

**Supplemental Material: Predicting the Cation- $\pi$  Binding of Substituted Benzenes: Energy Decomposition Calculations and the Development of a Cation- $\pi$  Substituent Constant.**

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**Table S1.** MP2(full)/6-311++G\*\* Total Energies (hartrees) and Number of Imaginary Frequencies (NI) for all Substituted Benzenes.

Aromatic	E <sub>Total</sub>	NI	Aromatic	E <sub>Total</sub>	NI
C <sub>6</sub> H <sub>6</sub>	-231.697672	1	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (NO <sub>2</sub> ) <sub>2</sub>	-640.020621	0
C <sub>6</sub> H <sub>5</sub> F	-330.795134	1	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (NO <sub>2</sub> ) <sub>2</sub>	-640.022271	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	-429.885239	1	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	-270.917303	0
<i>m</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	-429.891294	0	<i>o</i> -C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	-310.137196	0
<i>p</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	-429.890191	0	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	-310.136859	0
C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>	-528.986133	0	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	-310.136623	0
C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	-628.066687	1	C <sub>6</sub> H <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub>	-349.356311	0
C <sub>6</sub> H <sub>5</sub> Cl	-690.808194	1	C <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>4</sub>	-388.576381	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-1149.914885	1	C <sub>6</sub> H <sub>5</sub> OH	-306.799043	1
<i>m</i> -C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-1149.917729	1	<i>o</i> -C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	-381.902283	0
<i>p</i> -C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-1149.917362	0	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	-381.900413	2
C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	-1609.026463	1	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	-381.897781	3
C <sub>6</sub> H <sub>2</sub> Cl <sub>4</sub>	-2068.130396	0	C <sub>6</sub> H <sub>3</sub> (OH) <sub>3</sub>	-457.001939	3
C <sub>6</sub> H <sub>5</sub> Br	-2803.999965	1	C <sub>6</sub> H <sub>2</sub> (OH) <sub>4</sub>	-532.102522	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	-5376.298296	1	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	-286.949236	0
<i>m</i> -C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	-5376.301326	1	<i>o</i> -C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>	-342.203045	0
<i>p</i> -C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	-5376.301158	1	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>	-342.200032	0
C <sub>6</sub> H <sub>3</sub> Br <sub>3</sub>	-7948.602185	1	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>	-342.197394	0
C <sub>6</sub> H <sub>2</sub> Br <sub>4</sub>	-10520.896652	2	C <sub>6</sub> H <sub>3</sub> (NH <sub>2</sub> ) <sub>3</sub>	-397.450397	0
C <sub>6</sub> H <sub>5</sub> I	-7148.627628	1	C <sub>6</sub> H <sub>2</sub> (NH <sub>2</sub> ) <sub>4</sub>	-452.702496	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	-14065.553081	1	C <sub>6</sub> H <sub>5</sub> OCH <sub>3</sub>	-345.995264	0
<i>m</i> -C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	-14065.556928	1	<i>o</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>	-460.288401	2
<i>p</i> -C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	-14065.556711	1	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>	-460.293245	0
C <sub>6</sub> H <sub>3</sub> I <sub>3</sub>	-20982.485948	1	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>	-460.290409	0
C <sub>6</sub> H <sub>2</sub> I <sub>4</sub>	-27899.407594	2	C <sub>6</sub> H <sub>3</sub> (OCH <sub>3</sub> ) <sub>3</sub>	-574.591672	2
C <sub>6</sub> H <sub>5</sub> CN	-323.774436	0	C <sub>6</sub> H <sub>2</sub> (OCH <sub>3</sub> ) <sub>4</sub>	-688.873409	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> (CN) <sub>2</sub>	-415.845876	0	C <sub>6</sub> H <sub>5</sub> NMe <sub>2</sub>	-365.357468	0
<i>m</i> -C <sub>6</sub> H <sub>4</sub> (CN) <sub>2</sub>	-415.846494	1	<i>o</i> -C <sub>6</sub> H <sub>4</sub> (NMe <sub>2</sub> ) <sub>2</sub>	-499.018073	0
<i>p</i> -C <sub>6</sub> H <sub>4</sub> (CN) <sub>2</sub>	-415.847585	1	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (NMe <sub>2</sub> ) <sub>2</sub>	-499.016527	0
C <sub>6</sub> H <sub>3</sub> (CN) <sub>3</sub>	-507.914988	1	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (NMe <sub>2</sub> ) <sub>2</sub>	-499.014839	0
C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-435.861861	0	C <sub>6</sub> H <sub>3</sub> (NMe <sub>2</sub> ) <sub>3</sub>	-632.675462	0

**Table S2.** RHF/6-311++G\*\* Total Energies (hartrees) and Number of Imaginary Frequencies (NI) for Substituted Benzenes that Gave Negative Frequencies when Calculated at the MP2(full)/6-311++G\*\* level of theory.

<b>Aromatic</b>	<b>E<sub>Total</sub></b>	<b>NI</b>	<b>Aromatic</b>	<b>E<sub>Total</sub></b>	<b>NI</b>
C <sub>6</sub> H <sub>6</sub>	-230.756841	0	<i>o</i> -C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	-14063.197710	0
C <sub>6</sub> H <sub>5</sub> F	-329.637904	0	<i>m</i> -C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	-14063.204912	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	-428.511527	0	<i>p</i> -C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	-14063.205110	0
C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	-626.259936	0	C <sub>6</sub> H <sub>3</sub> I <sub>3</sub>	-20979.426872	0
C <sub>6</sub> H <sub>5</sub> Cl	-689.680676	0	C <sub>6</sub> H <sub>2</sub> I <sub>4</sub>	-27895.634663	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-1148.598118	0	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (CN) <sub>2</sub>	-414.260896	0
<i>m</i> -C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	-1148.602802	0	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (CN) <sub>2</sub>	-414.260880	0
C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	-1607.523415	0	C <sub>6</sub> H <sub>3</sub> (CN) <sub>3</sub>	-506.006070	0
C <sub>6</sub> H <sub>5</sub> Br	-2802.540575	0	C <sub>6</sub> H <sub>5</sub> OH	-305.640020	0
<i>o</i> -C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	-5374.316881	0	<i>m</i> -C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	-380.524874	0
<i>m</i> -C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	-5374.322517	0	<i>p</i> -C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	-380.51958	0
<i>p</i> -C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	-5374.322777	0	C <sub>6</sub> H <sub>3</sub> (OH) <sub>3</sub>	-455.411196	0
C <sub>6</sub> H <sub>3</sub> Br <sub>3</sub>	-7946.102998	0	<i>o</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>	-458.573340	0
C <sub>6</sub> H <sub>5</sub> I	-7146.981693	0	C <sub>6</sub> H <sub>3</sub> (OCH <sub>3</sub> ) <sub>3</sub>	-572.496213	0

**Table S3.** MP2(full)/6-311++G\*\* Total Energies (hartrees) and Number of Imaginary Frequencies (NI) for all Optimized Na<sup>+</sup>-Substituted Benzene Complexes.

<b>Aromatic</b>	<b>E<sub>Total</sub></b>	<b>NI</b>	<b>Aromatic</b>	<b>E<sub>Total</sub></b>	<b>NI</b>
<b>C<sub>6</sub>H<sub>6</sub></b>	-393.531737	0	<b>NO<sub>2</sub>2m</b>	-801.821904	2
<b>F1</b>	-492.621781	0	<b>NO<sub>2</sub>2p</b>	-801.822560	1
<b>F2o</b>	-591.705379	0	<b>CH<sub>3</sub>1</b>	-432.754284	0
<b>F2m</b>	-591.710969	0	<b>CH<sub>3</sub>2o</b>	-471.976454	0
<b>F2p</b>	-591.709326	0	<b>CH<sub>3</sub>2m</b>	-471.976244	0
<b>F3</b>	-690.799191	0	<b>CH<sub>3</sub>2p</b>	-471.976346	0
<b>F4</b>	-789.873289	0	<b>CH<sub>3</sub>3</b>	-511.198383	0
<b>Cl1</b>	-852.639986	0	<b>CH<sub>3</sub>4</b>	-550.419974	0
<b>Cl2o</b>	-1311.740849	0	<b>OH1</b>	-468.632651	0
<b>Cl2m</b>	-1311.742054	0	<b>OH2o</b>	-543.737427	0
<b>Cl2p</b>	-1311.741507	1	<b>OH2m</b>	-543.733937	0
<b>Cl3</b>	-1770.846871	1	<b>OH2p</b>	-543.732199	0
<b>Cl4</b>	-2229.948050	1	<b>OH3</b>	-618.837857	0
<b>Br1</b>	-2965.828932	0	<b>OH4</b>	-693.937407	0
<b>Br2o</b>	-5538.124476	1	<b>NH<sub>2</sub>1</b>	-448.789669	0
<b>Br2m</b>	-5538.126167	0	<b>NH<sub>2</sub>2o</b>	-504.045984	0
<b>Br2p</b>	-5538.125708	1	<b>NH<sub>2</sub>2m</b>	-504.049428	0
<b>Br3</b>	-8110.423571	0	<b>NH<sub>2</sub>2p</b>	-504.045378	0
<b>Br4</b>	-10682.717149	2	<b>NH<sub>2</sub>3</b>	-559.307522	0
<b>I1</b>	-7310.457595	0	<b>NH<sub>2</sub>4</b>	-614.551110	0
<b>I2o</b>	-14227.381730	1	<b>OCH<sub>3</sub>1</b>	-507.832694	0
<b>I2m</b>	-14227.383903	0	<b>OCH<sub>3</sub>2o</b>	-622.129753	0
<b>I2p</b>	-14227.383295	1	<b>OCH<sub>3</sub>2m</b>	-622.134098	0
<b>I3</b>	-21144.310855	0	<b>OCH<sub>3</sub>2p</b>	-622.130161	0
<b>I4</b>	-28061.233007	1	<b>OCH<sub>3</sub>3</b>	-736.435728	0
<b>CN1</b>	-485.593111	0	<b>OCH<sub>3</sub>4</b>	-850.718695	0
<b>CN2o</b>	-577.651944	1	<b>N(CH<sub>3</sub>)<sub>2</sub>1</b>	-527.202845	0
<b>CN2m</b>	-577.652093	0	<b>N(CH<sub>3</sub>)<sub>2</sub>2o</b>	-660.864043	0
<b>CN2p</b>	-577.652891	1	<b>N(CH<sub>3</sub>)<sub>2</sub>2m</b>	-660.870439	0
<b>CN3</b>	-669.709351	0	<b>N(CH<sub>3</sub>)<sub>2</sub>2p</b>	-660.864047	0
<b>NO<sub>2</sub>1</b>	-597.678202	1	<b>N(CH<sub>3</sub>)<sub>2</sub>3</b>	-794.539409	0

**Table S4.** RHF/6-311++G\*\* Total Energies (hartrees) and Number of Imaginary Frequencies (NI) for Optimized Na<sup>+</sup>-Substituted Benzene Complexes that Gave Negative Frequencies when Calculated at the MP2(full)/6-311++G\*\* level of theory.

<b>Aromatic</b>	<b>E<sub>Total</sub></b>	<b>NI</b>	<b>Aromatic</b>	<b>E<sub>Total</sub></b>	<b>NI</b>
<b>Cl2p</b>	-1310.290332	0	<b>I2p</b>	-14224.895188	0
<b>Cl3</b>	-1769.205467	0	<b>I4</b>	-28057.320143	0
<b>Cl4</b>	-2228.112814	0	<b>CN2o</b>	-575.980883	0
<b>Br2o</b>	-5536.006541	0	<b>CN2p</b>	-575.930854	0
<b>Br2p</b>	-5536.010873	0	<b>NO<sub>2</sub>1</b>	-595.965182	1
<b>Br4</b>	-10679.553090	0	<b>NO<sub>2</sub>2m</b>	-799.514159	0
<b>I2o</b>	-14224.889607	0	<b>NO<sub>2</sub>2p</b>	-799.468216	1

**Table S5.** MP2(full)/6-311++G\*\* Basis Set Superposition Error Corrected Total Energies (hartrees) for the Optimized Na<sup>+</sup>-Substituted Benzene Complexes.

<b>Aromatic</b>	<b>E<sub>Total</sub></b>	<b>Aromatic</b>	<b>E<sub>Total</sub></b>
<b>C<sub>6</sub>H<sub>6</sub></b>	-393.525943	<b>NO<sub>2</sub>2m</b>	-801.816819
<b>F1</b>	-492.616403	<b>NO<sub>2</sub>2p</b>	-801.817451
<b>F2o</b>	-591.700206	<b>CH<sub>3</sub>1</b>	-432.748439
<b>F2m</b>	-591.705948	<b>CH<sub>3</sub>2o</b>	-471.970308
<b>F2p</b>	-591.704247	<b>CH<sub>3</sub>2m</b>	-471.970330
<b>F3</b>	-690.794453	<b>CH<sub>3</sub>2p</b>	-471.970275
<b>F4</b>	-789.868594	<b>CH<sub>3</sub>3</b>	-511.192410
<b>Cl1</b>	-852.630708	<b>CH<sub>3</sub>4</b>	-550.413352
<b>Cl2o</b>	-1311.733734	<b>OH1</b>	-468.627009
<b>Cl2m</b>	-1311.735429	<b>OH2o</b>	-543.731657
<b>Cl2p</b>	-1311.734537	<b>OH2m</b>	-543.728435
<b>Cl3</b>	-1770.839520	<b>OH2p</b>	-543.726485
<b>Cl4</b>	-2229.937228	<b>OH3</b>	-618.832311
<b>Br1</b>	-2965.822801	<b>OH4</b>	-693.931554
<b>Br2o</b>	-5538.117762	<b>NH<sub>2</sub>1</b>	-448.783818
<b>Br2m</b>	-5538.120032	<b>NH<sub>2</sub>2o</b>	-504.040109
<b>Br2p</b>	-5538.119217	<b>NH<sub>2</sub>2m</b>	-504.043671
<b>Br3</b>	-8110.417351	<b>NH<sub>2</sub>2p</b>	-504.039305
<b>Br4</b>	-10682.709553	<b>NH<sub>2</sub>3</b>	-559.300587
<b>I1</b>	-7310.451271	<b>NH<sub>2</sub>4</b>	-614.544891
<b>I2o</b>	-14227.374648	<b>OCH<sub>3</sub>1</b>	-507.826948
<b>I2m</b>	-14227.377256	<b>OCH<sub>3</sub>2o</b>	-622.123554
<b>I2p</b>	-14227.376430	<b>OCH<sub>3</sub>2m</b>	-622.128175
<b>I3</b>	-21144.303948	<b>OCH<sub>3</sub>2p</b>	-622.124191
<b>I4</b>	-28061.224761	<b>OCH<sub>3</sub>3</b>	-736.429646
<b>CN1</b>	-485.588001	<b>OCH<sub>3</sub>4</b>	-850.712237
<b>CN2o</b>	-577.646989	<b>N(CH<sub>3</sub>)<sub>2</sub>1</b>	-527.196814
<b>CN2m</b>	-577.647464	<b>N(CH<sub>3</sub>)<sub>2</sub>2o</b>	-660.858015
<b>CN2p</b>	-577.648031	<b>N(CH<sub>3</sub>)<sub>2</sub>2m</b>	-660.864104
<b>CN3</b>	-669.705191	<b>N(CH<sub>3</sub>)<sub>2</sub>2p</b>	-660.857945
<b>NO<sub>2</sub>1</b>	-597.672836	<b>N(CH<sub>3</sub>)<sub>2</sub>3</b>	-794.532820

**Table S6.** MP2(full)/6-311++G\*\* Optimized Structures for All Substituted Benzenes.

C <sub>6</sub> H <sub>6</sub>							
6	0.000000	1.398984	-0.000055				
6	0.000000	-1.398984	-0.000055				
6	-1.211554	0.699492	-0.000055				
6	1.211554	0.699492	-0.000055				
6	-1.211554	-0.699492	-0.000055				
6	1.211554	-0.699492	-0.000055				
1	0.000000	2.485269	0.000329				
1	-2.152305	1.242633	0.000329				
1	-2.152305	-1.242633	0.000329				
1	0.000000	-2.485269	0.000329				
1	2.152305	-1.242633	0.000329				
1	2.152305	1.242633	0.000329				
C <sub>6</sub> H <sub>5</sub> F				<i>o</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>			
6	-0.930715	0.000000	0.000000	6	-0.537240	-0.697187	0.000022
6	-0.262331	-1.219138	-0.000002	6	-0.537242	0.697189	-0.000023
6	1.135963	-1.210303	0.000003	6	0.659618	1.402184	0.000034
6	1.837225	0.000000	-0.000004	6	1.868552	0.698894	-0.000042
6	1.135961	1.210303	0.000005	6	1.868555	-0.698894	0.000048
6	-0.262333	1.219139	-0.000004	6	0.659620	-1.402180	-0.000043
9	-2.281575	-0.000002	0.000000	9	-1.708616	-1.350743	0.000007
1	-0.830611	-2.143114	0.000001	9	-1.708622	1.350737	-0.000004
1	1.675122	-2.152843	0.000001	1	0.626562	2.486656	0.000011
1	2.922541	0.000001	-0.000002	1	2.805418	1.246172	-0.000003
1	1.675118	2.152844	0.000003	1	2.805423	-1.246167	0.000007
1	-0.830616	2.143114	-0.000001	1	0.626559	-2.486653	-0.000014
<i>m</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>				<i>p</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>			
6	1.185923	-0.305673	0.000000	6	0.000000	0.000000	1.370446
6	0.000000	-1.031716	0.000025	9	0.000000	0.000000	2.719667
6	-1.185924	-0.305671	0.000000	6	0.000000	1.217866	0.698807
6	-1.217112	1.084644	0.000005	6	0.000000	-1.217866	0.698807
6	0.000000	1.772292	-0.000002	6	0.000000	0.000000	-1.370446
6	1.217110	1.084641	0.000002	6	0.000000	-1.217866	-0.698807
9	2.349153	-0.985444	-0.000011	6	0.000000	1.217866	-0.698807
1	0.000000	-2.115281	0.000024	9	0.000000	0.000000	-2.719667
9	-2.349151	-0.985448	-0.000010	1	0.000000	2.144018	1.263108
1	-2.169492	1.602283	-0.000017	1	0.000000	-2.144018	1.263108
1	0.000001	2.857646	0.000010	1	0.000000	-2.144018	-1.263108
1	2.169490	1.602279	-0.000006	1	0.000000	2.144018	-1.263108
C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>				C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>			
6	0.000000	1.367731	0.000000	6	1.197681	0.696803	-0.000002

9	0.000000	2.712043	0.000000	6	1.197691	-0.696808	0.000005
6	-1.184490	-0.683866	0.000000	6	0.000005	-1.401831	0.000014
6	1.184490	-0.683866	0.000000	6	-1.197677	-0.696808	-0.000004
9	-2.348698	-1.356022	0.000000	6	-1.197684	0.696808	0.000006
9	2.348698	-1.356022	0.000000	6	-0.000007	1.401825	-0.000003
6	0.000000	-1.412191	0.000000	9	2.361682	1.356771	-0.000013
1	0.000000	-2.495070	0.000000	9	2.361705	-1.356755	0.000005
6	1.222993	0.706095	0.000000	1	-0.000008	-2.485826	0.000039
6	-1.222993	0.706095	0.000000	9	-2.361693	-1.356751	-0.000022
1	2.160794	1.247535	0.000000	9	-2.361703	1.356743	0.000015
1	-2.160794	1.247535	0.000000	1	0.000033	2.485820	-0.000001
$C_6H_5Cl$				$o-C_6H_4Cl_2$			
6	-0.515093	-0.000009	-0.000079	6	-0.036963	-0.701381	0.000032
6	0.172240	-1.215837	0.000081	6	-0.036909	0.701387	-0.000010
6	1.569999	-1.208985	-0.000042	6	1.178729	1.393771	0.000004
6	2.272779	0.000016	0.000092	6	2.388164	0.699035	0.000000
6	1.569962	1.208985	-0.000044	6	2.388103	-0.699141	0.000009
6	0.172198	1.215848	0.000083	6	1.178628	-1.393825	-0.000030
17	-2.250762	-0.000009	-0.000041	17	-1.509671	-1.602443	0.000000
1	-0.381333	-2.149186	0.000039	17	-1.509584	1.602510	-0.000003
1	2.107383	-2.152795	0.000009	1	1.161154	2.478923	0.000020
1	3.358414	0.000035	0.000082	1	3.323387	1.250114	0.000000
1	2.107347	2.152793	0.000000	1	3.323294	-1.250279	-0.000012
1	-0.381371	2.149199	0.000040	1	1.160983	-2.478977	0.000006
$m-C_6H_4Cl_2$				$p-C_6H_4Cl_2$			
6	-1.200493	-0.006832	-0.000003	6	0.000000	0.000000	1.389933
6	0.000019	-0.719393	-0.000025	17	0.000000	0.000000	3.122765
6	1.200528	-0.006805	0.000018	6	0.000000	1.213237	0.698107
6	1.215733	1.389714	-0.000009	6	0.000000	-1.213237	0.698107
6	-0.000066	2.078144	-0.000019	6	0.000000	0.000000	-1.389933
6	-1.215821	1.389683	0.000023	6	0.000000	-1.213237	-0.698107
17	-2.696742	-0.880929	0.000000	6	0.000000	1.213237	-0.698107
17	2.696786	-0.880887	0.000002	17	0.000000	0.000000	-3.122765
1	0.000009	-1.803793	0.000029	1	0.000000	2.149842	1.246102
1	2.160876	1.921816	0.000002	1	0.000000	-2.149842	1.246102
1	-0.000014	3.164072	0.000028	1	0.000000	-2.149842	-1.246102
1	-2.161018	1.921696	-0.000004	1	0.000000	2.149842	-1.246102
$C_6H_3Cl_3$				$C_6H_2Cl_4$			
6	0.000000	1.383926	0.000000	6	-1.214718	0.701070	-0.022423
17	-0.000493	3.114177	0.000000	6	-1.214696	-0.701071	0.022680
6	-1.198376	-0.692242	0.000000	6	0.000018	-1.386746	-0.006869
6	1.198774	-0.691943	0.000000	6	1.214724	-0.701078	0.022631
17	-2.697248	-1.556740	0.000000	6	1.214693	0.701078	-0.022372

17	2.697344	-1.557000	0.000000	6	-0.000017	1.386743	0.007334
6	0.000284	-1.408025	0.000000	17	-2.678899	1.607610	0.002831
1	0.000226	-2.492040	0.000000	17	-2.678839	-1.607655	-0.003015
6	1.218943	0.703717	0.000000	1	0.000017	-2.471252	0.013951
6	-1.218689	0.703484	0.000000	17	2.678903	-1.607622	-0.003185
1	2.158098	1.245155	0.000000	17	2.678834	1.607669	0.003000
1	-2.157196	1.245961	0.000000	1	-0.000032	2.471245	-0.013544
$C_6H_5Br$				<i>o</i> - $C_6H_4Br_2$			
6	0.091368	-0.000001	0.000010	6	-0.533386	0.701983	0.000112
6	0.777080	1.217670	-0.000011	6	-0.533349	-0.702007	-0.000115
6	2.175444	1.209132	0.000010	6	-1.751433	-1.394725	0.000084
6	2.877941	0.000001	-0.000007	6	-2.960576	-0.699088	-0.000033
6	2.175445	-1.209131	0.000003	6	-2.960612	0.698935	0.000032
6	0.777082	-1.217671	-0.000003	6	-1.751503	1.394638	-0.000090
35	-1.802594	0.000000	0.000000	35	1.060183	1.711120	0.000006
1	0.227402	2.153221	0.000003	35	1.060273	-1.711067	-0.000006
1	2.713080	2.152918	-0.000003	1	-1.739570	-2.479852	0.000088
1	3.963641	-0.000001	0.000004	1	-3.895734	-1.250638	0.000046
1	2.713086	-2.152914	0.000001	1	-3.895797	1.250436	-0.000029
1	0.227406	-2.153224	-0.000005	1	-1.739682	2.479766	-0.000065
<i>m</i> - $C_6H_4Br_2$				<i>p</i> - $C_6H_4Br_2$			
6	-1.199646	0.331393	-0.000078	6	0.000000	0.000000	1.389222
6	-0.000003	-0.385465	0.000081	35	0.000000	0.000000	3.279906
6	1.199643	0.331386	-0.000093	6	0.000000	1.214969	0.698715
6	1.216792	1.728698	0.000064	6	0.000000	-1.214969	0.698715
6	0.000007	2.416521	-0.000046	6	0.000000	0.000000	-1.389222
6	-1.216785	1.728703	0.000049	6	0.000000	-1.214969	-0.698715
35	-2.833819	-0.620989	0.000000	6	0.000000	1.214969	-0.698715
1	-0.000014	-1.469811	0.000042	35	0.000000	0.000000	-3.279906
35	2.833817	-0.620991	0.000000	1	0.000000	2.153874	1.242863
1	2.159880	2.264483	0.000014	1	0.000000	-2.153874	1.242863
1	0.000015	3.502699	0.000010	1	0.000000	-2.153874	-1.242863
1	-2.159867	2.264495	0.000025	1	0.000000	2.153874	-1.242863
$C_6H_3Br_3$				$C_6H_2Br_4$			
6	0.000000	0.000000	1.383470	6	0.000000	0.000000	1.389196
35	0.000000	0.000000	3.272685	1	0.000000	0.000000	2.473951
6	0.000000	1.198113	-0.691693	6	0.000000	1.217295	0.702179
6	0.000000	-1.198113	-0.691693	6	0.000000	-1.217295	0.702179
35	0.000000	2.834292	-1.636358	6	0.000000	0.000000	-1.389196
35	0.000000	-2.834292	-1.636358	6	0.000000	-1.217295	-0.702179
6	0.000000	0.000000	-1.410597	6	0.000000	1.217295	-0.702179
1	0.000000	0.000000	-2.494490	1	0.000000	0.000000	-2.473951
6	0.000000	-1.221685	0.705346	35	0.000000	2.802557	1.716397



6	0.000000	1.221685	0.705346	35	0.000000	-2.802557	1.716397
1	0.000000	-2.160426	1.247231	35	0.000000	-2.802557	-1.716397
1	0.000000	2.160426	1.247231	35	0.000000	2.802557	-1.716397
$C_6H_5I$				<i>o</i> - $C_6H_4I_2$			
6	-0.557813	0.000005	-0.000036	6	-0.703576	0.909553	0.000077
6	-1.248170	-1.217409	0.000053	6	0.703554	0.909568	-0.000087
6	-2.646852	-1.208650	-0.000047	6	1.392991	2.133637	0.000095
6	-3.349701	-0.000005	0.000037	6	0.698633	3.343276	-0.000014
6	-2.646858	1.208647	-0.000048	6	-0.698745	3.343259	0.000013
6	-1.248174	1.217414	0.000054	6	-1.393053	2.133595	-0.000092
53	1.554746	0.000000	-0.000002	53	-1.877402	-0.843959	0.000008
1	-0.706250	-2.157463	0.000044	53	1.877428	-0.843916	-0.000007
1	-3.184110	-2.152903	-0.000027	1	2.478121	2.132295	0.000125
1	-4.435391	-0.000007	0.000004	1	1.251673	4.277777	0.000034
1	-3.184120	2.152897	-0.000027	1	-1.251815	4.277743	-0.000023
1	-0.706258	2.157471	0.000044	1	-2.478182	2.132202	-0.000126
<i>m</i> - $C_6H_4I_2$				<i>p</i> - $C_6H_4I_2$			
6	1.203430	0.563630	0.000001	6	0.000000	0.000000	1.394615
6	0.000007	-0.151798	0.000074	53	0.000000	0.000000	3.504098
6	-1.203425	0.563617	0.000003	6	0.000000	1.214422	0.699162
6	-1.217049	1.962901	0.000016	6	0.000000	-1.214422	0.699162
6	-0.000001	2.650819	-0.000064	6	0.000000	0.000000	-1.394615
6	1.217054	1.962912	0.000015	6	0.000000	-1.214422	-0.699162
53	3.028505	-0.498358	-0.000005	6	0.000000	1.214422	-0.699162
53	-3.028507	-0.498356	-0.000002	53	0.000000	0.000000	-3.504098
1	0.000013	-1.236102	0.000115	1	0.000000	2.158084	1.235407
1	-2.156020	2.505981	-0.000002	1	0.000000	-2.158084	1.235407
1	-0.000005	3.737441	-0.000078	1	0.000000	-2.158084	-1.235407
1	2.156023	2.505995	-0.000006	1	0.000000	2.158084	-1.235407
$C_6H_3I_3$				$C_6H_2I_4$			
6	0.000000	1.387558	0.000000	6	0.000000	0.000000	1.386640
53	0.000000	3.498079	0.000000	1	0.000000	0.000000	2.471292
6	1.201660	-0.693779	0.000000	6	0.000000	1.223476	0.703541
6	-1.201660	-0.693779	0.000000	6	0.000000	-1.223476	0.703541
53	3.029425	-1.749039	0.000000	6	0.000000	0.000000	-1.386640
53	-3.029425	-1.749039	0.000000	6	0.000000	-1.223476	-0.703541
6	0.000000	-1.411350	0.000000	6	0.000000	1.223476	-0.703541
1	0.000000	-2.495415	0.000000	1	0.000000	0.000000	-2.471292
6	-1.222265	0.705675	0.000000	53	0.000000	2.968114	1.883533
6	1.222265	0.705675	0.000000	53	0.000000	-2.968114	1.883533
1	-2.161093	1.247707	0.000000	53	0.000000	-2.968114	-1.883533
1	2.161093	1.247707	0.000000	53	0.000000	2.968114	-1.883533

$C_6H_5CN$				$o-C_6H_4(CN)_2$			
6	-0.607338	-0.000003	0.015890	6	0.102078	0.705788	-0.024574
6	0.090273	-1.218904	-0.006209	6	0.102078	-0.705788	0.024572
6	1.486053	-1.211669	0.008252	6	-1.116830	-1.401582	0.001789
6	2.185231	0.000004	-0.013029	6	-2.322506	-0.699876	0.013580
6	1.486047	1.211672	0.008251	6	-2.322506	0.699876	-0.013579
6	0.090267	1.218901	-0.006207	6	-1.116830	1.401582	-0.001789
6	-2.042126	-0.000005	0.003221	6	1.336083	1.432129	0.000947
1	-0.461765	-2.153595	0.002491	6	1.336083	-1.432129	-0.000950
1	2.027309	-2.152901	-0.003675	1	-1.104823	-2.486855	0.018855
1	3.271101	0.000006	-0.006750	1	-3.261125	-1.245297	0.006949
1	2.027299	2.152908	-0.003675	1	-3.261124	1.245297	-0.006947
1	-0.461776	2.153589	0.002492	1	-1.104823	2.486855	-0.018855
7	-3.218944	0.000003	-0.007414	7	2.339000	2.049307	0.015583
				7	2.339000	-2.049307	-0.015580
$m-C_6H_4(CN)_2$				$p-C_6H_4(CN)_2$			
6	-1.208166	-0.054473	0.000033	6	1.395385	0.000011	0.000197
6	0.000053	-0.765172	0.000009	6	0.696335	1.219491	-0.000065
6	1.208161	-0.054395	-0.000012	6	-0.696260	1.219430	0.000077
6	1.213019	1.350120	-0.000026	6	-1.395461	0.000061	-0.000189
6	0.000035	2.041769	-0.000002	6	-0.696220	-1.219328	0.000097
6	-1.212889	1.350073	0.000018	6	0.696150	-1.219454	-0.000092
6	-2.451254	-0.771812	0.000044	6	2.829140	0.000092	0.000109
1	0.000096	-1.850542	0.000017	1	1.246570	2.155165	0.000017
6	2.451183	-0.771826	-0.000024	1	-1.246506	2.155097	0.000002
1	2.158175	1.883801	-0.000047	6	-2.829105	-0.000017	-0.000087
1	0.000015	3.127392	-0.000011	1	-1.246475	-2.154988	0.000003
1	-2.158027	1.883785	0.000038	1	1.246383	-2.155131	0.000036
7	-3.472262	-1.356357	-0.000055	7	4.006265	-0.000177	-0.000117
7	3.472104	-1.356520	0.000021	7	-4.006230	-0.000089	0.000070
$C_6H_3(CN)_3$							
6	1.120336	-0.832412	0.000064				
6	1.292125	0.558962	0.000078				
6	0.160537	1.386373	0.000093				
6	-1.130381	0.839751	0.000134				
6	-1.281166	-0.553787	0.000090				
6	-0.162097	-1.398359	0.000071				
6	2.272793	-1.687942	-0.000027				
1	2.288334	0.989856	0.000048				
6	0.325380	2.811888	-0.000015				
1	-2.001629	1.487098	0.000163				
6	-2.598247	-1.124013	-0.000018				
1	-0.287313	-2.476449	0.000035				
7	3.217628	-2.389002	-0.000117				

7	0.460638	3.980579	-0.000164				
7	-3.677562	-1.592045	-0.000157				
$C_6H_5NO_2$							
6	0.244685	0.000000	-0.000005				
6	-0.422182	-1.218326	-0.108948				
6	-1.819053	-1.206526	-0.112740				
6	-2.518485	0.000000	0.000005				
6	-1.819052	1.206527	0.112732				
6	-0.422182	1.218325	0.108955				
7	1.718337	0.000000	0.000000				
1	0.143372	-2.139694	-0.185609				
1	-2.360717	-2.142892	-0.204897				
1	-3.604217	0.000001	0.000001				
1	-2.360715	2.142893	0.204899				
1	0.143373	2.139693	0.185608				
8	2.284260	1.053610	-0.290520				
8	2.284259	-1.053610	0.290522				
$m-C_6H_4(NO_2)_2$				$p-C_6H_4(NO_2)_2$			
6	1.182172	0.151807	-0.015829	6	-1.365326	0.000000	-0.000004
6	0.000000	-0.580473	0.000047	6	-0.697044	-1.224085	0.003907
6	-1.182172	0.151810	0.015804	6	0.697044	-1.224084	-0.004109
6	-1.215326	1.543931	0.010539	6	1.365326	0.000000	0.000004
6	0.000000	2.233743	-0.000181	6	0.697044	1.224084	0.004113
6	1.215326	1.543929	-0.010790	6	-0.697044	1.224085	-0.003911
7	2.460014	-0.588627	-0.039585	7	-2.838749	0.000000	-0.000008
1	0.000000	-1.663368	0.000135	1	-1.262295	-2.148696	0.016516
7	-2.460014	-0.588621	0.039681	1	1.262295	-2.148694	-0.016871
1	-2.167250	2.061952	0.012391	7	2.838749	0.000000	0.000009
1	0.000000	3.319038	-0.000269	1	1.262295	2.148694	0.016879
1	2.167250	2.061950	-0.012726	1	-1.262295	2.148696	-0.016524
8	3.463791	0.015855	0.332630	8	-3.401160	1.034130	-0.358606
8	2.425498	-1.753820	-0.429623	8	-3.401162	-1.034130	0.358586
8	-2.425498	-1.753750	0.429909	8	3.401162	-1.034070	-0.358759
8	-3.463790	0.015801	-0.332634	8	3.401160	1.034070	0.358779
$C_6H_5CH_3$				$o-C_6H_4(CH_3)_2$			
6	-0.000339	0.915390	0.000000	6	0.478533	-0.705382	-0.010310
6	-0.008489	0.197206	1.204472	6	0.478533	0.705383	0.010310
6	-0.008489	-1.201118	1.208152	6	-0.745568	1.387631	-0.002740
6	-0.010696	-1.905259	0.000000	6	-1.961854	0.698286	0.011760
6	-0.008489	-1.201118	-1.208152	6	-1.961854	-0.698287	-0.011759
6	-0.008489	0.197206	-1.204472	6	-0.745567	-1.387631	0.002738
6	0.033538	2.422412	0.000000	6	1.776979	-1.469633	0.006705
1	-0.010456	0.738629	2.148009	6	1.776979	1.469633	-0.006705

1	-0.015794	-1.739027	2.152079	1	-0.743462	2.475316	0.014454
1	-0.013623	-2.991378	0.000000	1	-2.898720	1.248081	0.003461
1	-0.015794	-1.739027	-2.152079	1	-2.898719	-1.248082	-0.003460
1	-0.010456	0.738629	-2.148009	1	-0.743460	-2.475316	-0.014456
1	-0.464878	2.825976	0.885397	1	2.440302	-1.142815	-0.800654
1	1.064585	2.791913	0.000000	1	2.315045	-1.320071	0.949397
1	-0.464878	2.825976	-0.885397	1	1.598290	-2.540997	-0.113025
				1	1.598288	2.541003	0.112974
				1	2.440280	1.142849	0.800686
				1	2.315069	1.320029	-0.949376
<i>m</i> -C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>				<i>p</i> -C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>			
6	1.225896	-0.272032	-0.003615	6	1.421771	0.000000	0.014535
6	1.211382	1.129599	-0.008194	6	0.698903	-1.201100	0.008875
6	0.000000	-0.951377	-0.025505	6	-0.698903	-1.201100	-0.008875
6	0.000001	1.826817	0.013264	6	-1.421771	0.000000	-0.014535
6	-1.225897	-0.272031	-0.003608	6	-0.698903	1.201100	-0.008875
6	-1.211382	1.129599	-0.008193	6	0.698903	1.201100	0.008875
6	2.527908	-1.032322	0.011815	6	2.928927	0.000000	-0.006406
6	-2.527908	-1.032322	0.011813	1	1.235315	-2.147821	0.014373
1	2.861362	-1.217940	1.038601	1	-1.235315	-2.147821	-0.014373
1	3.315993	-0.471330	-0.497729	6	-2.928927	0.000000	0.006406
1	2.423267	-2.000904	-0.484487	1	-1.235315	2.147821	-0.014373
1	-2.861351	-1.217974	1.038596	1	1.235315	2.147821	0.014373
1	-3.315999	-0.471313	-0.497704	1	3.328103	-0.885444	0.495669
1	-2.423273	-2.000887	-0.484522	1	3.307975	0.000000	-1.034059
1	2.151837	1.676026	-0.002485	1	3.328103	0.885445	0.495669
1	-0.000001	-2.040788	-0.037383	1	-3.328103	0.885444	-0.495669
1	0.000001	2.913496	0.002938	1	-3.328103	-0.885445	-0.495669
1	-2.151836	1.676027	-0.002480	1	-3.307975	0.000001	1.034059
C <sub>6</sub> H <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub>				C <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>4</sub>			
6	1.222447	-0.705726	-0.011238	6	1.228470	0.703935	-0.015281
6	0.000042	-1.390101	-0.028897	6	1.228470	-0.703935	0.015281
6	-1.222404	-0.705800	-0.011237	6	0.000000	-1.376387	-0.005611
6	-1.203971	0.694954	0.008038	6	-1.228470	-0.703935	0.015281
6	-0.000042	1.411363	0.015965	6	-1.228470	0.703935	-0.015281
6	1.203929	0.695026	0.008034	6	0.000000	1.376387	0.005610
6	2.528478	-1.459402	0.011335	6	2.523185	1.474366	0.003179
1	0.000075	-2.479126	-0.052428	6	2.523185	-1.474366	-0.003179
6	-2.528390	-1.459554	0.011334	1	0.000000	-2.465616	0.017348
1	-2.147349	1.239526	0.014257	6	-2.523185	-1.474366	-0.003179
6	-0.000088	2.919169	-0.009709	6	-2.523185	1.474366	0.003179
1	2.147275	1.239656	0.014254	1	0.000000	2.465616	-0.017348
1	2.434933	-2.421777	-0.499364	1	2.338454	2.547059	-0.095335
1	3.320239	-0.887900	-0.480802	1	3.071124	1.310250	0.937896

1	2.850433	-1.657635	1.039474	1	3.181239	1.165794	-0.816106
1	-3.320183	-0.888102	-0.480812	1	2.338454	-2.547059	0.095335
1	-2.434785	-2.421926	-0.499359	1	3.071124	-1.310250	-0.937896
1	-2.850340	-1.657800	1.039472	1	3.181239	-1.165793	0.816106
1	0.885461	3.320157	0.491071	1	-2.338454	-2.547059	0.095335
1	-0.000094	3.295249	-1.038569	1	-3.181239	-1.165794	0.816106
1	-0.885665	3.320103	0.491062	1	-3.071124	-1.310250	-0.937896
				1	-2.338454	2.547059	-0.095335
				1	-3.071124	1.310250	0.937896
				1	-3.181239	1.165793	-0.816106
$C_6H_5OH$				$o-C_6H_4(OH)_2$			
6	-0.941326	-0.021951	0.000001	6	0.530715	0.675536	-0.018489
6	-0.224841	-1.222766	-0.000003	6	0.506590	-0.727381	0.009887
6	1.170438	-1.194027	0.000004	6	-0.717801	-1.393234	-0.014159
6	1.858601	0.024823	-0.000003	6	-1.910998	-0.663929	0.010819
6	1.135307	1.220078	0.000004	6	-1.883534	0.733272	-0.003979
6	-0.263198	1.201235	-0.000004	6	-0.655410	1.405356	0.008057
8	-2.307932	-0.110557	0.000000	8	1.790771	1.233862	-0.039621
1	-0.771925	-2.160172	0.000000	8	1.667053	-1.440280	0.005952
1	1.721579	-2.130033	0.000002	1	-0.716680	-2.478689	-0.001223
1	2.943715	0.041915	0.000000	1	-2.860276	-1.190208	0.000001
1	1.654707	2.174043	0.000002	1	-2.807241	1.302578	0.015217
1	-0.823496	2.133988	-0.000005	1	-0.618214	2.492269	-0.015461
1	-2.671006	0.780363	0.000016	1	1.733031	2.150644	0.244817
				1	2.389415	-0.802973	0.073182
$m-C_6H_4(OH)_2$				$p-C_6H_4(OH)_2$			
6	1.197743	-0.318591	-0.000020	6	1.401204	0.023362	0.000004
6	-0.020023	-1.004182	0.000059	6	0.681646	1.219859	-0.000025
6	-1.215221	-0.283980	-0.000018	6	-0.714953	1.195633	0.000001
6	-1.205621	1.115039	0.000034	6	-1.401202	-0.023360	-0.000011
6	0.017761	1.782360	-0.000038	6	-0.681646	-1.219851	0.000000
6	1.226640	1.077753	0.000040	6	0.714950	-1.195637	-0.000025
8	2.331409	-1.087486	-0.000021	8	2.770468	0.110646	0.000021
1	-0.012211	-2.091131	0.000051	1	1.221219	2.161507	-0.000028
8	-2.437820	-0.899375	-0.000023	1	-1.267757	2.132718	-0.000014
1	-2.147663	1.652125	-0.000001	8	-2.770466	-0.110651	0.000015
1	0.034598	2.868260	-0.000017	1	-1.221224	-2.161496	-0.000014
1	2.175619	1.607821	0.000000	1	1.267752	-2.132722	-0.000024
1	3.093967	-0.500877	-0.000032	1	3.131651	-0.780684	0.000063
1	-2.300688	-1.851701	0.000003	1	-3.131653	0.780677	0.000066
$C_6H_3(OH)_3$				$C_6H_2(OH)_4$			
6	-0.452311	1.311605	-0.000013	6	-1.213400	-0.672704	-0.000023
6	0.922679	1.058215	0.000041	6	-1.198924	0.727196	-0.009914

6	1.362074	-0.264096	-0.000009	6	0.023454	1.398345	0.026619
6	0.455101	-1.328160	0.000012	6	1.213400	0.672704	0.000023
6	-0.909756	-1.047511	-0.000005	6	1.198924	-0.727197	0.009914
6	-1.377810	0.269960	0.000021	6	-0.023454	-1.398345	-0.026619
8	-0.829358	2.627116	-0.000025	8	-2.468425	-1.248899	-0.044116
1	1.617643	1.892702	0.000028	8	-2.359920	1.444491	-0.002885
8	2.689863	-0.595320	-0.000010	1	0.029250	2.484613	0.048578
1	0.830287	-2.347268	-0.000021	8	2.468425	1.248899	0.044116
8	-1.860487	-2.031810	-0.000022	8	2.359920	-1.444491	0.002885
1	-2.447971	0.454608	0.000000	1	-0.029250	-2.484613	-0.048578
1	-1.790712	2.666850	0.000077	1	-2.422961	-2.123920	0.351867
1	3.204950	0.217370	-0.000025	1	-3.080073	0.803068	0.048612
1	-1.414212	-2.884229	0.000114	1	2.422961	2.123921	-0.351865
				1	3.080073	-0.803068	-0.048611
$C_6H_5NH_2$				$o-C_6H_4(NH_2)_2$			
6	0.937690	0.000000	0.003142	6	-0.505117	0.705150	-0.013622
6	0.222805	1.207404	-0.020988	6	-0.505118	-0.705150	0.013623
6	-1.173224	1.205674	0.013960	6	0.711605	-1.392169	-0.042799
6	-1.881689	0.000000	0.002176	6	1.925786	-0.698575	-0.014222
6	-1.173224	-1.205674	0.013960	6	1.925786	0.698575	0.014222
6	0.222805	-1.207404	-0.020988	6	0.711606	1.392169	0.042799
7	2.340093	0.000000	-0.079664	7	-1.752568	1.360293	0.037627
1	0.765519	2.150080	-0.021836	7	-1.752569	-1.360292	-0.037627
1	-1.707091	2.151900	0.006942	1	0.704547	-2.480260	-0.045586
1	-2.966820	0.000000	0.026200	1	2.861773	-1.248002	-0.044370
1	-1.707091	-2.151900	0.006942	1	2.861773	1.248001	0.044370
1	0.765519	-2.150080	-0.021836	1	0.704548	2.480260	0.045586
1	2.769173	0.830196	0.306833	1	-1.676006	2.356697	-0.125672
1	2.769173	-0.830196	0.306833	1	-2.415980	0.956532	-0.616845
				1	-1.676007	-2.356696	0.125670
				1	-2.415980	-0.956532	0.616846
$m-C_6H_4(NH_2)_2$				$p-C_6H_4(NH_2)_2$			
6	1.218870	-0.291293	0.002683	6	1.418823	0.000000	0.002967
6	0.000000	-0.979533	-0.033815	6	0.698121	1.202253	-0.009177
6	-1.218870	-0.291293	0.002683	6	-0.698121	1.202253	-0.009180
6	-1.214923	1.110990	-0.008172	6	-1.418823	0.000000	0.002969
6	0.000000	1.797505	0.018248	6	-0.698121	-1.202253	-0.009180
6	1.214923	1.110991	-0.008172	6	0.698121	-1.202253	-0.009177
7	2.430634	-1.001142	-0.077005	7	2.827284	0.000000	-0.075779
1	0.000000	-2.068334	-0.053334	1	1.232804	2.149573	-0.019329
7	-2.430634	-1.001141	-0.077005	1	-1.232804	2.149573	-0.019329
1	-2.155316	1.655561	0.005201	7	-2.827284	0.000000	-0.075779
1	0.000000	2.884103	0.019382	1	-1.232804	-2.149573	-0.019329
1	2.155316	1.655561	0.005201	1	1.232804	-2.149573	-0.019329

1	3.216349	-0.496818	0.311914	1	3.246467	0.826401	0.330721
1	2.382250	-1.930736	0.318537	1	3.246467	-0.826401	0.330721
1	-2.382250	-1.930737	0.318535	1	-3.246468	-0.826401	0.330721
1	-3.216349	-0.496818	0.311915	1	-3.246468	0.826401	0.330721
$C_6H_3(NH_2)_3$				$C_6H_2(NH_2)_4$			
6	0.653863	1.237508	0.001579	6	-1.218883	-0.702455	-0.027513
6	-0.744179	1.184057	-0.018109	6	-1.218911	0.702445	0.027502
6	-1.398644	-0.052492	0.001579	6	-0.000021	1.387399	0.000062
6	-0.653334	-1.236507	-0.018107	6	1.218898	0.702463	-0.027519
6	0.744782	-1.185015	0.001580	6	1.218905	-0.702437	0.027519
6	1.397513	0.052450	-0.018107	6	0.000009	-1.387382	0.000015
7	1.310420	2.480116	-0.073884	7	-2.468416	-1.366076	0.008681
1	-1.323052	2.105096	-0.027145	7	-2.468470	1.366030	-0.008707
7	-2.803054	-0.105201	-0.073884	1	-0.000043	2.476940	0.000073
1	-1.161540	-2.198345	-0.027142	7	2.468432	1.366078	0.008668
7	1.492633	-2.374915	-0.073881	7	2.468462	-1.366040	-0.008693
1	2.484593	0.093249	-0.027142	1	0.000017	-2.476920	0.000052
1	0.775185	3.241651	0.321744	1	-2.382005	-2.358243	-0.176327
1	2.241141	2.467084	0.321745	1	-3.119732	-0.958915	-0.656616
1	-3.194945	-0.949495	0.321746	1	-3.119759	0.958891	0.656632
1	-3.257128	0.707344	0.321745	1	-2.382078	2.358207	0.176254
1	2.419759	-2.292156	0.321749	1	3.119757	0.958872	-0.656589
1	1.015986	-3.174427	0.321749	1	2.382025	2.358233	-0.176408
				1	3.119728	-0.958970	0.656710
				1	2.382052	-2.358232	0.176180
$C_6H_5OCH_3$				<i>o</i> - $C_6H_4(OCH_3)_2$			
6	0.460195	-0.278141	-0.000019	6	0.709079	-0.143239	0.000007
6	0.045122	1.059842	-0.000002	6	-0.709135	-0.143112	-0.000008
6	-1.325479	1.355550	-0.000014	6	-1.397446	1.071447	0.000008
6	-2.278364	0.337376	0.000020	6	-0.694678	2.287330	-0.000008
6	-1.853181	-0.998176	-0.000005	6	0.695044	2.287192	0.000011
6	-0.495127	-1.305990	0.000014	6	1.397584	1.071189	-0.000014
8	1.762371	-0.685307	-0.000026	8	1.290726	-1.371186	0.000006
1	0.762226	1.872045	-0.000026	8	-1.290924	-1.371000	-0.000006
1	-1.639287	2.395627	0.000000	1	-2.480807	1.085676	0.000000
1	-3.337011	0.577085	0.000007	1	-1.246668	3.222125	0.000004
1	-2.582373	-1.803306	0.000020	1	1.247208	3.221883	-0.000002
1	-0.146315	-2.334134	0.000000	1	2.480949	1.085226	0.000006
6	2.746675	0.334578	0.000023	6	2.707947	-1.394339	0.000000
1	3.706778	-0.179469	0.000029	6	-2.708146	-1.394108	0.000002
1	2.669002	0.962210	-0.894544	1	2.984570	-2.447696	0.000000
1	2.668962	0.962161	0.894622	1	3.113859	-0.909221	0.894704
				1	3.113850	-0.909223	-0.894709
				1	-2.984790	-2.447459	0.000000

	1	-3.114045	-0.908982	-0.894701			
	1	-3.114034	-0.908990	0.894716			
<i>m</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>				<i>p</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>			
6	-1.052978	-0.212204	-0.000011	6	1.375615	-0.297309	-0.000063
6	0.281589	-0.652603	-0.000006	6	0.942016	1.036932	-0.000071
6	1.317226	0.280983	-0.000011	6	-0.425305	1.323142	-0.000050
6	1.029110	1.656498	0.000006	6	-1.375616	0.297313	-0.000029
6	-0.295250	2.073412	-0.000002	6	-0.942016	-1.036928	-0.000033
6	-1.354706	1.151247	0.000007	6	0.425303	-1.323137	-0.000028
8	-1.981281	-1.214545	-0.000018	8	2.684600	-0.692876	-0.000087
1	0.454925	-1.721552	-0.000019	1	1.646445	1.860334	-0.000094
8	2.641891	-0.044837	-0.000008	1	-0.773411	2.351648	-0.000053
1	1.851414	2.363993	0.000000	8	-2.684603	0.692874	-0.000015
1	-0.520417	3.136107	0.000012	1	-1.646444	-1.860330	-0.000010
1	-2.376418	1.509158	0.000002	1	0.773408	-2.351642	-0.000027
6	-3.341801	-0.815937	0.000015	6	3.654111	0.339613	0.000158
6	2.954883	-1.427712	0.000015	1	4.621765	-0.160466	0.000206
1	-3.921287	-1.738139	0.000005	1	3.568884	0.967072	-0.894254
1	-3.584125	-0.232064	-0.894578	1	3.568663	0.966840	0.894711
1	-3.584091	-0.232102	0.894642	6	-3.654108	-0.339621	0.000104
1	4.042417	-1.485869	0.000018	1	-4.621765	0.160451	0.000134
1	2.562136	-1.923304	-0.894457	1	-3.568822	-0.967017	-0.894346
1	2.562133	-1.923271	0.894505	1	-3.568708	-0.966912	0.894618
C <sub>6</sub> H <sub>3</sub> (OCH <sub>3</sub> ) <sub>3</sub>				C <sub>6</sub> H <sub>2</sub> (OCH <sub>3</sub> ) <sub>4</sub>			
6	0.069047	1.388351	-0.000007	6	-1.220152	-0.702616	0.002975
6	1.256909	0.633134	0.000052	6	-1.220147	0.702623	-0.002980
6	1.167901	-0.753863	0.000005	6	0.000005	1.390932	0.000100
6	-0.080173	-1.404835	-0.000014	6	1.220155	0.702616	0.002829
6	-1.236895	-0.634461	-0.000046	6	1.220150	-0.702624	-0.002846
6	-1.176584	0.771860	0.000006	6	-0.000004	-1.390932	-0.000106
8	0.255958	2.740946	0.000009	8	-2.445012	-1.303742	0.015101
1	2.197580	1.167828	0.000068	8	-2.445002	1.303759	-0.015104
8	2.245720	-1.592156	0.000023	1	0.000003	2.471552	-0.000055
1	-0.087410	-2.486828	-0.000058	8	2.445013	1.303744	0.014998
8	-2.501746	-1.148791	-0.000058	8	2.445003	-1.303762	-0.015018
1	-2.109961	1.319186	-0.000051	1	-0.000014	-2.471553	0.000039
6	-0.915447	3.540021	0.000002	6	-2.455760	-2.710955	-0.138575
6	3.523506	-0.977368	-0.000031	6	-2.455738	2.710971	0.138585
6	-2.608155	-2.562788	0.000054	6	2.455756	2.710973	-0.138540
1	-0.570256	4.573061	0.000056	6	2.455736	-2.710987	0.138565
1	-1.520222	3.355729	0.894434	1	-3.506680	-2.996930	-0.163761
1	-1.520166	3.355801	-0.894482	1	-1.966641	-3.212885	0.704580
1	4.245459	-1.792915	-0.000036	1	-1.970732	-3.012151	-1.074375
1	3.666410	-0.361514	0.894413	1	-3.506655	2.996955	0.163776



1	3.666347	-0.361549	-0.894507	1	-1.966618	3.212904	-0.704568
1	-3.675406	-2.780280	0.000047	1	-1.970704	3.012155	1.074385
1	-2.146262	-2.994333	0.894562	1	3.506675	2.996953	-0.163698
1	-2.146223	-2.994488	-0.894360	1	1.966635	3.212811	0.704669
				1	1.970730	3.012269	-1.074308
				1	3.506653	-2.996973	0.163733
				1	1.966612	-3.212849	-0.704627
				1	1.970708	-3.012249	1.074343
$C_6H_5NMe_2$				$o-C_6H_4(NMe_2)_2$			
6	-0.188218	-0.000001	-0.123724	6	0.713196	0.240588	0.031804
6	0.542467	-1.207239	-0.064696	6	1.383984	1.472630	0.100740
6	1.935924	-1.201079	0.028945	6	0.695406	2.689951	0.059737
6	2.647706	0.000001	0.077156	6	-0.692413	2.690729	-0.059790
6	1.935922	1.201081	0.028951	6	-1.382418	1.474203	-0.100748
6	0.542465	1.207238	-0.064690	6	-0.713076	0.241350	-0.031757
7	-1.580664	-0.000002	-0.275049	7	1.413952	-0.990656	0.045787
1	0.032124	-2.161977	-0.096497	1	2.467014	1.486587	0.152457
1	2.463267	-2.150307	0.072460	1	1.248742	3.623590	0.104610
1	3.730481	0.000002	0.153163	1	-1.244708	3.624985	-0.104702
1	2.463264	2.150309	0.072471	1	-2.465413	1.489515	-0.152430
1	0.032121	2.161976	-0.096484	6	1.280547	-1.744030	-1.202593
6	-2.276494	-1.217648	0.110457	6	2.802775	-0.926152	0.465944
6	-2.276494	1.217648	0.110444	1	1.819458	-1.247257	-2.026979
1	-2.103581	-1.489621	1.164493	1	0.226325	-1.840037	-1.461751
1	-3.346577	-1.069003	-0.043009	1	1.705198	-2.742674	-1.061103
1	-1.967988	-2.053668	-0.519874	1	3.457576	-0.422481	-0.266510
1	-2.103579	1.489634	1.164477	1	2.879182	-0.406196	1.423751
1	-1.967991	2.053661	-0.519897	1	3.167810	-1.949021	0.594042
1	-3.346577	1.069000	-0.043017	7	-1.415058	-0.989209	-0.045741
				6	-1.282319	-1.742718	1.202642
				1	-1.820789	-1.245446	2.027013
				1	-0.228170	-1.839604	1.461802
				1	-1.707878	-2.740971	1.061127
				6	-2.803833	-0.923649	-0.465997
				1	-3.458312	-0.419604	0.266476
				1	-3.169591	-1.946234	-0.594271
				1	-2.879790	-0.403511	-1.423739
$m-C_6H_4(NMe_2)_2$				$p-C_6H_4(NMe_2)_2$			
6	1.233251	0.216136	-0.148155	6	-1.440894	-0.000001	-0.167609
6	0.000000	-0.463758	-0.188958	6	-0.698136	-1.197125	-0.154655
6	-1.233251	0.216137	-0.148156	6	0.698137	-1.197125	-0.154655
6	-1.219622	1.621373	-0.041030	6	1.440894	0.000000	-0.167609
6	0.000000	2.295161	0.012198	6	0.698137	1.197123	-0.154638
6	1.219622	1.621372	-0.041028	6	-0.698137	1.197123	-0.154638

7	2.441176	-0.492218	-0.251751	7	-2.845955	-0.000002	-0.233058
1	-0.000001	-1.540009	-0.261282	1	-1.198283	-2.158307	-0.144781
7	-2.441177	-0.492217	-0.251753	1	1.198283	-2.158306	-0.144781
1	-2.137833	2.192105	0.007229	7	2.845955	-0.000001	-0.233058
1	0.000001	3.378511	0.102613	1	1.198282	2.158305	-0.144749
1	2.137834	2.192104	0.007232	1	-1.198283	2.158305	-0.144749
6	3.627633	0.180533	0.254222	6	-3.502668	-1.212683	0.228675
6	2.397498	-1.909194	0.069440	6	-3.502670	1.212686	0.228653
6	-2.397499	-1.909194	0.069436	1	-3.255880	-1.457768	1.275483
6	-3.627632	0.180532	0.254227	1	-4.582424	-1.076295	0.144599
1	4.484905	-0.482319	0.123959	1	-3.229365	-2.061396	-0.400850
1	3.542617	0.446373	1.320544	1	-3.255887	1.457788	1.275459
1	3.826946	1.089503	-0.315922	1	-3.229362	2.061388	-0.400883
1	3.405003	-2.317874	-0.025751	1	-4.582425	1.076297	0.144575
1	2.031082	-2.102931	1.091194	6	3.502669	1.212686	0.228658
1	1.759676	-2.445877	-0.636242	6	3.502669	-1.212683	0.228670
1	-3.405004	-2.317874	-0.025759	1	3.255885	1.457784	1.275464
1	-2.031086	-2.102931	1.091191	1	4.582425	1.076298	0.144581
1	-1.759674	-2.445875	-0.636245	1	3.229362	2.061391	-0.400875
1	-4.484905	-0.482317	0.123960	1	3.255882	-1.457773	1.275477
1	-3.542613	0.446365	1.320550	1	3.229365	-2.061394	-0.400858
1	-3.826945	1.089507	-0.315911	1	4.582425	-1.076295	0.144594
$C_6H_3(NMe_2)_3$							
6	-0.186869	1.398104	-0.196687				
6	1.109877	0.855120	-0.191658				
6	1.304229	-0.537219	-0.196688				
6	0.185618	-1.388742	-0.191659				
6	-1.117359	-0.860886	-0.196687				
6	-1.295494	0.533621	-0.191658				
7	-0.373126	2.791635	-0.244064				
1	1.963652	1.512923	-0.185660				
7	2.604190	-1.072681	-0.244066				
1	0.328404	-2.457034	-0.185664				
7	-2.231063	-1.718955	-0.244065				
1	-2.292056	0.944110	-0.185660				
6	-1.665346	3.289071	0.199308				
6	0.743092	3.610980	0.199313				
6	3.681093	-0.202303	0.199304				
6	2.755655	-2.449026	0.199314				
6	-2.015747	-3.086767	0.199313				
6	-3.498748	-1.161953	0.199306				
1	-1.659022	4.378698	0.134643				
1	-1.901391	2.995850	1.235632				
1	-2.462654	2.928656	-0.454044				
1	0.450826	4.660698	0.134648				

1	1.047855	3.390041	1.235638	
1	1.607069	3.472611	-0.454036	
1	4.621576	-0.752594	0.134638	
1	3.545180	0.148729	1.235627	
1	3.767617	0.668392	-0.454050	
1	3.810870	-2.720775	0.134648	
1	2.411935	-2.602488	1.235638	
1	2.203835	-3.128069	-0.454035	
1	-2.962553	-3.626104	0.134648	
1	-1.643789	-3.144572	1.235637	
1	-1.304963	-3.597051	-0.454036	
1	-4.261697	-1.939922	0.134640	
1	-3.459795	-0.787548	1.235629	
1	-3.810903	-0.344544	-0.454047	

**Table S7.** RHF/6-311++G\*\* Optimized Structures for Substituted Benzenes that Gave Negative Frequencies when Calculated at the MP2(full)/6-311++G\*\* level of theory.

C <sub>6</sub> H <sub>6</sub>							
6	0.000000	1.385858	-0.000004				
6	0.000000	-1.385858	-0.000004				
6	-1.200188	0.692929	-0.000004				
6	1.200188	0.692929	-0.000004				
6	-1.200188	-0.692929	-0.000004				
6	1.200188	-0.692929	-0.000004				
1	0.000000	2.461273	0.000024				
1	-2.131525	1.230636	0.000024				
1	-2.131525	-1.230636	0.000024				
1	0.000000	-2.461273	0.000024				
1	2.131525	-1.230636	0.000024				
1	2.131525	1.230636	0.000024				
C <sub>6</sub> H <sub>5</sub> F				<i>o</i> -C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>			
6	0.924979	0.000000	0.000000	6	0.534555	-0.689065	0.000001
6	0.261902	1.206900	0.000000	6	0.534555	0.689065	-0.000001
6	-1.123697	1.198267	0.000000	6	-0.650061	1.388248	0.000001
6	-1.819930	0.000000	0.000000	6	-1.848483	0.692093	-0.000001
6	-1.123697	-1.198267	0.000000	6	-1.848483	-0.692093	0.000001
6	0.261902	-1.206900	0.000000	6	-0.650061	-1.388248	-0.000001
9	2.252929	0.000000	0.000000	9	1.686706	-1.333838	0.000000
1	0.822498	2.123090	0.000000	9	1.686706	1.333838	0.000000
1	-1.657729	2.131460	0.000000	1	-0.619958	2.461993	0.000000
1	-2.894647	0.000000	0.000000	1	-2.776462	1.233494	0.000001
1	-1.657729	-2.131460	0.000000	1	-2.776462	-1.233494	-0.000001
1	0.822498	-2.123090	0.000000	1	-0.619958	-2.461993	0.000000
C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>				C <sub>6</sub> H <sub>5</sub> Cl			
6	1.185418	-0.688187	0.000003	6	0.500398	0.000000	-0.000005
6	1.185418	0.688187	-0.000002	6	-0.176608	1.204936	0.000002
6	0.000000	1.387441	-0.000005	6	-1.562015	1.198071	0.000019
6	-1.185418	0.688187	-0.000003	6	-2.257306	0.000000	0.000025
6	-1.185418	-0.688187	0.000003	6	-1.562015	-1.198071	0.000018
6	0.000000	-1.387441	0.000005	6	-0.176608	-1.204936	0.000000
9	2.330124	-1.338868	0.000005	17	2.246348	0.000000	-0.000026
9	2.330124	1.338868	-0.000005	1	0.369404	2.129328	-0.000003
1	0.000000	2.460576	-0.000008	1	-2.094764	2.132010	0.000025
9	-2.330124	1.338868	-0.000006	1	-3.332271	0.000000	0.000038
9	-2.330124	-1.338869	0.000006	1	-2.094764	-2.132010	0.000023
1	0.000000	-2.460576	0.000009	1	0.369404	-2.129328	-0.000006
<i>o</i> -C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>				<i>m</i> -C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>			
6	-0.028095	0.692723	0.000002	6	1.186501	-0.001111	0.000000

6	-0.028095	-0.692723	-0.000002	6	0.000000	-0.709898	0.000000
6	1.174631	-1.381768	-0.000002	6	-1.186501	-0.001111	0.000000
6	2.371451	-0.692687	0.000001	6	-1.204076	1.380413	0.000000
6	2.371451	0.692687	0.000004	6	0.000000	2.063542	0.000000
6	1.174631	1.381768	0.000004	6	1.204075	1.380413	0.000000
17	-1.503884	1.606099	0.000002	17	2.692049	-0.877847	0.000000
17	-1.503884	-1.606099	-0.000005	17	-2.692049	-0.877847	0.000000
1	1.160068	-2.455111	-0.000004	1	0.000000	-1.781991	0.000001
1	3.298033	-1.237018	0.000001	1	-2.138307	1.908457	0.000000
1	3.298033	1.237018	0.000006	1	0.000000	3.138388	0.000000
1	1.160068	2.455111	0.000007	1	2.138307	1.908457	0.000000
$C_6H_3Cl_3$				$C_6H_5Br$			
6	-1.184970	-0.684143	0.000000	6	-0.103038	0.000000	0.000000
17	-2.690918	-1.553602	0.000000	6	-0.780695	-1.205369	0.000001
6	1.184971	-0.684144	0.000000	6	-2.166443	-1.198233	0.000001
6	0.000000	1.368286	0.000000	6	-2.861257	0.000000	0.000000
17	2.690918	-1.553602	0.000000	6	-2.1664430	1.198233	0.000000
17	0.000000	3.107204	0.000000	6	-0.780695	1.205369	0.000000
6	1.207554	0.697181	0.000000	35	1.798983	0.000000	0.000000
1	2.135724	1.233061	0.000000	1	-0.239061	-2.132104	0.000001
6	-1.207554	0.697181	0.000000	1	-2.699294	-2.132146	0.000001
6	0.000000	-1.394363	0.000000	1	-3.936258	0.000000	0.000000
1	-2.135725	1.233059	0.000000	1	-2.699294	2.132146	0.000000
1	0.000001	-2.466122	0.000000	1	-0.239061	2.132104	-0.000001
$o-C_6H_4Br_2$				$m-C_6H_4Br_2$			
6	0.538126	-0.693267	-0.000013	6	1.187510	0.335439	-0.000002
6	0.538126	0.693266	0.000015	6	0.000000	-0.373640	0.000001
6	1.743613	1.381177	0.000027	6	-1.187510	0.335439	0.000000
6	2.940573	0.692494	0.000017	6	-1.204056	1.717618	0.000002
6	2.940572	-0.692497	-0.000009	6	0.000000	2.401262	0.000000
6	1.743612	-1.381179	-0.000022	6	1.204056	1.717618	0.000000
35	-1.055310	-1.716859	-0.000033	35	2.828744	-0.619042	-0.000002
35	-1.055308	1.716860	0.000030	1	0.000000	-1.445436	0.000000
1	1.735062	2.454299	0.000046	35	-2.828744	-0.619042	0.000002
1	3.866878	1.237459	0.000027	1	-2.135753	2.249875	0.000002
1	3.866877	-1.237462	-0.000016	1	0.000000	3.476208	0.000001
1	1.735060	-2.454301	-0.000042	1	2.135753	2.249875	-0.000001
$p-C_6H_4Br_2$				$C_6H_3Br_3$			
6	0.000000	0.000000	1.373876	6	0.000000	0.000000	1.369788
35	0.000000	0.000000	3.272178	35	0.000000	0.000000	3.265594
6	0.000000	1.202678	0.692556	6	0.000000	-1.186272	-0.684894
6	0.000000	-1.202678	0.692556	6	0.000000	1.186272	-0.684894
6	0.000000	0.000000	-1.373876	35	0.000000	-2.828087	-1.632797

6	0.000000	-1.202678	-0.692556	35	0.000000	2.828087	-1.632797
6	0.000000	1.202678	-0.692556	6	0.000000	0.000000	-1.394762
35	0.000000	0.000000	-3.272178	1	0.000000	0.000000	-2.466297
1	0.000000	2.132291	1.228962	6	0.000000	1.207899	0.697381
1	0.000000	-2.132291	1.228962	6	0.000000	-1.207899	0.697381
1	0.000000	-2.132291	-1.228962	1	0.000000	2.135876	1.233149
1	0.000000	2.132291	-1.228962	1	0.000000	-2.135876	1.233149
$C_6H_2Br_4$				$C_6H_5I$			
6	0.000000	0.000000	1.375022	6	-0.566562	0.000000	0.000000
1	0.000000	0.000000	2.446568	6	-1.250500	1.204424	0.000001
6	0.000000	1.203798	0.693365	6	-2.636453	1.197943	-0.000001
6	0.000000	-1.203798	0.693365	6	-3.331254	0.000000	0.000000
6	0.000000	0.000000	-1.375022	6	-2.636453	-1.197943	-0.000001
6	0.000000	-1.203798	-0.693365	6	-1.250500	-1.204424	0.000001
6	0.000000	1.203798	-0.693365	53	1.551084	0.000000	0.000000
1	0.000000	0.000000	-2.446568	1	-0.716498	2.135565	0.000000
35	0.000000	2.789603	1.719980	1	-3.168881	2.132191	0.000000
35	0.000000	-2.789603	1.719980	1	-4.406337	0.000000	0.000000
35	0.000000	-2.789603	-1.719980	1	-3.168881	-2.132191	0.000000
35	0.000000	2.789603	-1.719980	1	-0.716497	-2.135565	0.000000
$o-C_6H_4I_2$				$m-C_6H_4I_2$			
6	0.695180	0.911120	0.000001	6	-1.192803	0.565796	0.000014
6	-0.695180	0.911120	-0.000001	6	0.000000	-0.139193	-0.000002
6	-1.378794	2.122630	0.000001	6	1.192803	0.565796	0.000013
6	-0.691853	3.320638	0.000000	6	1.203537	1.950059	0.000046
6	0.691853	3.320638	0.000000	6	0.000000	2.634478	0.000062
6	1.378794	2.122629	-0.000001	6	-1.203537	1.950059	0.000048
53	1.884077	-0.839573	0.000000	53	-3.022179	-0.496606	-0.000010
53	-1.884078	-0.839573	0.000000	53	3.022179	-0.496606	-0.000014
1	-2.451767	2.124826	0.000001	1	0.000000	-1.210923	-0.000027
1	-1.238361	4.246198	0.000001	1	2.130997	2.489813	0.000058
1	1.238362	4.246197	0.000000	1	0.000000	3.709601	0.000088
1	2.451767	2.124825	-0.000002	1	-2.130997	2.489814	0.000061
$p-C_6H_4I_2$				$C_6H_3I_3$			
6	0.000000	0.000000	1.380707	6	0.000000	1.375775	0.000000
53	0.000000	0.000000	3.494757	53	0.000000	3.489754	0.000000
6	0.000000	1.201222	0.692830	6	1.191456	-0.687888	0.000000
6	0.000000	-1.201222	0.692830	6	-1.191456	-0.687888	0.000000
6	0.000000	0.000000	-1.380707	53	3.022216	-1.744877	0.000000
6	0.000000	-1.201222	-0.692830	53	-3.022216	-1.744877	0.000000
6	0.000000	1.201222	-0.692830	6	0.000000	-1.393318	0.000000
53	0.000000	0.000000	-3.494757	1	0.000000	-2.464868	0.000000
1	0.000000	2.135603	1.221040	6	-1.206649	0.696659	0.000000

1	0.000000	-2.135603	1.221040	6	1.206649	0.696659	0.000000
1	0.000000	-2.135603	-1.221040	1	-2.134638	1.232434	0.000000
1	0.000000	2.135603	-1.221040	1	2.134638	1.232434	0.000000
$C_6H_2I_4$				$m-C_6H_4(CN)_2$			
6	0.000000	0.000000	1.370685	6	1.195831	-0.054836	-0.000006
1	0.000000	0.000000	2.441817	6	0.000000	-0.756561	-0.000002
6	0.000000	1.210647	0.694652	6	-1.195831	-0.054836	0.000005
6	0.000000	-1.210647	0.694652	6	-1.198229	1.335037	0.000009
6	0.000000	0.000000	-1.370685	6	0.000000	2.025701	0.000005
6	0.000000	-1.210647	-0.694652	6	1.198229	1.335037	-0.000002
6	0.000000	1.210647	-0.694652	6	2.446473	-0.774486	-0.000012
1	0.000000	0.000000	-2.441817	1	0.000000	-1.830047	-0.000005
53	0.000000	2.953941	1.887624	6	-2.446473	-0.774485	0.000008
53	0.000000	-2.953941	1.887624	1	-2.132444	1.865073	0.000014
53	0.000000	-2.953941	-1.887624	1	0.000000	3.099660	0.000008
53	0.000000	2.953941	-1.887624	1	2.132444	1.865073	-0.000005
				7	3.428265	-1.334513	-0.000014
				7	-3.428265	-1.334513	0.000009
$p-C_6H_4(CN)_2$				$C_6H_3(CN)_3$			
6	1.377470	0.000000	0.000010	6	-0.150956	1.375102	-0.000006
6	0.690397	1.207226	0.000000	6	-1.272887	0.559692	-0.000001
6	-0.690397	1.207226	-0.000002	6	-1.115395	-0.818283	0.000007
6	-1.377470	0.000000	-0.000009	6	0.151735	-1.382199	0.000011
6	-0.690397	-1.207226	0.000002	6	1.266352	-0.556819	0.000005
6	0.690397	-1.207226	0.000003	6	1.121151	0.822506	-0.000003
6	2.821131	0.000000	0.000010	6	-0.308354	2.808878	-0.000016
1	1.232702	2.133840	0.000004	1	-2.255600	0.991795	-0.000004
1	-1.232703	2.133840	-0.000008	6	-2.278383	-1.671482	0.000008
6	-2.821131	0.000000	-0.000010	1	0.268880	-2.449305	0.000018
1	-1.232702	-2.133840	-0.000003	6	2.586737	-1.137397	0.000006
1	1.232703	-2.133840	0.000011	1	1.986720	1.457509	-0.000007
7	3.951383	-0.000001	0.000007	7	-0.431632	3.931831	-0.000024
7	-3.951383	0.000000	-0.000009	7	-3.189250	-2.339718	0.000008
				7	3.620882	-1.592110	0.000005
$C_6H_5OH$							
				6	0.934018	-0.024350	-0.000001
				6	0.219791	-1.213932	0.000000
				6	-1.161331	-1.179831	0.000001
				6	-1.843925	0.029299	0.000002
				6	-1.121867	1.208387	0.000001
				6	0.265163	1.188431	0.000000
				8	2.282560	-0.107551	-0.000002
				1	0.756340	-2.144688	-0.000001

	1	-1.710063	-2.105051	0.000001				
	1	-2.918362	0.048250	0.000003				
	1	-1.633656	2.154478	0.000002				
	1	0.819743	2.111909	-0.000001				
	1	2.674423	0.747485	-0.000001				
<i>m</i> -C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>					<i>p</i> -C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>			
6	-1.185866	-0.318940	0.000001	6	1.390568	-0.026289	0.000001	
6	0.024640	-0.997910	-0.000003	6	0.672759	-1.207524	0.000001	
6	1.205835	-0.279764	-0.000004	6	-0.711504	-1.180362	0.000000	
6	1.194582	1.110664	0.000003	6	-1.390568	0.026289	-0.000001	
6	-0.019951	1.762277	0.000007	6	-0.672759	1.207524	-0.000001	
6	-1.220526	1.064255	0.000009	6	0.711504	1.180362	0.000000	
8	-2.304246	-1.071614	-0.000001	8	2.744891	-0.107863	0.000003	
1	0.021517	-2.073579	-0.000008	1	1.201288	-2.142893	0.000001	
8	2.407132	-0.889247	-0.000010	1	-1.258405	-2.108416	-0.000001	
1	2.124532	1.646596	0.000002	8	-2.744891	0.107863	-0.000002	
1	-0.040301	2.837730	0.000013	1	-1.201288	2.142893	-0.000002	
1	-2.160277	1.588545	0.000011	1	1.258405	2.108416	0.000000	
1	-3.073841	-0.530564	0.000003	1	3.134423	0.747868	0.000005	
1	2.312991	-1.825323	-0.000013	1	-3.134423	-0.747868	0.000001	
C <sub>6</sub> H <sub>3</sub> (OH) <sub>3</sub>					<i>o</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>			
6	1.271195	-0.524531	-0.000003	6	-0.705110	-0.125386	0.000001	
6	1.103156	0.855115	0.000009	6	0.705110	-0.125386	0.000000	
6	-0.181340	1.363153	0.000010	6	1.380998	1.073916	-0.000001	
6	-1.292129	0.527804	0.000003	6	0.684989	2.285115	-0.000001	
6	-1.089855	-0.838622	-0.000007	6	-0.684991	2.285114	0.000000	
6	0.188973	-1.382918	-0.000010	6	-1.380999	1.073915	0.000001	
8	2.536601	-0.978894	-0.000006	8	-1.290007	-1.335214	0.000001	
1	1.966591	1.494935	0.000014	8	1.290008	-1.335213	-0.000001	
8	-0.420554	2.686208	0.000020	1	2.453507	1.089367	-0.000002	
1	-2.277947	0.955651	0.000004	1	1.234141	3.209181	-0.000001	
8	-2.116047	-1.707314	-0.000016	1	-1.234143	3.209180	0.000001	
1	0.311356	-2.450585	-0.000019	1	-2.453508	1.089365	0.000002	
1	2.557218	-1.919636	-0.000008	6	-2.683631	-1.430891	0.000002	
1	0.383845	3.174434	0.000023	6	2.683631	-1.430890	-0.000002	
1	-2.941063	-1.254798	-0.000006	1	-2.912471	-2.486640	0.000002	
				1	-3.114012	-0.973361	-0.886567	
				1	-3.114011	-0.973360	0.886572	
				1	2.912472	-2.486639	-0.000002	
				1	3.114013	-0.973359	0.886567	
				1	3.114011	-0.973360	-0.886572	
<i>m</i> -C <sub>6</sub> H <sub>4</sub> (OCH <sub>3</sub> ) <sub>2</sub>					C <sub>6</sub> H <sub>3</sub> (OCH <sub>3</sub> ) <sub>3</sub>			
6	1.052989	-0.212240	0.009942	6	0.111721	1.374499	0.000005	



6	-0.281397	-0.652733	-0.006222	6	-1.158836	0.780625	0.000010
6	-1.317046	0.280842	-0.011174	6	-1.246211	-0.590497	0.000004
6	-1.029090	1.656286	-0.002044	6	-0.096623	-1.393894	-0.000006
6	0.295253	2.073316	0.004434	6	1.134491	-0.784002	-0.000009
6	1.354636	1.151220	0.016686	6	1.255459	0.613269	-0.000004
8	1.981474	-1.214451	0.017317	8	0.102519	2.716974	0.000011
1	-0.454644	-1.721665	-0.014394	1	-2.016459	1.421263	0.000017
8	-2.641696	-0.045037	-0.023574	8	-2.404228	-1.269703	0.000007
1	-1.851381	2.363747	-0.008478	1	-0.222620	-2.456936	-0.000009
1	0.520262	3.136027	0.010417	8	2.301709	-1.447271	-0.000019
1	2.376305	1.509116	0.026503	1	2.239079	1.035674	-0.000008
6	3.341561	-0.815858	-0.019770	6	1.310478	3.425605	0.000008
6	-2.955125	-1.427291	0.015877	6	-3.621901	-0.577895	0.000017
1	3.921108	-1.737980	-0.029456	6	2.311423	-2.847710	-0.000025
1	3.608018	-0.227664	0.865073	1	1.044582	4.472642	0.000013
1	3.559161	-0.236313	-0.923456	1	1.896883	3.204943	-0.886368
1	-4.042686	-1.485084	0.018888	1	1.896892	3.204936	0.886375
1	-2.560095	-1.896608	0.923395	1	-4.395713	-1.331687	0.000018
1	-2.564954	-1.948919	-0.864806	1	-3.724008	0.040287	-0.886351
				1	-3.723998	0.040279	0.886392
				1	3.351131	-3.140955	-0.000032
				1	1.827111	-3.245219	-0.886396
				1	1.827120	-3.245227	0.886347

**Table S8.** MP2(full)/6-311++G\*\* Optimized Structures for All Na<sup>+</sup>-Substituted Benzene Complexes.

<b>C<sub>6</sub>H<sub>6</sub></b>							
11	0.000000	0.000000	1.907003				
6	0.000000	1.404744	-0.494199				
6	0.000000	-1.404744	-0.494199				
6	1.216544	0.702372	-0.494199				
6	-1.216544	0.702372	-0.494199				
6	1.216544	-0.702372	-0.494199				
6	-1.216544	-0.702372	-0.494199				
1	0.000000	2.490473	-0.530980				
1	2.156813	1.245237	-0.530980				
1	2.156813	-1.245237	-0.530980				
1	0.000000	-2.490473	-0.530980				
1	-2.156813	-1.245237	-0.530980				
1	-2.156813	1.245237	-0.530980				
<b>F1</b>				<b>F2o</b>			
11	-2.008533	-0.423690	0.000000	11	2.094070	-0.697085	0.000000
6	0.443509	1.037810	0.000000	6	-0.392746	0.678040	0.701534
6	0.425854	-1.753292	0.000000	6	-0.392746	0.678040	-0.701534
6	0.430763	-1.045723	1.212654	6	-0.382933	-1.740736	-0.701752
6	0.430763	-1.045723	-1.212654	6	-0.382933	-1.740736	0.701752
6	0.430763	0.359154	1.221071	6	-0.382933	-0.526047	-1.407059
6	0.430763	0.359154	-1.221071	6	-0.382933	-0.526047	1.407059
9	0.466460	2.372081	0.000000	9	-0.413251	1.837534	1.347412
1	0.464964	-2.838332	0.000000	9	-0.413251	1.837534	-1.347412
1	0.464679	-1.574455	2.160984	1	-0.424054	-2.677226	-1.249540
1	0.464679	-1.574455	-2.160984	1	-0.424054	-2.677226	1.249540
1	0.473461	0.915408	2.152718	1	-0.422399	-0.494154	-2.492151
1	0.473461	0.915408	-2.152718	1	-0.422399	-0.494154	2.492151
<b>F2m</b>				<b>F2p</b>			
11	0.000000	0.000000	0.000000	11	0.000000	0.000000	0.000000
0	0.000000	0.000000	2.237349	0	0.000000	0.000000	2.230622
6	1.431566	0.000000	2.528022	6	1.386756	0.000000	2.487667
6	-1.373972	0.000000	2.441543	6	-1.386756	0.000000	2.487667
1	2.514194	0.000000	2.608064	9	2.721280	0.000000	2.506588
1	-2.460078	0.000000	2.439079	9	-2.721280	0.000000	2.506588
6	0.708487	1.195993	2.519543	6	0.702747	1.217694	2.480330
6	0.708487	-1.195993	2.519543	6	0.702747	-1.217694	2.480330
9	1.387257	2.341821	2.559960	6	-0.702747	-1.217694	2.480330
9	1.387257	-2.341821	2.559960	6	-0.702747	1.217694	2.480330
6	-0.686835	1.224382	2.457067	1	1.245159	2.157565	2.519201
6	-0.686835	-1.224382	2.457067	1	1.245159	-2.157565	2.519201
1	-1.217582	2.170513	2.486900	1	-1.245159	-2.157565	2.519201

1	-1.217582	-2.170513	2.486900	1	-1.245159	2.157565	2.519201
<b>F3</b>				<b>F4</b>			
11	0.000000	0.000000	2.185553	11	0.000000	0.000000	2.259108
6	0.000000	-1.375965	-0.360902	6	0.000000	1.401284	-0.317652
6	-1.191620	0.687982	-0.360902	6	0.000000	-1.401284	-0.317652
6	1.191620	0.687982	-0.360902	1	0.000000	2.486725	-0.361009
6	0.000000	1.417104	-0.340812	1	0.000000	-2.486725	-0.361009
6	-1.227248	-0.708552	-0.340812	6	1.208091	0.699930	-0.327062
6	1.227248	-0.708552	-0.340812	6	-1.208091	0.699930	-0.327062
9	0.000000	-2.706615	-0.378840	6	-1.208091	-0.699930	-0.327062
9	-2.343998	1.353308	-0.378840	6	1.208091	-0.699930	-0.327062
9	2.343998	1.353308	-0.378840	9	2.355854	1.364909	-0.346302
1	0.000000	2.500805	-0.393850	9	-2.355854	1.364909	-0.346302
1	-2.165761	-1.250403	-0.393850	9	-2.355854	-1.364909	-0.346302
1	2.165761	-1.250403	-0.393850	9	2.355854	-1.364909	-0.346302
<b>C11</b>				<b>C12o</b>			
11	-2.041774	-0.693552	0.000000	11	1.298696	0.003328	1.929971
6	0.382377	0.659778	0.000000	6	0.965923	-1.399781	-0.493194
6	0.371048	-2.148990	0.000000	6	0.972777	1.396203	-0.479411
6	0.379454	-1.441887	1.212851	6	-0.234259	-0.706222	-0.256751
6	0.379454	-1.441887	-1.212851	6	-0.237776	0.705634	-0.291543
6	0.379454	-0.038510	1.218837	6	2.167453	0.698022	-0.693617
6	0.379454	-0.038510	-1.218837	6	2.166110	-0.705663	-0.688561
17	0.398026	2.382098	0.000000	1	0.943347	-2.485594	-0.520294
1	0.402380	-3.234443	0.000000	1	0.952652	2.481906	-0.512646
1	0.413341	-1.977302	2.157637	17	-1.682826	-1.598007	-0.027912
1	0.413341	-1.977302	-2.157637	17	-1.678831	1.600836	-0.031630
1	0.418282	0.511244	2.154847	1	3.085546	1.247897	-0.878263
1	0.418282	0.511244	-2.154847	1	3.079606	-1.258060	-0.887801
<b>C12m</b>				<b>C12p</b>			
11	2.125135	0.581749	0.000000	11	0.000000	0.000000	2.126043
6	-0.291431	-0.806751	0.000000	6	0.000000	1.403234	-0.305885
6	-0.330414	1.996682	0.000000	6	0.000000	-1.403234	-0.305885
1	-0.319583	-1.892515	0.000000	6	1.215974	0.7007010	-0.313943
1	-0.368245	3.082574	0.000000	6	-1.215974	-0.700701	-0.313943
6	-0.315714	-0.097437	1.211074	6	-1.215974	0.700701	-0.313943
6	-0.315714	-0.097437	-1.211074	6	1.215974	-0.700701	-0.313943
17	-0.315714	-0.968373	2.695074	17	0.000000	3.124240	-0.317082
17	-0.315714	-0.968373	-2.695074	17	0.000000	-3.124240	-0.317082
6	-0.310690	1.306624	1.220892	1	2.154482	1.246590	-0.350109
6	-0.310690	1.306624	-1.220892	1	-2.154482	-1.246590	-0.350109
1	-0.353239	1.842777	2.163991	1	-2.154482	1.246590	-0.350109
1	-0.353239	1.842777	-2.163991	1	2.154482	-1.246590	-0.350109

<b>CI3</b>				<b>CI4</b>			
11	0.000000	0.000000	2.190721	0	0.000000	0.000000	0.000000
6	0.000000	-1.394140	-0.261953	11	0.000000	0.000000	2.457507
6	-1.207361	0.697070	-0.261953	6	1.390741	0.000000	0.000000
6	1.207361	0.697070	-0.261953	6	-1.390741	0.000000	0.000000
6	0.000000	1.411792	-0.258689	6	0.705764	-1.223538	0.005047
6	-1.222648	-0.705896	-0.258689	6	-0.705764	1.223538	0.005047
6	1.222648	-0.705896	-0.258689	6	-0.706013	-1.223604	0.005107
17	0.000000	-3.113735	-0.271520	6	0.706013	1.223604	0.005107
17	-2.696574	1.556868	-0.271520	1	2.476792	-0.000060	-0.031210
17	2.696574	1.556868	-0.271520	1	-2.476792	0.000060	-0.031210
1	0.000000	2.496907	-0.292958	17	1.606257	-2.681410	-0.005491
1	-2.162385	-1.248453	-0.292958	17	-1.606257	2.681410	-0.005491
1	2.162385	-1.248453	-0.292958	17	-1.606598	-2.681444	-0.005309
				17	1.606598	2.681444	-0.005309
<b>Br1</b>				<b>Br2o</b>			
11	2.121998	1.240286	0.000000	11	2.220247	-1.482232	0.000000
6	-0.299600	-0.100794	0.000000	6	-0.215810	-0.378452	0.706790
6	-0.292971	2.707312	0.000000	6	-0.215810	-0.378452	-0.706790
6	-0.300589	2.000982	1.213291	6	-0.207859	-2.820002	-0.702046
6	-0.300589	2.000982	-1.213291	6	-0.207859	-2.820002	0.702046
6	-0.300589	0.597400	1.220033	6	-0.215810	-1.605975	-1.398754
6	-0.300589	0.597400	-1.220033	6	-0.215810	-1.605975	1.398754
35	-0.311582	-1.983786	0.000000	35	-0.225444	1.209449	1.710468
1	-0.324565	3.792808	0.000000	35	-0.225444	1.209449	-1.710468
1	-0.334397	2.538483	2.157045	1	-0.235765	-3.757112	-1.250433
1	-0.334397	2.538483	-2.157045	1	-0.235765	-3.757112	1.250433
1	-0.336835	0.049949	2.157497	1	-0.248179	-1.594759	-2.484539
1	-0.336835	0.049949	-2.157497	1	-0.248179	-1.594759	2.484539
<b>Br2m</b>				<b>Br2p</b>			
11	0.000000	0.000000	0.000000	11	0.000000	0.000000	2.216569
0	0.000000	0.000000	2.840190	6	0.000000	1.404626	-0.214070
6	1.418456	0.000000	2.393095	6	0.000000	-1.404626	-0.214070
6	-1.387520	0.000000	2.484683	6	1.216692	0.701298	-0.224781
1	2.504582	0.000000	2.396035	6	-1.216692	-0.701298	-0.224781
1	-2.472747	0.000000	2.543550	6	-1.216692	0.701298	-0.224781
6	0.707460	1.211619	2.426980	6	1.216692	-0.701298	-0.224781
6	0.707460	-1.211619	2.426980	35	0.000000	3.285584	-0.219761
35	1.656194	2.836453	2.404352	35	0.000000	-3.285584	-0.219761
35	1.656194	-2.836453	2.404352	1	2.158085	1.242575	-0.258858
6	-0.697583	1.221159	2.451999	1	-2.158085	-1.242575	-0.258858
6	-0.697583	-1.221159	2.451999	1	-2.158085	1.242575	-0.258858
1	-1.235577	2.162947	2.501443	1	2.158085	-1.242575	-0.258858

1	-1.235577	-2.162947	2.501443				
<b>Br3</b>				<b>Br4</b>			
11	0.000000	0.000000	2.289824	11	0.000000	0.000000	2.456116
6	0.000000	-1.395558	-0.176980	6	1.391173	0.000000	0.000000
6	-1.208589	0.697779	-0.176980	6	-1.391173	0.000000	0.000000
6	1.208589	0.697779	-0.176980	6	0.706583	-1.226681	0.006981
6	0.000000	1.413193	-0.151481	6	-0.706583	1.226681	0.006981
6	-1.223861	-0.706596	-0.151481	6	-0.706541	-1.226681	0.006971
6	1.223861	-0.706596	-0.151481	6	0.706541	1.226681	0.006971
35	0.000000	-3.276139	-0.178273	1	2.477282	0.000010	-0.027394
35	-2.837220	1.638070	-0.178273	1	-2.477282	-0.000010	-0.027394
35	2.837220	1.638070	-0.178273	35	1.716569	-2.807149	0.004107
1	0.000000	2.498372	-0.185699	35	-1.716569	2.807149	0.004107
1	-2.163653	-1.249186	-0.185699	35	-1.716483	-2.807173	0.004081
1	2.163653	-1.249186	-0.185699	35	1.716483	2.807173	0.004081
<b>I1</b>				<b>I2o</b>			
11	2.160468	1.658414	0.000000	0	0.000000	0.000000	0.000000
6	-0.252565	0.354359	0.000000	11	0.000000	0.000000	2.440980
6	-0.260393	1.057553	1.220181	6	1.396256	0.000000	-0.000014
6	-0.260393	1.057553	-1.220181	0	-0.000010	0.000000	-1.000000
6	-0.260393	2.461154	1.213901	6	-1.396256	0.000000	0.000028
6	-0.260393	2.461154	-1.213901	6	0.708284	-1.229737	0.104698
6	-0.252177	3.166688	0.000000	6	-0.708297	-1.229755	0.104710
53	-0.245791	-1.752416	0.000000	6	-0.701581	1.211777	-0.089938
1	-0.294382	0.513837	2.159921	6	0.701575	1.211775	-0.089953
1	-0.294382	0.513837	-2.159921	1	2.482033	-0.001546	-0.031190
1	-0.294968	3.002371	2.155619	1	-2.482033	-0.001526	-0.031137
1	-0.294968	3.002371	-2.155619	53	1.878912	-2.975287	0.250528
1	-0.281651	4.252299	0.000000	53	-1.878916	-2.975312	0.250562
				1	-1.254585	2.141289	-0.191879
				1	1.254578	2.141287	-0.191899
<b>I2m</b>				<b>I2p</b>			
11	2.269830	1.048888	0.000000	11	0.000000	0.000000	2.244520
6	-0.173601	-0.226274	0.000000	6	0.000000	1.411257	-0.172160
6	-0.147207	2.580777	0.000000	6	0.000000	-1.411257	-0.172160
1	-0.220184	-1.311488	0.000000	53	0.000000	3.514829	-0.162722
1	-0.159150	3.667833	0.000000	53	0.000000	-3.514829	-0.162722
6	-0.175056	0.482299	1.216542	6	1.215480	0.701688	-0.187302
6	-0.175056	0.482299	-1.216542	6	-1.215480	0.701688	-0.187302
53	-0.175056	-0.578783	3.035613	6	-1.215480	-0.701688	-0.187302
53	-0.175056	-0.578783	-3.035613	6	1.215480	-0.701688	-0.187302
6	-0.140140	1.889209	1.220909	1	2.161554	1.235269	-0.220007
6	-0.140140	1.889209	-1.220909	1	-2.161554	1.235269	-0.220007

1	-0.162806	2.435866	2.158894	1	-2.161554	-1.235269	-0.220007
1	-0.162806	2.435866	-2.158894	1	2.161554	-1.235269	-0.220007
<b>I3</b>				<b>I4</b>			
11	0.000000	0.000000	2.309444	6	1.388921	0.000177	0.993919
6	0.000000	-1.401122	-0.141507	1	2.475275	0.000328	1.002781
6	-1.213407	0.700561	-0.141507	6	0.708882	-1.232717	0.958491
6	1.213407	0.700561	-0.141507	6	0.708285	1.232665	0.958128
6	0.000000	1.412551	-0.116253	6	-1.387090	-0.000501	0.986392
6	-1.223305	-0.706275	-0.116253	6	-0.707176	1.232741	1.000826
6	1.223305	-0.706275	-0.116253	6	-0.706608	-1.233501	1.001109
53	0.000000	-3.506496	-0.127842	1	-2.472764	-0.000691	1.024321
53	-3.036714	1.753248	-0.127842	53	1.884889	-2.977036	0.966209
53	3.036714	1.753248	-0.127842	53	1.883748	2.977356	0.965416
1	0.000000	2.498011	-0.145777	53	-1.882609	2.976790	0.973546
1	-2.163341	-1.249005	-0.145777	53	-1.881369	-2.977968	0.973826
1	2.163341	-1.249005	-0.145777	11	-0.009419	-0.001835	-1.453156
<b>CN1</b>				<b>CN2o</b>			
11	0.000000	0.000000	0.000000	11	0.000000	0.000000	2.556094
0	0.000000	0.000000	3.292083	6	1.407315	0.000000	0.000005
6	1.417416	0.000000	2.432927	0	0.000004	0.000000	-1.000000
6	-1.392190	0.000000	2.498975	6	-1.407315	0.000000	-0.000010
6	-0.688028	1.215087	2.487760	6	0.709575	-1.222847	0.067859
6	-0.688028	-1.215087	2.487760	6	-0.709478	-1.222956	0.067828
6	0.713834	1.222235	2.452677	6	-0.702660	1.208728	-0.058890
6	0.713834	-1.222235	2.452677	6	0.702526	1.208654	-0.058907
6	2.851894	0.000000	2.410080	1	2.493514	-0.012790	-0.034503
7	4.027914	0.000000	2.358444	1	-2.493516	-0.012963	-0.034500
1	-2.476707	0.000000	2.559712	6	1.430764	-2.458402	0.127843
1	-1.222799	2.159518	2.536339	6	-1.429881	-2.458917	0.127794
1	-1.222799	-2.159518	2.536339	7	2.038402	-3.464361	0.212816
1	1.261683	2.160268	2.477751	7	-2.036909	-3.465240	0.212774
1	1.261683	-2.160268	2.477751	1	-1.247805	2.144799	-0.140019
				1	1.247660	2.144730	-0.140051
<b>CN2m</b>				<b>CN2p</b>			
11	0.000000	0.000000	0.000000	11	0.000000	0.000000	2.180653
0	0.000000	0.000000	2.796266	6	0.000000	1.406725	-0.363463
6	1.420527	0.000000	2.507613	6	0.000000	-1.406725	-0.363463
6	-1.389926	0.000000	2.606689	6	0.000000	2.839834	-0.365617
1	2.507519	0.000000	2.512016	6	0.000000	-2.839834	-0.365617
1	-2.474484	0.000000	2.672094	7	0.000000	4.017049	-0.331924
6	0.711164	1.216269	2.537991	7	0.000000	-4.017049	-0.331924
6	0.711164	-1.216269	2.537991	6	1.220642	0.699671	-0.373081
6	1.435237	2.454615	2.521506	6	-1.220642	0.699671	-0.373081

6	1.435237	-2.454615	2.521506	6	-1.220642	-0.699671	-0.373081
7	2.027493	3.470904	2.472726	6	1.220642	-0.699671	-0.373081
7	2.027493	-3.470904	2.472726	1	2.162967	1.239811	-0.409336
6	-0.698120	1.219018	2.574286	1	-2.162967	1.239811	-0.409336
6	-0.698120	-1.219018	2.574286	1	-2.162967	-1.239811	-0.409336
1	-1.237438	2.160744	2.627423	1	2.162967	-1.239811	-0.409336
1	-1.237438	-2.160744	2.627423				
<b>CN3</b>							
11	0.000000	0.000000	2.657924				
6	1.412555	0.000000	0.000000				
6	-0.706277	-1.223308	0.000000				
6	-0.706277	1.223308	0.000000				
6	0.701330	-1.214742	-0.017235				
6	-1.402663	0.000001	-0.017235				
6	0.701332	1.214741	-0.017235				
1	2.498903	-0.000002	-0.036450				
1	-1.249453	-2.164112	-0.036450				
1	-1.249450	2.164114	-0.036450				
6	1.418390	-2.456973	-0.017017				
6	-2.836996	0.000125	-0.017017				
6	1.418606	2.456848	-0.017017				
7	2.006652	-3.476305	0.020809				
7	-4.013895	0.000341	0.020809				
7	2.007243	3.475964	0.020809				
<b>NO<sub>2</sub>1</b>							
11	-2.118432	-0.974539	0.000000				
6	0.348137	0.416334	0.000000				
6	0.364799	-2.362782	0.000000				
7	0.364716	1.904699	0.000000				
1	0.406420	-3.448247	0.000000				
6	0.359992	-0.256422	1.225967				
6	0.359992	-0.256422	-1.225967				
1	0.396854	0.309637	2.151256				
1	0.396854	0.309637	-2.151256				
6	0.365096	-1.659584	-1.216040				
6	0.365096	-1.659584	1.216040				
1	0.405541	-2.200029	-2.157512				
1	0.405541	-2.200029	2.157512				
8	0.359992	2.455426	1.096476				
8	0.359992	2.455426	-1.096476				
<b>NO<sub>2</sub>2m</b>				<b>NO<sub>2</sub>2p</b>			
11	1.269671	2.050508	0.000000	11	0.000000	0.000000	2.265104
6	-0.713871	-0.123410	0.000000	6	0.000661	1.366551	-0.333717

6	2.018984	-0.788562	0.000000	6	-0.000661	-1.366551	-0.333717
1	-1.777122	0.094407	0.000000	6	1.229108	0.700282	-0.370243
1	3.063345	-1.087989	0.000000	6	-1.229108	-0.700282	-0.370243
6	1.349711	-0.623042	1.223208	6	1.228660	-0.699109	-0.337117
6	1.349711	-0.623042	-1.223208	6	-1.228660	0.699109	-0.337117
1	1.859383	-0.786506	2.167472	7	0.000000	2.837029	-0.265163
1	1.859383	-0.786506	-2.167472	7	0.000000	-2.837029	-0.265163
6	-0.003010	-0.278947	-1.192411	1	2.153607	1.267656	-0.430947
6	-0.003010	-0.278947	1.192411	1	-2.153607	-1.267656	-0.430947
7	-0.746225	-0.126757	-2.476118	1	2.154684	-1.266578	-0.339369
7	-0.746225	-0.126757	2.476118	1	-2.154684	1.266578	-0.339369
8	-0.096233	-0.276754	-3.505011	8	0.833416	3.428424	-0.942724
8	-1.935973	0.156835	-2.388471	8	-0.833416	-3.428424	-0.942724
8	-1.935973	0.156835	2.388471	8	-0.833219	3.333990	0.494580
8	-0.096233	-0.276754	3.505011	8	0.833219	-3.333990	0.494580
<b>CH<sub>3</sub>1</b>				<b>CH<sub>3</sub>2o</b>			
11	0.000000	0.000000	2.494346	11	-1.113980	-0.004790	1.819461
6	1.401424	0.000000	0.073974	6	-0.525611	-1.391164	-0.476104
6	0.676747	-1.208886	0.097202	6	-0.525117	1.393858	-0.468129
6	0.676747	1.208886	0.097202	6	-1.716613	-0.698870	-0.748497
6	-0.727324	-1.212638	0.125721	6	-1.716485	0.703637	-0.744042
6	-0.727324	1.212638	0.125721	6	0.677380	-0.709321	-0.206583
6	-1.435252	0.000000	0.138565	6	0.677427	0.709967	-0.201706
6	2.900618	0.000000	-0.073812	1	-0.518185	-2.478226	-0.514193
1	3.164090	0.000000	-1.136124	1	-0.517362	2.481183	-0.498726
1	3.348137	-0.888315	0.377856	1	-2.620811	-1.248128	-0.995546
1	3.348137	0.888315	0.377856	1	-2.620500	1.254650	-0.987858
1	1.214786	-2.153148	0.051567	6	1.958854	-1.476936	-0.010412
1	1.214786	2.153148	0.051567	6	1.960250	1.476273	-0.010907
1	-1.265017	-2.156642	0.104825	1	1.778906	-2.553281	-0.035571
1	-1.265017	2.156642	0.104825	1	2.668801	-1.232268	-0.806630
1	-2.521299	0.000000	0.123987	1	2.445282	-1.229967	0.938381
				1	2.626536	1.309046	-0.863486
				1	1.770318	2.548759	0.062902
				1	2.500285	1.156260	0.884941
<b>CH<sub>3</sub>2m</b>				<b>CH<sub>3</sub>2p</b>			
11	0.000000	0.000000	2.585062	11	0.000000	0.000000	2.373099
6	1.418318	0.000000	0.222560	6	1.432480	0.000000	0.000000
6	0.696145	-1.209828	0.224884	6	-1.432480	0.000000	0.000000
6	0.696145	1.209828	0.224884	6	0.702116	-1.204919	0.008614
6	-0.709811	-1.222240	0.209062	6	-0.702116	1.204919	0.008614
6	-0.709811	1.222240	0.209062	6	0.702116	1.204919	0.008614
6	-1.405800	0.000000	0.206150	6	-0.702116	-1.204919	0.008614



6	2.921041	0.000000	0.122497	6	2.934634	0.000000	-0.117002
6	-1.466950	2.525973	0.122497	6	-2.934634	0.000000	-0.117002
1	3.202313	0.000000	-0.935322	1	3.221383	0.000000	-1.173223
1	3.361969	-0.888243	0.581052	1	-3.221383	0.000000	-1.173223
1	3.361969	0.888243	0.581052	1	3.372726	-0.888102	0.344442
1	-1.631845	2.807489	-0.922324	1	-3.372726	0.888102	0.344442
1	-2.445898	2.445565	0.600890	1	3.372726	0.888102	0.344442
1	-0.908496	3.335672	0.598085	1	-3.372726	-0.888102	0.344442
1	1.239149	-2.152761	0.197536	1	1.235565	-2.152817	-0.020415
1	1.239149	2.152761	0.197536	1	-1.235565	2.152817	-0.020415
1	-1.249733	-2.164344	0.176854	1	1.235565	2.152817	-0.020415
1	-2.492627	0.000000	0.165979	1	-1.235565	-2.152817	-0.020415
<b>CH<sub>3</sub></b>				<b>CH<sub>3</sub></b>			
11	0.000000	0.000000	2.062645	11	0.000000	0.000000	2.085819
6	0.000000	1.419945	-0.295600	6	0.000000	1.380525	-0.248358
6	1.229708	-0.709972	-0.295600	6	0.000000	-1.380525	-0.248358
6	-1.229708	-0.709972	-0.295600	6	1.237317	0.708063	-0.256170
6	0.000000	-1.396255	-0.289274	6	-1.237317	-0.708063	-0.256170
6	1.209193	0.698128	-0.289274	6	1.237301	-0.708000	-0.255989
6	-1.209193	0.698128	-0.289274	6	-1.237301	0.708000	-0.255989
6	0.000000	2.923833	-0.400905	1	-0.000067	2.469299	-0.281215
6	2.532113	-1.461916	-0.400905	1	0.000067	-2.469299	-0.281215
6	-2.532113	-1.461916	-0.400905	6	2.526724	1.482143	-0.354032
1	0.000000	-2.484896	-0.321102	6	-2.526724	-1.482143	-0.354032
1	2.151983	1.242448	-0.321102	6	2.526226	-1.482182	-0.358023
1	-2.151983	1.242448	-0.321102	6	-2.526226	1.482182	-0.358023
1	0.000000	3.219394	-1.454819	1	3.231389	1.211459	0.438462
1	2.788077	-1.609697	-1.454819	1	-3.231389	-1.211459	0.438462
1	-2.788077	-1.609697	-1.454819	1	2.344143	2.557266	-0.300353
1	0.888223	3.358614	0.063782	1	-2.344143	-2.557266	-0.300353
1	2.464533	-2.448531	0.063782	1	3.021506	1.269866	-1.307223
1	-3.352757	-0.910083	0.063782	1	-3.021506	-1.269866	-1.307223
1	-0.888223	3.358614	0.063782	1	3.000357	-1.296617	-1.327319
1	3.352757	-0.910083	0.063782	1	-3.000357	1.296617	-1.327319
1	-2.464533	-2.448531	0.063782	1	3.246160	-1.186864	0.411329
				1	-3.246166	1.186864	0.411329
				1	2.347764	-2.555792	-0.270256
				1	-2.347764	2.555792	-0.270256
<b>OH1</b>				<b>OH2o</b>			
11	-0.738912	-0.077211	1.877006	11	1.167927	-0.126414	1.811499
6	1.100036	-0.047553	-0.246398	6	-0.709515	-0.717101	-0.252527
6	-1.669358	0.092430	-0.736998	6	-0.755434	0.694482	-0.173686
8	2.429774	-0.115494	0.003685	6	0.398670	1.452079	-0.404943
6	0.350314	-1.227047	-0.410201	6	0.502118	-1.350781	-0.560062

6	0.451491	1.200534	-0.288671	6	1.606136	0.811192	-0.735732
6	-0.924315	1.268002	-0.552417	6	1.655102	-0.588616	-0.812271
6	-1.025236	-1.153451	-0.673640	8	-1.979839	1.202363	0.143734
1	0.850245	-2.190526	-0.391500	8	-1.808046	-1.462615	-0.026339
1	1.029588	2.112510	-0.176082	1	-2.060224	2.115678	-0.155796
1	-1.413088	2.237443	-0.638049	1	-2.575923	-0.874346	0.019274
1	-1.592431	-2.065593	-0.853468	1	0.344949	2.537969	-0.367262
1	-2.724474	0.148411	-0.976813	1	0.506308	-2.432868	-0.657728
1	2.842410	0.733548	-0.190686	1	2.484402	1.406800	-0.964447
				1	2.573903	-1.088202	-1.104371
<b>OH2m</b>				<b>OH2p</b>			
11	2.044606	0.458758	0.000000	11	0.000000	0.000000	2.037703
6	-0.352645	-1.092029	0.000000	6	-1.223411	-0.706152	-0.383910
6	-0.363771	1.703130	0.000000	6	1.223411	0.706152	-0.383910
1	-0.373114	-2.180861	0.000000	6	-1.213885	0.697979	-0.375735
1	-0.396845	2.789146	0.000000	6	1.213885	-0.697979	-0.375735
6	-0.362016	1.016717	1.222107	6	0.000000	1.400244	-0.361447
6	-0.362016	1.016717	-1.222107	6	0.000000	-1.400244	-0.361447
1	-0.416954	1.541258	2.170637	8	-2.437565	-1.317024	-0.372489
1	-0.416954	1.541258	-2.170637	8	2.437565	1.317024	-0.372489
6	-0.390103	-0.387721	-1.217055	1	-2.160704	1.228761	-0.417407
6	-0.390103	-0.387721	1.217055	1	2.160704	-1.228761	-0.417407
8	-0.390103	-1.006115	-2.422504	1	-0.011673	2.487806	-0.386350
8	-0.390103	-1.006115	2.422504	1	0.011673	-2.487806	-0.386350
1	-0.660613	-1.926935	-2.328056	1	-2.356433	-2.221222	-0.697139
1	-0.660613	-1.926935	2.328056	1	2.356433	2.221222	-0.697139
<b>OH3</b>				<b>OH4</b>			
11	0.000000	0.000000	2.090629	11	0.000000	0.000000	2.126932
6	0.000000	1.409990	-0.304719	6	0.000000	1.401950	-0.280488
6	1.221087	-0.704995	-0.304719	6	0.000000	-1.401950	-0.280488
6	-1.221087	-0.704995	-0.304719	6	1.212541	0.699784	-0.300880
6	1.207506	0.701248	-0.343773	6	-1.212541	-0.699784	-0.300880
6	0.003546	-1.396355	-0.343773	6	1.219635	-0.709359	-0.307160
6	-1.211052	0.695107	-0.343773	6	-1.219635	0.709359	-0.307160
1	-2.146716	-1.271090	-0.361819	1	-0.017767	2.488919	-0.310346
1	-0.027438	2.494655	-0.361819	1	0.017767	-2.488919	-0.310346
1	2.174154	-1.223565	-0.361819	8	2.449681	1.284657	-0.291339
8	2.418358	1.307760	-0.353876	8	-2.449681	-1.284657	-0.291339
8	-0.076625	-2.748239	-0.353876	8	2.373734	-1.414116	-0.314571
8	-2.341733	1.440479	-0.353876	8	-2.373734	1.414116	-0.314571
1	2.319062	2.239947	-0.581865	1	2.418823	2.145826	-0.724315
1	0.780320	-3.128340	-0.581865	1	-2.418823	-2.145826	-0.724315
1	-3.099382	0.888393	-0.581865	1	3.101769	-0.799164	-0.485017
				1	-3.101769	0.799164	-0.485017

<b>NH<sub>2</sub>1</b>				<b>NH<sub>2</sub>o</b>			
11	0.000000	0.000000	0.000000	11	1.184991	-0.000508	1.784144
6	1.421630	0.000000	2.397888	6	-0.724406	-0.710441	-0.192850
6	-1.409989	0.000000	2.389709	6	-0.722240	0.714018	-0.218777
7	2.819124	0.000000	2.335068	6	0.484428	1.394781	-0.454514
1	-2.494638	0.000000	2.430218	6	0.467022	-1.398802	-0.487249
6	0.701371	1.214809	2.378510	6	1.667108	0.695194	-0.751031
6	0.701371	-1.214809	2.378510	6	1.656012	-0.706697	-0.773471
1	1.245167	2.156693	2.393500	7	-1.914135	1.372891	0.077911
1	1.245167	-2.156693	2.393500	7	-1.938184	-1.358991	-0.013849
6	-0.699451	-1.211484	2.390454	1	-1.894252	2.369150	-0.104230
6	-0.699451	1.211484	2.390454	1	-2.725053	0.951244	-0.364684
1	-1.242579	-2.152211	2.414742	1	-2.563036	-0.952188	0.671237
1	-1.242579	2.152211	2.414742	1	-1.901963	-2.367742	0.042481
1	3.221728	0.809270	2.798875	1	0.475473	2.482066	-0.491304
1	3.221728	-0.809270	2.798875	1	0.452129	-2.486243	-0.519593
				1	2.570552	1.244795	-0.997734
				1	2.549932	-1.261118	-1.042844
<b>NH<sub>2</sub>2m</b>				<b>NH<sub>2</sub>2p</b>			
11	-2.019880	0.157837	0.000000	11	0.000000	0.000000	1.993927
6	0.447447	-1.017711	0.000000	6	0.000000	1.427385	-0.383543
6	0.210401	1.762741	0.000000	6	0.000000	-1.427385	-0.383543
1	0.573093	-2.099146	0.000000	7	0.000000	2.820526	-0.297928
1	0.139019	2.847096	0.000000	7	0.000000	-2.820526	-0.297928
6	0.260365	1.077958	1.219954	6	1.209223	0.699808	-0.371639
6	0.260365	1.077958	-1.219954	6	-1.209223	0.699808	-0.371639
1	0.248305	1.620473	2.161218	6	-1.209223	-0.699808	-0.371639
1	0.248305	1.620473	-2.161218	6	1.209223	-0.699808	-0.371639
6	0.416304	-0.326177	-1.226795	1	2.150482	1.244538	-0.397479
6	0.416304	-0.326177	1.226795	1	-2.150482	1.244538	-0.397479
7	0.416304	-1.024571	-2.426353	1	-2.150482	-1.244538	-0.397479
7	0.416304	-1.024571	2.426353	1	2.150482	-1.244538	-0.397479
1	0.710490	-0.497007	-3.237544	1	0.832296	3.266107	-0.662606
1	0.846799	-1.939317	-2.397818	1	-0.832296	3.266107	-0.662606
1	0.846799	-1.939317	2.397818	1	-0.832296	-3.266107	-0.662606
1	0.710490	-0.497007	3.237544	1	0.832296	-3.266107	-0.662606
<b>NH<sub>2</sub>3</b>				<b>NH<sub>2</sub>4</b>			
11	0.000000	0.000000	2.028876	11	0.000000	0.000000	2.324285
6	0.000000	1.408860	-0.341694	6	1.389498	0.000000	0.000000
6	1.220109	-0.704430	-0.341694	6	-1.389498	0.000000	0.000000
6	-1.220109	-0.704430	-0.341694	6	0.707114	-1.228846	-0.045356
6	1.217436	0.702887	-0.305174	6	-0.707114	1.228846	-0.045356
6	-1.217436	0.702887	-0.305174	6	-0.708743	-1.232405	-0.006251

6	0.000000	-1.405774	-0.305174	6	0.708743	1.232405	-0.006251
7	0.000000	2.796773	-0.280392	1	2.478180	-0.000859	-0.036137
7	2.422076	-1.398386	-0.280392	1	-2.478180	0.000859	-0.036137
7	-2.422076	-1.398386	-0.280392	7	1.371217	-2.464870	-0.031579
1	2.158706	1.246330	-0.340018	7	-1.371217	2.464870	-0.031579
1	-2.158706	1.246330	-0.340018	7	-1.372058	-2.458388	-0.117097
1	0.000000	-2.492660	-0.340018	7	1.372058	2.458388	-0.117097
1	0.836999	3.245686	-0.627623	1	2.362498	-2.393941	-0.229363
1	-0.836999	3.245686	-0.627623	1	-2.362498	2.393941	-0.229363
1	2.392347	-2.347706	-0.627623	1	-0.987433	-3.207195	0.447142
1	3.229346	-0.897980	-0.627623	1	0.987433	3.207195	0.447142
1	-3.229346	-0.897980	-0.627623	1	0.946310	-3.134384	-0.667423
1	-2.392347	-2.347706	-0.627623	1	-0.946310	3.134384	-0.667423
				1	-2.380102	-2.415599	-0.047446
				1	2.380102	2.415599	-0.047446
<b>OCH<sub>3</sub>1</b>				<b>OCH<sub>3</sub>2o</b>			
11	-1.162530	-0.247248	1.843979	11	0.000000	0.000000	0.000000
6	0.674101	-0.242890	-0.243119	0	0.000000	0.000000	1.845904
6	-2.031990	0.431433	-0.708009	6	1.551821	0.000000	2.382394
6	-0.271076	-1.245653	-0.554441	6	0.891388	1.270266	2.382394
6	-1.607113	-0.907911	-0.791250	6	-0.511834	1.314846	2.363783
6	-1.097043	1.423003	-0.385140	6	0.782282	-1.174235	2.363783
6	0.250121	1.097841	-0.139853	6	-0.627752	-1.112762	2.376541
8	1.937845	-0.668338	-0.059463	6	-1.271458	0.125331	2.376541
1	-3.060421	0.697471	-0.930805	8	2.891098	0.053151	2.413509
1	0.080404	-2.268323	-0.659258	8	1.704194	2.336020	2.413509
1	-2.309653	-1.686341	-1.075910	1	-1.023530	2.270193	2.401648
1	-1.401234	2.465435	-0.346997	1	1.270371	-2.141856	2.401648
1	0.957134	1.892413	0.071259	1	-1.201405	-2.033541	2.422984
6	2.967135	0.326878	0.002057	1	-2.354689	0.184666	2.422984
1	2.871468	0.937124	0.905124	6	3.589489	-1.177583	2.632691
1	3.901981	-0.227381	0.035747	6	1.097924	3.614650	2.632691
1	2.940583	0.959820	-0.888694	1	4.637589	-0.900575	2.717227
				1	3.456478	-1.855995	1.784970
				1	3.253205	-1.655712	3.557285
				1	1.926716	4.313471	2.717227
				1	0.513379	3.614024	3.557285
				1	0.466196	3.895461	1.784970
<b>OCH<sub>3</sub>2m</b>				<b>OCH<sub>3</sub>2p</b>			
6	-1.068698	-0.383186	-0.119534	11	0.000000	0.000000	2.390226
6	0.273854	-0.790595	0.059835	6	1.420703	0.000000	0.000000
6	1.324651	0.068438	-0.293931	6	-1.420703	0.000000	0.000000
6	1.038123	1.373764	-0.759451	6	0.704511	-1.215973	0.016427
6	-0.290160	1.770183	-0.908112	6	-0.704511	1.215973	0.016427

6	-1.360190	0.914262	-0.575073	6	-0.698363	-1.207686	0.009461
8	-1.987891	-1.316058	0.197349	6	0.698363	1.207686	0.009461
1	0.443681	-1.810015	0.387569	8	2.767517	0.108435	-0.016245
8	2.630253	-0.249542	-0.211732	8	-2.767517	-0.108435	-0.016245
1	1.861653	2.014313	-1.059033	1	1.219412	-2.169889	-0.020003
1	-0.509161	2.755410	-1.310900	1	-1.219412	2.169889	-0.020003
1	-2.379257	1.239363	-0.746119	1	-1.253107	-2.141095	-0.031072
6	-3.350533	-1.039878	-0.146524	1	1.253107	2.141095	-0.031072
6	2.960553	-1.620789	0.037776	6	3.510293	-1.071976	-0.338155
1	-3.900709	-1.942534	0.108479	6	-3.510293	1.071976	-0.338155
1	-3.442349	-0.837236	-1.216666	1	3.431716	-1.818524	0.458270
1	-3.739419	-0.197863	0.433964	1	-3.431716	1.818524	0.458270
1	4.044568	-1.673105	-0.030185	1	3.167910	-1.494094	-1.286946
1	2.506907	-2.267163	-0.718013	1	-3.167910	1.494094	-1.286946
1	2.641396	-1.926233	1.038803	1	4.544579	-0.748178	-0.428568
11	0.015289	1.401515	1.768841	1	-4.544579	0.748178	-0.428568
<b>OCH<sub>3</sub></b>				<b>OCH<sub>3</sub></b>			
11	0.000000	0.000000	2.354837	11	-0.000015	-0.000002	2.265834
6	1.413720	0.000000	0.000000	6	0.000000	-1.393698	-0.082638
6	-0.706860	-1.224318	0.000000	6	0.000000	1.393698	-0.082634
6	-0.706860	1.224318	0.000000	1	0.000001	-2.475821	-0.113471
6	0.691094	-1.218502	-0.031999	1	0.000000	2.475822	-0.113464
6	-1.400801	0.010746	-0.031999	6	-1.231070	-0.707981	-0.109061
6	0.709706	1.207756	-0.031999	6	1.231072	-0.707980	-0.109050
1	-1.201265	2.186025	-0.062805	6	1.231072	0.707981	-0.109048
1	2.493786	-0.052686	-0.062805	6	-1.231070	0.707981	-0.109059
1	-1.292520	-2.133339	-0.062805	8	-2.442602	-1.304865	-0.125830
8	1.458128	-2.326933	-0.064601	8	2.442605	-1.304865	-0.125810
8	-2.744247	-0.099309	-0.064601	8	2.442604	1.304865	-0.125806
8	1.286119	2.426243	-0.064601	8	-2.442602	1.304866	-0.125827
6	0.796328	-3.576598	-0.288690	6	-2.475032	-2.696645	-0.447001
6	-3.495589	1.098659	-0.288690	6	2.475037	-2.696646	-0.446976
6	2.699261	2.477939	-0.288690	6	2.475038	2.696646	-0.446973
1	0.136910	-3.827619	0.547660	6	-2.475032	2.696647	-0.446995
1	-3.383271	1.795242	0.547660	1	-2.025437	-3.300370	0.348510
1	3.246360	2.032378	0.547660	1	-3.529848	-2.947762	-0.535175
1	0.228251	-3.547575	-1.222024	1	-1.966510	-2.885588	-1.396996
1	-3.186416	1.576116	-1.222024	1	2.025437	-3.300367	0.348535
1	2.958164	1.971459	-1.222024	1	1.966521	-2.885593	-1.396973
1	1.591364	-4.315193	-0.360073	1	3.529853	-2.947762	-0.535142
1	-4.532749	0.779435	-0.360073	1	2.025436	3.300367	0.348537
1	2.941385	3.535758	-0.360073	1	3.529854	2.947763	-0.535137
				1	1.966523	2.885591	-1.396971
				1	-2.025437	3.300368	0.348518
				1	-1.966509	2.885590	-1.396989

	1	-3.529848	2.947763	-0.535169			
<b>N(CH<sub>3</sub>)<sub>2</sub>1</b>				<b>N(CH<sub>3</sub>)<sub>2</sub>2o</b>			
6	0.202417	0.422496	0.000000	11	1.827161	-0.363831	1.770356
6	0.282200	-0.319262	1.213746	6	0.763891	-1.733212	-0.343748
6	0.467575	-1.708123	1.204947	6	1.575533	0.907905	-0.622809
6	0.552377	-2.423131	0.000000	6	-0.211595	-0.719425	-0.192326
6	0.467575	-1.708123	-1.204947	6	0.224715	0.657954	-0.279469
6	0.282200	-0.319262	-1.213746	6	2.101054	-1.452164	-0.671906
7	0.019663	1.785023	0.000000	6	2.504226	-0.123921	-0.837685
1	0.265562	0.191778	2.169020	7	-1.549493	-1.034358	0.052901
1	0.572239	-2.226898	2.154312	7	-0.674416	1.709157	-0.092521
1	0.736286	-3.492650	0.000000	1	0.452456	-2.770691	-0.299392
1	0.572239	-2.226898	-2.154312	1	1.907043	1.933994	-0.736784
1	0.265562	0.191778	-2.169020	1	2.793038	-2.271047	-0.847006
6	0.282200	2.513637	1.239202	1	3.519456	0.117253	-1.139118
6	0.282200	2.513637	-1.239202	6	-1.852435	-2.423848	0.373987
1	1.319857	2.392845	1.577681	6	-2.509731	-0.500082	-0.927373
1	0.089116	3.571277	1.064301	6	-1.357685	1.732881	1.201190
1	-0.392113	2.183297	2.032484	6	-0.242502	3.037989	-0.503742
1	1.319857	2.392845	-1.577681	1	-1.225743	-2.769624	1.200074
1	-0.392113	2.183297	-2.032484	1	-1.723071	-3.101039	-0.484217
1	0.089116	3.571277	-1.064301	1	-2.895473	-2.474159	0.692052
11	-1.954155	-1.368940	0.000000	1	-3.518060	-0.617487	-0.524528
				1	-2.439458	-1.052766	-1.874716
				1	-2.317217	0.555213	-1.113108
				1	-0.669194	2.054727	2.002958
				1	-1.762454	0.747785	1.435503
				1	-2.179341	2.451280	1.159418
				1	-1.109821	3.699942	-0.467252
				1	0.536165	3.459745	0.153167
				1	0.127446	3.010958	-1.530342
<b>N(CH<sub>3</sub>)<sub>2</sub>2m</b>				<b>N(CH<sub>3</sub>)<sub>2</sub>2p</b>			
11	1.395233	1.905678	0.000000	11	0.000000	0.000000	2.088614
6	-0.607130	0.069031	0.000000	6	0.000000	1.455976	-0.298939
6	2.076077	-0.710982	0.000000	6	0.000000	-1.455976	-0.298939
1	-1.659915	0.308124	0.000000	6	1.202119	0.701421	-0.232060
1	3.110722	-1.044916	0.000000	6	-1.202119	-0.701421	-0.232060
6	1.426469	-0.510626	1.221118	6	1.202119	-0.701421	-0.232060
6	1.426469	-0.510626	-1.221118	6	-1.202119	0.701421	-0.232060
1	1.936831	-0.711968	2.153349	7	0.000000	2.825644	-0.463002
1	1.936831	-0.711968	-2.153349	7	0.000000	-2.825644	-0.463002
6	0.050313	-0.138866	-1.238961	1	2.164852	1.200218	-0.235626
6	0.050313	-0.138866	1.238961	1	-2.164852	-1.200218	-0.235626
7	-0.606735	0.056406	-2.436444	1	2.164852	-1.200218	-0.235626

7	-0.606735	0.056406	2.436444	1	-2.164852	1.200218	-0.235626
6	-0.008998	-0.505063	-3.645229	6	1.234956	3.547193	-0.197178
6	-2.066544	0.104085	-2.416940	6	-1.234956	-3.547193	-0.197178
6	-2.066544	0.104085	2.416940	6	-1.234956	3.547193	-0.197178
6	-0.008998	-0.505063	3.645229	6	1.234956	-3.547193	-0.197178
1	0.118775	-1.586127	-3.542434	1	2.034848	3.194071	-0.851003
1	-0.640789	-0.302353	-4.514334	1	-2.034848	-3.194071	-0.851003
1	0.965516	-0.048198	-3.838078	1	1.074674	4.602841	-0.414798
1	-2.413870	0.952288	-1.820693	1	-1.074674	-4.602841	-0.414798
1	-2.458758	0.235867	-3.429064	1	1.564089	3.452123	0.850489
1	-2.474030	-0.818513	-1.994612	1	-1.564089	-3.452123	0.850489
1	-2.474030	-0.818513	1.994612	1	-1.074674	4.602841	-0.414798
1	-2.458758	0.235867	3.429064	1	1.074674	-4.602841	-0.414798
1	-2.413870	0.952288	1.820693	1	-2.034848	3.194071	-0.851003
1	0.965516	-0.048198	3.838078	1	2.034848	-3.194071	-0.851003
1	-0.640789	-0.302353	4.514334	1	-1.564089	3.452123	0.850489
1	0.118775	-1.586127	3.542434	1	1.564089	-3.452123	0.850489
<b>N(CH<sub>3</sub>)<sub>2</sub>3</b>							
11	0.000000	0.000000	2.278942				
6	0.000000	1.410335	-0.012661				
6	1.221386	-0.705167	-0.012661				
6	-1.221386	-0.705167	-0.012661				
6	1.231022	0.710727	-0.037970				
6	-0.000003	-1.421460	-0.037970				
6	-1.231019	0.710733	-0.037970				
1	0.000012	2.486265	-0.082032				
1	2.153163	-1.243143	-0.082032				
1	-2.153175	-1.243122	-0.082032				
7	2.431047	1.403584	-0.026593				
7	0.000016	-2.807140	-0.026593				
7	-2.431063	1.403557	-0.026593				
6	2.407165	2.813311	-0.403455				
6	1.232816	-3.491321	-0.403455				
6	-3.639981	0.678011	-0.403455				
6	3.640099	0.677934	-0.402788				
6	-1.232941	-3.491385	-0.402788				
6	-2.407158	2.813451	-0.402788				
1	1.803556	3.392284	0.299463				
1	2.036026	-3.258067	0.299463				
1	-3.839582	-0.134217	0.299463				
1	3.424537	3.200857	-0.355011				
1	1.059755	-4.566164	-0.355011				
1	-4.484292	1.365308	-0.355011				
1	2.016646	2.966493	-1.419082				
1	1.560735	-3.229713	-1.419082				

1	-3.577381	0.263220	-1.419082	
1	3.577998	0.263054	-1.418413	
1	-1.561188	-3.230164	-1.418413	
1	-2.016810	2.967110	-1.418413	
1	4.484459	1.365144	-0.353937	
1	-1.059980	-4.566227	-0.353937	
1	-3.424479	3.201083	-0.353937	
1	3.839226	-0.134272	0.300285	
1	-2.035896	-3.257731	0.300285	
1	-1.803330	3.392003	0.300285	

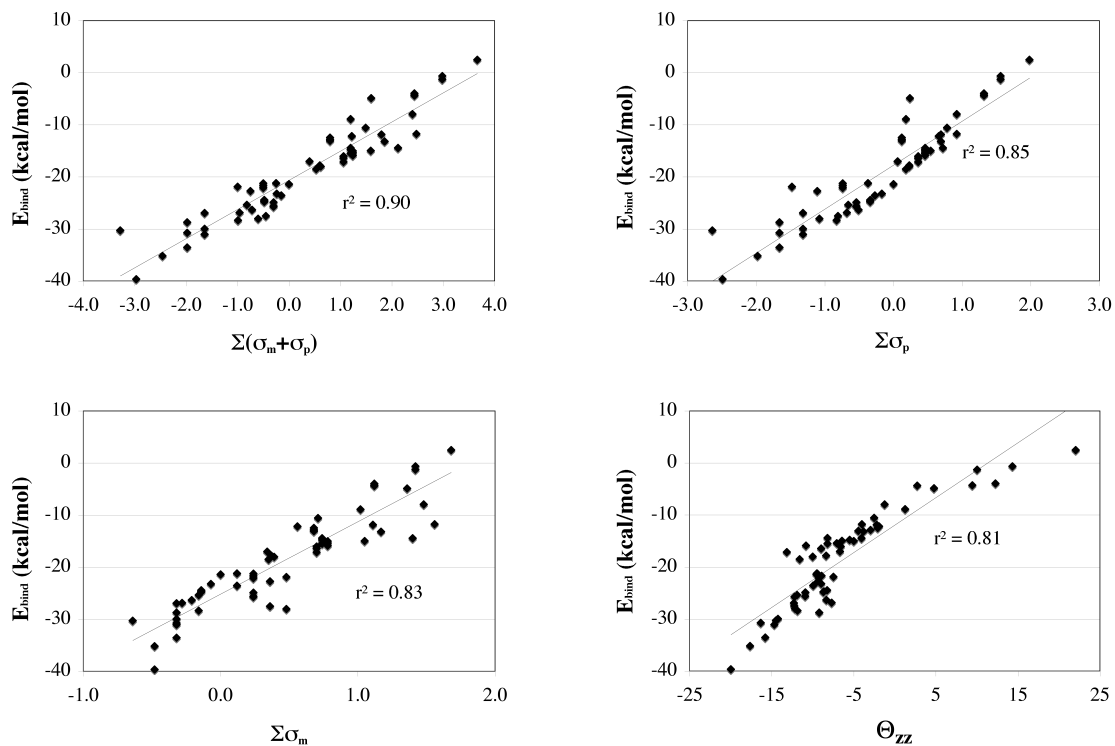


**Table S9.** RHF/6-311++G\*\* Optimized Structures for Na<sup>+</sup>-Substituted Benzene Complexes that Gave Negative Frequencies when Calculated at the MP2(full)/6-311++G\*\* level of theory.

<b>Cl2p</b>				<b>Cl3</b>			
11	0.000000	0.000000	2.228731	11	0.000000	0.000000	2.320319
6	0.000000	1.385930	-0.323333	6	0.000000	-1.378380	-0.276270
6	0.000000	-1.385930	-0.323333	6	-1.193712	0.689190	-0.276270
6	1.204727	0.694760	-0.328600	6	1.193712	0.689190	-0.276270
6	-1.204727	-0.694760	-0.328600	6	0.000000	1.398356	-0.271182
6	1.204727	-0.694760	-0.328600	6	-1.211012	-0.699178	-0.271182
6	-1.204727	0.694760	-0.328600	6	1.211012	-0.699178	-0.271182
17	0.000000	3.115989	-0.332774	17	0.000000	-3.105593	-0.289508
17	0.000000	-3.115989	-0.332774	17	-2.689522	1.552796	-0.289508
1	2.133727	1.233329	-0.358836	17	2.689522	1.552796	-0.289508
1	-2.133727	-1.233329	-0.358836	1	0.000000	2.470995	-0.301480
1	2.133727	-1.233329	-0.358836	1	-2.139945	-1.235498	-0.301480
1	-2.133727	1.233329	-0.358836	1	2.139945	-1.235498	-0.301480
<b>Cl4</b>				<b>Br2o</b>			
11	0.000000	0.000000	2.384436	11	1.840062	-0.000001	2.023975
6	-1.194432	0.688337	-0.244031	6	1.534606	-1.384473	-0.510629
6	1.194432	-0.688337	-0.244031	6	1.534607	1.384472	-0.510629
6	0.000000	1.395643	-0.240529	6	0.339521	-0.697557	-0.293620
6	0.000000	-1.395643	-0.240529	6	0.339522	0.697557	-0.293619
6	1.207550	0.699747	-0.240520	6	2.718609	0.695216	-0.719584
6	-1.207550	-0.699747	-0.240520	6	2.718608	-0.695217	-0.719584
1	-2.124204	1.224154	-0.271518	1	1.523054	-2.458056	-0.536291
1	2.124204	-1.224154	-0.271518	1	1.523055	2.458055	-0.536291
17	-0.060236	3.116837	-0.249801	35	-1.223576	-1.716544	-0.015538
17	0.060236	-3.1168370	-0.249801	35	-1.223575	1.716544	-0.015538
17	2.726976	1.510600	-0.249753	1	3.625342	1.240339	-0.908742
17	-2.726976	-1.510600	-0.249753	1	3.625341	-1.240342	-0.908742
<b>Br2p</b>				<b>Br4</b>			
11	0.000000	0.000000	2.318076	11	0.000000	0.000000	2.456316
6	0.000000	1.388458	-0.226976	6	0.000000	1.376633	-0.153936
6	0.000000	-1.388458	-0.226976	6	0.000000	-1.376633	-0.153936
6	1.204406	0.695125	-0.233852	6	1.212677	0.697338	-0.149428
6	-1.204406	-0.695125	-0.233852	6	-1.212677	-0.697338	-0.149428
6	-1.204406	0.695125	-0.233852	6	1.212677	-0.697338	-0.149428
6	1.204406	-0.695125	-0.233852	6	-1.212677	0.697338	-0.149428
35	0.000000	3.276435	-0.230196	1	0.000000	2.449359	-0.177167
35	0.000000	-3.276435	-0.230196	1	0.000000	-2.449359	-0.177167
1	2.136134	1.228909	-0.262232	35	2.793816	1.720639	-0.151655
1	-2.136134	-1.228909	-0.262232	35	-2.793816	-1.720639	-0.151655
1	-2.136134	1.228909	-0.262232	35	2.793816	-1.720639	-0.151655

1	2.136134	-1.228909	-0.262232	35	-2.793816	1.720639	-0.151655
<b>I2o</b>				<b>I2p</b>			
11	-0.001729	2.103150	2.050685	11	0.000000	0.000000	2.350551
6	1.381098	1.942549	-0.501650	6	0.000000	1.396798	-0.179672
6	-1.382213	1.941684	-0.501546	6	0.000000	-1.396798	-0.179672
6	0.699367	0.737402	-0.302203	53	0.000000	3.505136	-0.172563
6	-0.699668	0.736966	-0.302232	53	0.000000	-3.505136	-0.172563
6	-0.695544	3.130167	-0.689834	6	1.202179	0.695408	-0.189439
6	0.693653	3.130583	-0.689906	6	-1.202179	0.695408	-0.189439
1	2.454566	1.943050	-0.526731	6	-1.202179	-0.695408	-0.189439
1	-2.455686	1.941484	-0.526451	6	1.202179	-0.695408	-0.189439
53	1.886800	-0.988182	-0.017395	1	2.138910	1.220666	-0.215450
53	-1.885999	-0.989466	-0.017668	1	-2.138910	1.220666	-0.215450
1	-1.242265	4.039662	-0.860774	1	-2.138910	-1.220666	-0.215450
1	1.239804	4.040398	-0.860968	1	2.138910	-1.220666	-0.215450
<b>I4</b>				<b>CN2o</b>			
11	0.000000	0.000000	2.463224	11	0.000005	3.581919	0.000000
6	-1.156155	0.737948	-0.116959	6	-0.000003	-1.734467	-1.399969
6	1.156155	-0.737948	-0.116959	6	-0.000003	-1.734467	1.399969
6	0.067388	1.404402	-0.109777	6	-0.000010	-0.545203	-0.703067
6	-0.067388	-1.404402	-0.109777	6	-0.000010	-0.545203	0.703067
6	1.245468	0.652462	-0.109808	6	0.000008	-2.930863	0.690760
6	-1.245468	-0.652462	-0.109808	6	0.000008	-2.930863	-0.690760
1	-2.060012	1.314863	-0.137064	1	-0.000007	-1.733242	-2.473668
1	2.060012	-1.314863	-0.137064	1	-0.000007	-1.733242	2.473668
53	0.000000	3.514675	-0.107359	6	-0.000003	0.741491	-1.352620
53	0.000000	-3.514675	-0.107359	6	-0.000003	0.741491	1.352620
53	3.187926	1.479893	-0.107572	7	0.000003	1.815475	-1.707749
53	-3.187926	-1.479893	-0.107572	7	0.000003	1.815475	1.707749
				1	0.000015	-3.861387	1.227007
				1	0.000015	-3.861387	-1.227007
<b>CN2p</b>							
11	0.000000	0.000000	2.298434				
6	0.000000	1.385202	-0.394983				
6	0.000000	-1.385202	-0.394983				
6	0.000000	2.827681	-0.376276				
6	0.000000	-2.827681	-0.376276				
7	0.000000	3.955669	-0.328211				
7	0.000000	-3.955669	-0.328211				
6	1.210624	0.693082	-0.404152				
6	-1.210624	0.693082	-0.404152				
6	-1.210624	-0.693082	-0.404152				
6	1.210624	-0.693082	-0.404152				

1	2.138164	1.234766	-0.433267				
1	-2.138164	1.234766	-0.433267				
1	-2.138164	-1.234766	-0.433267				
1	2.138164	-1.234766	-0.433267				
<b>NO<sub>2</sub>1</b>							
11	-2.215805	-0.968221	0.000000				
6	0.371676	0.416190	0.000000				
6	0.389335	-2.333361	0.000000				
7	0.375142	1.889869	0.000000				
1	0.422905	-3.408138	0.000000				
6	0.386656	-0.251735	1.214707				
6	0.386656	-0.251735	-1.214707				
1	0.416307	0.304297	2.131742				
1	0.416307	0.304297	-2.131742				
6	0.386656	-1.641220	-1.207443				
6	0.386656	-1.641220	1.207443				
1	0.424184	-2.177329	-2.138066				
1	0.424184	-2.177329	2.138066				
8	0.362386	2.424627	1.055316				
8	0.362386	2.424627	-1.055316				
<b>NO<sub>2</sub>2m</b>				<b>NO<sub>2</sub>2p</b>			
11	4.510362	-0.918389	0.005808	11	0.000000	0.000000	2.466789
6	-0.471501	-0.448011	-0.001471	6	0.378292	1.301143	-0.334563
6	-1.005465	2.301146	0.001390	6	-0.378292	-1.301143	-0.334563
1	-0.274843	-1.500158	-0.002666	6	1.361691	0.327038	-0.358870
1	-1.218076	3.352854	0.002402	6	-1.361691	-0.327038	-0.358870
6	-2.047691	1.384788	0.001686	6	0.974530	-1.005371	-0.338149
6	0.302310	1.862926	-0.000287	6	-0.974530	1.005371	-0.338149
1	-3.070198	1.708639	0.003011	7	0.787848	2.714348	-0.305213
1	1.118536	2.557913	-0.000620	7	-0.787848	-2.714348	-0.305213
6	0.540916	0.494326	-0.001509	1	2.397090	0.605254	-0.406416
6	-1.760802	0.031429	0.000273	1	-2.397090	-0.605254	-0.406416
7	1.905722	0.024707	-0.003437	1	1.700322	-1.795492	-0.349203
7	-2.863606	-0.938371	0.000570	1	-1.700322	1.795492	-0.349203
8	2.803212	0.817587	-0.002947	8	1.868612	2.967108	-0.703733
8	2.124366	-1.153254	-0.004250	8	-1.868612	-2.967108	-0.703733
8	-2.567407	-2.085771	-0.000277	8	0.000000	3.479264	0.143016
8	-3.961523	-0.501180	0.001669	8	0.000000	-3.479264	0.143016



**Figure S1.** Correlation between cation- $\pi$  binding energies ( $E_{\text{bind}}$ ) and either (a)  $\Sigma(\sigma_m + \sigma_p)$ , (b)  $\Sigma\sigma_p$ , (c)  $\Sigma\sigma_m$ , or (d)  $\Theta_{zz}$ , for the substituted benzenes in Table 1 of the manuscript.