 -0.169016 -1.224277 -0.004313
1 -0.710920 2.165642 -0.006706
1 1.769738 2.152844 0.000465
1 3.005799 -0.001549 0.006952
1 1.766634 -2.154269 0.000545
1 -0.713835 -2.165082 -0.007047
7 -2.325644 0.000215 0.006115
1 -2.699039 0.915341 -0.276219
1 -2.710799 -0.697614 -0.643944
1 -2.705390 -0.209014 0.940207

X = BH_2

6 1.018800 0.000241 0.000004
6 0.285346 1.208517 0.000003
6 -1.106975 1.213235 -0.000080
6 -1.802262 -0.000133 -0.000001
6 -1.106823 -1.213366 0.000065
6 0.285477 -1.208268 0.000002
1 0.827317 2.151229 0.000111
1 -1.653251 2.152752 -0.000160
1 -2.889575 -0.000275 0.000016
1 -1.653000 -2.152966 0.000166
1 0.827628 -2.150874 -0.000111
5 2.554910 -0.000065 0.000052
1 3.161854 -1.032797 -0.000735
1 3.163099 1.031899 0.000497

X = Li

6 1.280143 0.000003 -0.000006
6 0.515424 1.191150 -0.000002
6 -0.883540 1.204008 0.000002
6 -1.590280 -0.000003 0.000002
6 -0.883535 -1.204011 -0.000002
6 0.515428 -1.191148 -0.000006
1 1.021118 2.160256 -0.000003
1 -1.423706 2.149942 0.000004
1 -2.678483 -0.000005 0.000006
1 -1.423697 -2.149947 -0.000002
1 1.021127 -2.160251 -0.000010
3 3.253936 0.000001 0.000025

X = Et

6 0.434894 -0.000131 -0.328628
6 -0.270166 1.202595 -0.185279
6 -1.637046 1.205979 0.095843
6 -2.325920 0.000121 0.238248
6 -1.637259 -1.205837 0.095987
6 -0.270341 -1.202701 -0.185144
1 0.258438 2.146989 -0.299829
1 -2.165002 2.150709 0.198839
1 -3.391174 0.000254 0.453552
1 -2.165317 -2.150497 0.199091
1 0.258070 -2.147214 -0.299562
6 1.926557 -0.000210 -0.592048
1 2.193400 -0.879513 -1.192099
1 2.193424 0.878755 -1.192594
6 2.762265 0.000149 0.700795
1 3.834900 0.000153 0.474501
1 2.542632 0.884518 1.309510
1 2.542732 -0.883940 1.309952

X= Pr

6 0.121695 -0.000081 0.371724
6 0.820827 1.202590 0.200488
6 2.175607 1.205935 -0.134166
6 2.858376 0.000088 -0.303364
6 2.175732 -1.205839 -0.134273
6 0.820947 -1.202662 0.200383
1 0.297156 2.146948 0.335770
1 2.699067 2.150665 -0.258026
1 3.914355 0.000155 -0.560348
1 2.699284 -2.150507 -0.258215
1 0.297374 -2.147085 0.335578
6 -1.357839 -0.000162 0.692952
1 -1.603996 -0.879859 1.302986
1 -1.604013 0.879271 1.303361
6 -2.250876 0.000099 -0.564085
1 -2.004747 0.877636 -1.176740
1 -2.004737 -0.877179 -1.177107
6 -3.745834 0.000023 -0.232023
1 -4.355943 0.000214 -1.142589
1 -4.022799 -0.884942 0.354571
1 -4.022805 0.884736 0.354947

X = CHF_2

6 0.178152 -0.000014 -0.151539
6 -0.519353 1.210176 -0.088343
6 -1.908418 1.208446 0.038186
6 -2.605053 0.000008 0.100499
6 -1.908442 -1.208428 0.038244
6 -0.519365 -1.210179 -0.088290
1 0.026643 2.147304 -0.127710
1 -2.445948 2.151172 0.092750

1 -3.687210 0.000020 0.199484
1 -2.445971 -2.151153 0.092867
1 0.026607 -2.147319 -0.127648
6 1.673058 0.000040 -0.343805
1 1.976012 0.000005 -1.398116
9 2.233668 -1.108482 0.235415
9 2.233708 1.108446 0.235547

X = CH_2Cl

6 -0.021229 -0.000091 0.445051
6 0.659838 -1.207151 0.241067
6 1.996059 -1.208256 -0.157275
6 2.666839 0.000076 -0.357239
6 1.995937 1.208355 -0.157172
6 0.659745 1.207079 0.241172
1 0.138031 -2.149036 0.393409
1 2.513972 -2.151266 -0.309575
1 3.708741 0.000150 -0.665835
1 2.513793 2.151406 -0.309410
1 0.137821 2.148880 0.393629
6 -1.455817 -0.000128 0.879746
1 -1.709432 0.889557 1.457493
1 -1.709482 -0.889924 1.457283
17 -2.623628 0.000054 -0.542888

X = Cl

6 0.503962 0.000003 0.000003
6 -0.178617 1.215754 0.000003
6 -1.574703 1.207600 -0.000002
6 -2.274992 -0.000001 -0.000002
6 -1.574693 -1.207605 0.000002
6 -0.178616 -1.215752 0.000001
17 2.265049 0.000001 -0.000002
1 0.373660 2.149455 0.000012
1 -2.113016 2.151285 -0.000006
1 -3.361196 -0.000006 -0.000006
1 -2.113013 -2.151287 -0.000003
1 0.373675 -2.149447 0.000003

X = SiH_3

6 -0.468423 -0.000020 -0.012632
6 0.256627 -1.205137 -0.010088
6 1.652109 -1.207656 0.003357
6 2.352273 0.000019 0.010977
6 1.652084 1.207666 0.003354
6 0.256589 1.205109 -0.010090
1 -0.272024 -2.156069 -0.023802
1 2.192337 -2.150924 0.003692
1 3.439182 0.000030 0.018554
1 2.192283 2.150950 0.003687
1 -0.272104 2.156013 -0.023804
14 -2.347617 -0.000001 0.006121
1 -2.863858 -1.212692 -0.685494
1 -2.893223 -0.002654 1.393053
1 -2.863501 1.215468 -0.680852

X = SiH_2Me

6 0.045269 -0.000661 -0.263806
6 -0.670006 1.203907 -0.134720
6 -2.041433 1.208062 0.124036
6 -2.730057 0.000857 0.256173
6 -2.042356 -1.207096 0.126189
6 -0.670915 -1.204446 -0.132576
1 -0.152181 2.154953 -0.244020
1 -2.573202 2.151624 0.217681
1 -3.798761 0.001443 0.454862
1 -2.574837 -2.150087 0.221518
1 -0.153789 -2.156059 -0.240176
14 1.903717 -0.001665 -0.564701
1 2.257046 1.205974 -1.365320
1 2.256523 -1.213742 -1.358805
6 2.902001 0.002538 1.041017
1 2.677115 -0.881094 1.648845
1 3.977678 0.001835 0.829286
1 2.677353 0.889493 1.644077

X = CCH

6 -0.594106 0.000016 0.000009
6 0.119909 1.213144 0.000040
6 1.512552 1.208607 -0.000005
6 2.212960 -0.000017 -0.000055
6 1.512525 -1.208625 -0.000006
6 0.119881 -1.213128 0.000040
1 -0.428533 2.150028 0.000108
1 2.052996 2.151314 0.000016
1 3.299550 -0.000029 -0.000107
1 2.052946 -2.151345 0.000016
1 -0.428583 -2.150001 0.000108
6 -2.024169 0.000015 0.000011
6 -3.234213 -0.000001 -0.000025
1 -4.300410 -0.000031 -0.000192

X = AlH_2

6 0.540623 -0.000122 -0.000053
6 -0.195082 1.204975 -0.000036
6 -1.590394 1.209572 0.000014
6 -2.289225 0.000132 0.000032
6 -1.590598 -1.209476 -0.000008

6 -0.195325 -1.205133 -0.000009
1 0.331297 2.158171 -0.000038
1 -2.133359 2.151565 0.000044
1 -3.376469 0.000209 0.000058
1 -2.133791 -2.151337 -0.000016
1 0.330896 -2.158417 -0.000039
13 2.489334 -0.000053 0.000024
1 3.270680 -1.386559 0.000048
1 3.269401 1.387376 -0.000014

X = Ph

6 -0.742882 0.000042 0.000040
6 -1.465802 1.138771 0.394210
6 -2.859944 1.139458 0.393710
6 -3.563829 -0.000015 -0.000006
6 -2.859869 -1.139504 -0.393755
6 -1.465779 -1.138761 -0.394205
1 -0.928550 2.022014 0.728540
1 -3.397114 2.029730 0.710496
1 -4.650493 -0.000077 -0.000035
1 -3.397080 -2.029745 -0.710553
1 -0.928399 -2.021919 -0.728540
6 0.742880 0.000002 0.000028
6 1.465770 -1.138747 0.394224
6 1.465813 1.138782 -0.394195
6 2.859913 -1.139477 0.393727
1 0.928480 -2.021952 0.728577
6 2.859901 1.139479 -0.393739
1 0.928471 2.021972 -0.728504
6 3.563831 -0.000027 -0.000022
1 3.397067 -2.029754 0.710512
1 3.397116 2.029719 -0.710538
1 4.650493 -0.000013 -0.000054

X = BF_2

6 0.192218 -0.000119 0.000002
6 -0.527005 1.209253 0.000015
6 -1.920434 1.211662 0.000013
6 -2.616890 0.000064 -0.000002
6 -1.920570 -1.211604 -0.000013
6 -0.527136 -1.209369 -0.000010
1 0.015326 2.151099 0.000036
1 -2.464715 2.152212 0.000016
1 -3.703964 0.000104 -0.000009
1 -2.464965 -2.152090 -0.000014
1 0.015086 -2.151283 -0.000026
5 1.737450 -0.000002 -0.000005
9 2.435391 -1.132747 0.000027
9 2.435153 1.132819 -0.000028

X = BMe_2

6 0.137061 0.000399 0.000269
6 -0.603451 -1.200651 -0.035847
6 -1.997069 -1.207553 -0.043149
6 -2.697824 -0.000042 -0.000190
6 -1.997453 1.207655 0.043003
6 -0.603803 1.201194 0.036179
1 -0.076407 -2.150321 -0.064461
1 -2.537867 -2.149971 -0.077978
1 -3.785119 -0.000208 -0.000356
1 -2.538543 2.149913 0.077659
1 -0.077109 2.151036 0.064969
5 1.705606 0.000381 0.000360
6 2.534800 -1.347254 0.072516
1 2.798760 -1.636275 -0.958771
1 3.492127 -1.212600 0.591976
1 2.021075 -2.206135 0.517374
6 2.536408 1.346782 -0.072604
1 2.019600 2.211385 -0.502373
1 2.818145 1.625270 0.956844
1 3.485290 1.212823 -0.607744

X = CC-F

6 -0.007929 -0.000021 0.000077
6 0.706658 1.212362 -0.000115
6 2.099435 1.208074 0.000057
6 2.800605 0.000030 0.000066
6 2.099477 -1.208041 0.000057
6 0.706703 -1.212380 -0.000115
1 0.159033 2.149871 -0.000179
1 2.639180 2.151217 -0.000179
1 3.887143 0.000049 0.000054
1 2.639259 -2.151162 -0.000179
1 0.159108 -2.149907 -0.000179
6 -1.439915 -0.000054 0.000039
6 -2.644684 -0.000034 0.000071
9 -3.933981 0.000034 -0.000019

X = CC-Cl

6 0.530871 0.000228 -0.000165
6 1.245080 1.213669 -0.000020
6 2.637547 1.208461 0.000221
6 3.337750 -0.000313 0.000360
6 2.637091 -1.208819 0.000221
6 1.244622 -1.213487 -0.000021
1 0.697207 2.150872 -0.000181
1 3.178042 2.151086 0.000332
1 4.424269 -0.000519 0.000569
1 3.177229 -2.151649 0.000331

1 0.696391 -2.150481 -0.000182
6 -0.898272 0.000517 -0.000313
6 -2.108997 0.000316 -0.002935
17 -3.760429 -0.000161 0.000885

X = CC-Me

6 -0.035561 -0.000073 -0.000102
6 -0.753009 1.211926 0.000004
6 -2.145698 1.207944 0.000069
6 -2.847381 0.000064 0.000077
6 -2.145816 -1.207884 0.000066

1 4.465158 0.907559 -0.46943
6 -0.753127 -1.212001 0.000006
1 -0.205309 2.149431 0.000091
1 -2.685561 2.151201 0.000145
1 -3.934016 0.000118 0.000159
1 -2.685771 -2.151089 0.000141
1 -0.205515 -2.149545 0.000094
6 1.394306 -0.000117 -0.000250
6 2.606743 0.000252 -0.000520
6 4.066259 -0.000047 0.000208
1 4.465682 -0.046696 1.021429
1 4.465034 -0.861368 -0.549966