

## **SUPPLEMENTARY MATERIAL**

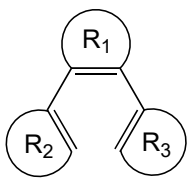
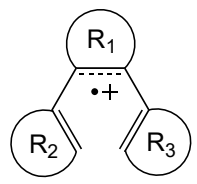
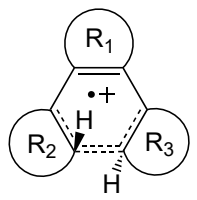
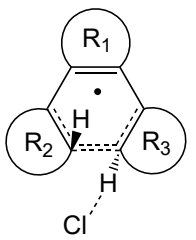
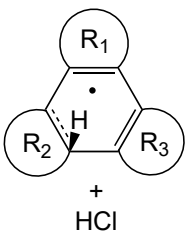
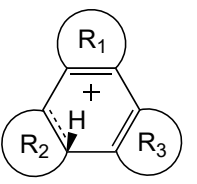
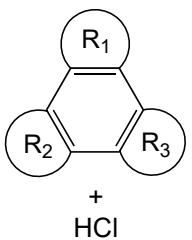
### **Beyond the Woodward-Hoffman rules: what controls reactivity in eliminative aromatic ring-forming reactions?**

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Detailed mechanism for Scholl reaction

(S <sub>1</sub> ) 	$- e^-$ →	(S <sub>2</sub> ) 	via TS (S <sub>3</sub> ) →	(S <sub>4</sub> ) 	$+ Cl^-$ →	(S <sub>5</sub> ) 	via TS (S <sub>6</sub> ) →	(S <sub>7</sub> ) 	$- e^-$ →	(S <sub>8</sub> ) 	$+ Cl^-$ →	(S <sub>9</sub> ) 
$[Fe(III)Cl_3(H_2O)_3] + H_2O$	$+ e^-$ →	$[Fe(II)Cl_3(H_2O)_3]^- + H_2O$		$[Fe(II)Cl_3(H_2O)_3]^- + H_2O$	$- Cl^-$ →	$[Fe(II)Cl_2(H_2O)_4]$		$[Fe(II)Cl_2(H_2O)_4]$		$[Fe(II)Cl_2(H_2O)_4]$		$[Fe(II)Cl_2(H_2O)_4]$
$[Fe(III)Cl_3(H_2O)_3] + H_2O$		$[Fe(III)Cl_3(H_2O)_3] + H_2O$		$[Fe(III)Cl_3(H_2O)_3] + H_2O$		$[Fe(III)Cl_3(H_2O)_3] + H_2O$		$[Fe(III)Cl_3(H_2O)_3] + H_2O$	$+ e^-$ →	$[Fe(II)Cl_3(H_2O)_3]^- + H_2O$	$- Cl^-$ →	$[Fe(II)Cl_2(H_2O)_4]$

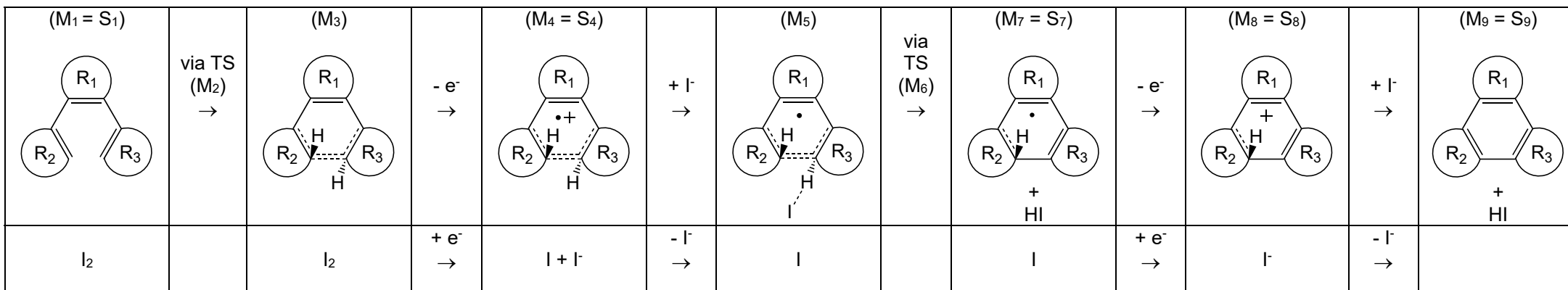
F<sub>1</sub>:  $[Fe(III)Cl_3(H_2O)_3]$

F<sub>2</sub>:  $[Fe(II)Cl_3(H_2O)_3]^-$

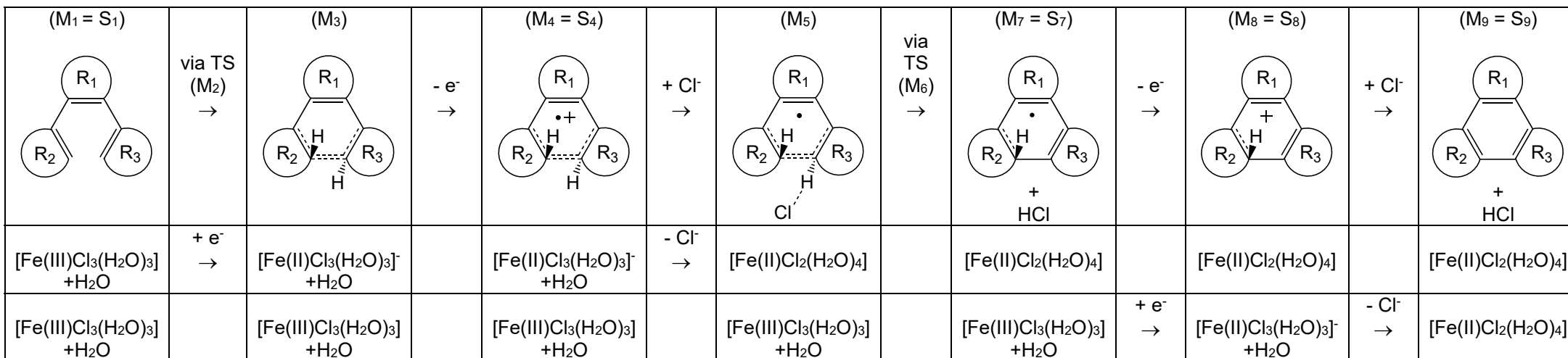
F<sub>3</sub>:  $[Fe(II)Cl_2(H_2O)_4]$

Small molecules: H<sub>2</sub>O, HCl

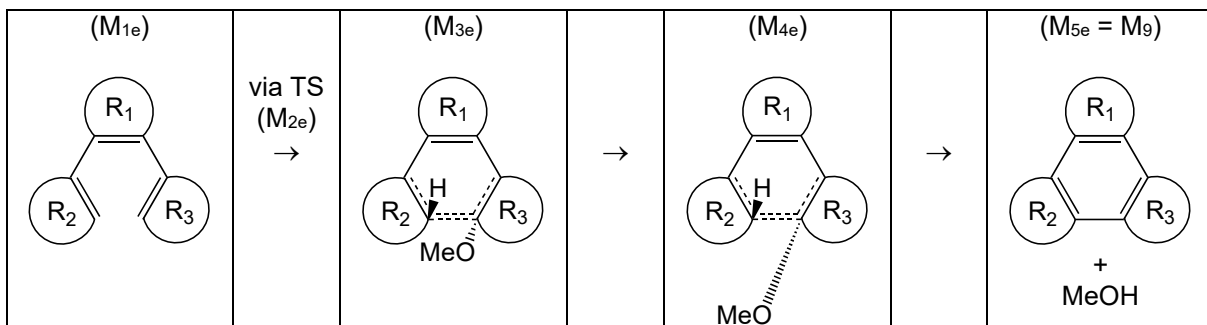
Detailed mechanism for Mallory reaction (oxidative pathway)



Computed mechanism for Mallory reaction (oxidative pathway) – Fe(III)Cl<sub>3</sub>(H<sub>2</sub>O)<sub>3</sub> used as oxidant to optimize cancellation of solvation model errors



### Detailed mechanism for Mallory reaction (eliminative pathway)



Small molecules: MeOH

# Geometries, energies and thermochemical data for reaction pathway minima, transition states and intermediates

Common reactants, redox species

Energies & thermochemical data:

Compound	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
[FeCl3(H2O)3]	-1732.641787	49.987	9.338	-34.7058526	-0.03890442
[FeCl3(H2O)3]-	-1732.738749	49.601	8.982	-35.00907115	-0.11881448
[FeCl2(H2O)4]	-1348.858737	64.27	10.411	-37.35849315	-0.04264669
HCL	-460.7997862	4.273	2.074	-13.2992789	-0.006443977
H2O	-76.4188287	13.411	2.371	-13.4513354	-0.010888571

S<sub>1</sub>

Energies & thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-540.7210023	135.187	7.524	-31.68589125	-0.006222913
pyrrole	phenyl	-672.2832085	153.689	8.791	-34.27919995	-0.033129726
thiophene	phenyl	-1015.078583	143.59	8.95	-34.8435979	-0.063181801
benzene	phenyl	-694.3760609	164.632	9.135	-35.0242768	-0.010489987
benzene	3-pyridine	-726.4291731	149.907	8.992	-34.84151085	-0.031780496
benzene	2-thiophene	-1335.883339	122.473	8.775	-34.29649265	-0.007340811
benzene	2-pyrrole	-649.9825591	142.531	8.421	-33.2884475	-0.254414051
benzene	3-pyridine	-726.4291731	149.907	8.992	-34.84151085	-0.031780496
benzene	3-thiophene	-1335.882225	122.246	8.809	-34.686771	-0.007871462
benzene	3-pyrrole	-650.2184884	142.34	8.522	-33.7225539	-0.015690785
benzene	phenyl/2-methoxyphenyl	-808.9016287	185.113	10.8	-39.10326695	-0.01014625

S<sub>2</sub>

Energies & thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-540.4607245	135.382	7.542	-31.38893385	-0.062665404
pyrrole	phenyl	-672.045994	152.475	8.534	-33.3099143	-0.069288739
thiophene	phenyl	-1014.864398	143.148	9.032	-34.8519461	-0.060290762
benzene	phenyl	-694.1140343	164.863	9.125	-34.633104	-0.059109131
benzene	3-pyridine	-726.1503721	149.687	9.034	-34.5126514	-0.08703688
benzene	2-thiophene	-1335.62935	122.597	8.694	-33.59882165	-0.061049978
benzene	2-pyrrole	-649.9918036	142.927	8.323	-32.4613794	-0.067792689
benzene	3-pyridine	-726.1503721	149.687	9.034	-34.5126514	-0.08703688
benzene	3-thiophene	-1335.624801	122.51	8.657	-33.54694355	-0.062601505
benzene	3-pyrrole	-649.9881672	143.001	8.293	-32.32572115	-0.068102815
benzene	phenyl/2-methoxyphenyl	-808.6456339	185.318	10.792	-38.4213979	-0.05833202

S<sub>3</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-540.4077051	133.608	7.121	-29.8549521	-0.064645218
pyrrole	phenyl	-672.0028293	153.318	7.902	-31.3439132	-0.06438645
thiophene	phenyl	-1014.829416	143.332	8.264	-32.4542238	-0.062801788
benzene	phenyl	-694.0531455	164.564	8.274	-32.21898345	-0.07565697
benzene	3-pyridine	-726.1107284	149.606	8.364	-32.65905285	-0.089256095
benzene	2-thiophene	-1335.591498	122.472	8.072	-31.830494	-0.063365324
benzene	2-pyrrole	-649.9524916	142.771	7.614	-30.43366125	-0.069182036
benzene	3-pyridine	-726.1107284	149.606	8.364	-32.65905285	-0.089256095
benzene	3-thiophene	-1335.610964	122.532	8.058	-31.78308815	-0.064292881
benzene	3-pyrrole	-649.9698156	142.86	7.631	-30.42412045	-0.070880307
benzene	phenyl/2-methoxyphenyl	-808.6003239	185.094	10.072	-36.2353621	-0.06009548

S<sub>4</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-540.4330416	135.432	6.999	-29.0481582	-0.064437704
pyrrole	phenyl	-671.9968008	153.471	8.337	-32.59524875	-0.076851873
thiophene	phenyl	-1014.809171	143.188	8.563	-33.28278265	-0.078081109
benzene	phenyl	-694.0566796	164.794	8.776	-33.7487911	-0.082231703
benzene	3-pyridine	-726.110944	149.461	8.696	-33.8913068	-0.091367151
benzene	2-thiophene	-1335.612718	123.175	8.264	-32.16114235	-0.063411291
benzene	2-pyrrole	-649.9457262	143.396	7.789	-30.6134457	-0.094194583
benzene	3-pyridine	-726.110944	149.461	8.696	-33.8913068	-0.091367151
benzene	3-thiophene	-1335.624057	123.742	8.179	-32.0582806	-0.077040553
benzene	3-pyrrole	-649.953649	143.663	7.769	-30.58154365	-0.098755949
benzene	phenyl/2-methoxyphenyl	-808.6018609	185.286	10.379	-37.256824	-0.05928582

S<sub>5</sub>=S<sub>6</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-1000.839361	132.516	7.922	-32.22912055	-0.025624889
pyrrole	phenyl	-1132.40018	151.904	9.255	-35.16351285	-0.036438373
thiophene	phenyl	-1475.236956	140.636	9.277	-35.15218315	-0.022423046
benzene	phenyl	-1154.468756	163.128	9.703	-36.08897045	-0.032435024
benzene	3-pyridine	-1186.512179	146.827	9.302	-35.169774	-0.063011468
benzene	2-thiophene	-1796.009139	119.908	9.204	-35.4393016	-0.022958386
benzene	2-pyrrole	-1110.358426	139.336	8.964	-34.2562424	-0.030096307
benzene	3-pyridine	-1186.512179	146.827	9.302	-35.169774	-0.063011468
benzene	3-thiophene	-1796.026784	120.146	9.25	-35.4691166	-0.026091699
benzene	3-pyrrole	-1110.369466	140.02	8.901	-34.32034465	-0.034886653
benzene	phenyl/2-methoxyphenyl	-1268.994954	183.344	11.218	-39.5245529	-0.02931753

S<sub>7</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-1000.876749	132.536	9.014	-36.1220651	-0.008995311
pyrrole	phenyl	-1132.44545	151.207	10.34	-38.9729754	-0.015051395
thiophene	phenyl	-1475.2751	141.308	10.468	-39.4207967	-0.010762293
benzene	phenyl	-1154.524429	162.584	10.591	-39.05138885	-0.010564946
benzene	3-pyridine	-1186.573451	148.003	9.965	-37.6014854	-0.052802241
benzene	2-thiophene	-1796.037352	120.394	10.356	-38.8578895	-0.011221123
benzene	2-pyrrole	-1110.375878	140.531	9.729	-36.93512015	-0.016911855
benzene	3-pyridine	-1186.573451	148.003	9.965	-37.6014854	-0.052802241
benzene	3-thiophene	-1796.049448	120.567	10.376	-39.12234855	-0.011560372
benzene	3-pyrrole	-1110.382154	140.636	9.764	-36.9318405	-0.018220966
benzene	phenyl/2-methoxyphenyl	-1269.043731	183.055	12.198	-42.58744785	-0.01192554

S<sub>8</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-539.8273506	128.807	6.781	-28.986143	-0.10888675
pyrrole	phenyl	-671.4469804	147.688	8.031	-31.925902	-0.075976981
thiophene	phenyl	-1014.265753	137.261	8.267	-32.66441955	-0.072216431
benzene	phenyl	-693.4892257	158.534	8.487	-33.0374052	-0.095338482
benzene	3-pyridine	-725.5528965	143.128	8.383	-32.91784705	-0.093608564
benzene	2-thiophene	-1335.041975	116.308	8.023	-32.0517213	-0.064585008
benzene	2-pyrrole	-649.3927529	136.892	7.56	-30.64117365	-0.082010725
benzene	3-pyridine	-725.5528965	143.128	8.383	-32.91784705	-0.093608564
benzene	3-thiophene	-1335.049329	116.816	7.999	-32.0892882	-0.065906014
benzene	3-pyrrole	-649.3925838	137.064	7.623	-30.79442275	-0.082873261
benzene	phenyl/2-methoxyphenyl	-808.038175	178.956	10.098	-36.55289185	-0.06763671

S<sub>9</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol (Hartree)
ethene	phenyl	-539.5545665	122.099	6.517	-28.3755318	-0.006467846
pyrrole	phenyl	-671.1214265	140.498	7.87	-31.42530815	-0.013200534
thiophene	phenyl	-1013.951808	130.449	8.056	-32.12476805	-0.008354125
benzene	phenyl	-693.2002024	151.342	8.363	-33.0719906	-0.00813524
benzene	3-pyridine	-725.2483137	136.621	8.104	-32.34003235	-0.036781617
benzene	2-thiophene	-1334.717814	109.551	7.834	-31.5615627	-0.007858693
benzene	2-pyrrole	-649.0517601	129.262	7.567	-30.4923968	-0.016106302
benzene	3-pyridine	-725.2483137	136.621	8.104	-32.34003235	-0.036781617
benzene	3-thiophene	-1334.716315	109.538	7.846	-31.60717965	-0.008068084
benzene	3-pyrrole	-649.0483365	129.081	7.681	-30.7297242	-0.018239623
benzene	phenyl/2-methoxyphenyl	-807.6653005	172.019	9.997	-37.1846717	-0.06173623

M<sub>1</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_G (Hartree)
ethene	phenyl	-540.5630382	-540.7210023	135.187	7.524	-31.68589125	-0.009825297	-0.006222913
pyrrole	phenyl	-672.1283483	-672.2832085	153.689	8.791	-34.27919995	-0.01489319	-0.033129726
thiophene	phenyl	-1014.959443	-1015.078583	143.59	8.95	-34.8435979	-0.00772539	-0.063181801
benzene	phenyl	-694.2058859	-694.3760609	164.632	9.135	-35.0242768	-0.00870518	-0.010489987
benzene	3-pyridine	-726.2799348	-726.4291731	149.907	8.992	-34.84151085	-0.012468044	-0.031780516
benzene	2-thiophene	-1335.733701	-1335.883339	122.473	8.775	-34.29649265	-0.00915008	-0.007340811
benzene	2-pyrrole	-650.0792488	-649.9825591	142.531	8.421	-33.2884475	-0.01496667	-0.254414051
benzene	3-pyridine	-726.2799348	-726.4291731	149.907	8.992	-34.84151085	-0.012468044	-0.031780516
benzene	3-thiophene	-1335.719251	-1335.882225	122.246	8.809	-34.686771	-0.0087605	-0.007871462
benzene	3-pyrrole	-650.0576134	-649.9779604	142.343	8.521	-33.72642985	-0.02041668	-0.256199654
benzene	phenyl/2- methoxyphenyl	-808.7321264	-808.9016287	185.113	10.8	-39.10326695	-0.012699139	-0.010149093

M<sub>2</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_G (Hartree)
ethene	phenyl	-540.56072	-540.6143142	134.308	6.942	-29.04130075	-0.00699632	-0.01164231
pyrrole	phenyl	-	-	-	-	-	-	-
thiophene	phenyl	-	-	-	-	-	-	-
benzene	phenyl	-	-	-	-	-	-	-
benzene	3-pyridine	-726.2780277	-726.3373576	149.457	8.334	-32.73001255	-0.016317177	-0.033662885
benzene	2-thiophene	-1335.720849	-1335.7847	121.949	8.135	-32.23150575	-0.0096105	-0.007677989
benzene	2-pyrrole	-	-	-	-	-	-	-
benzene	3-pyridine	-726.2780277	-726.3373576	149.457	8.334	-32.73001255	-0.016317177	-0.033662885
benzene	3-thiophene	-1335.747696	-1335.813966	121.859	8.153	-32.0785548	-0.01101825	-0.007639963
benzene	3-pyrrole	-	-	-	-	-	-	-
benzene	phenyl/2- methoxyphenyl	-	-	-	-	-	-	-



M<sub>3</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_G (Hartree)
ethene	phenyl	-540.558798	-540.6578209	134.785	7.074	-29.70080855	-0.00969612	-0.005826782
pyrrole	phenyl	-672.1158017	-672.1928594	152.417	8.372	-32.456609	-0.02199998	-0.012801238
thiophene	phenyl	-1014.944966	-1015.018655	142.165	8.59	-33.21957485	-0.01512718	-0.007524966
benzene	phenyl	-694.1977628	-694.282947	164.027	8.807	-33.73120025	-0.01339075	-0.007482271
benzene	3-pyridine	-726.2708269	-726.3386618	149.37	8.597	-33.2753289	-0.020435601	-0.034882262
benzene	2-thiophene	-1335.733579	-1335.826769	122.582	8.374	-32.33228045	-0.01220785	-0.008460893
benzene	2-pyrrole	-650.0663899	-650.1513359	141.876	8.053	-31.04725395	-0.01763243	-0.013651042
benzene	3-pyridine	-726.2708269	-726.3386618	149.37	8.597	-33.2753289	-0.020435601	-0.034882262
benzene	3-thiophene	-1335.760321	-1335.84832	123.022	8.278	-32.2079519	-0.01348783	-0.008921109
benzene	3-pyrrole	-650.0694087	-650.158884	142.207	7.95	-31.3379502	-0.01955899	-0.012663841
benzene	phenyl/2-methoxyphenyl	-808.7163664	-808.7051832	184.605	10.394	-37.22372935	-0.014605255	-0.106791514

M<sub>4</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_G (Hartree)
ethene	phenyl	-540.3825427	-540.4330424	135.431	7	-29.04845635	-0.065062568	-0.064439138
pyrrole	phenyl	-671.962611	-672.0049572	153.469	8.338	-32.5949506	-0.068745184	-0.068764161
thiophene	phenyl	-1014.782757	-1014.820521	143.189	8.564	-33.2872549	-0.066544802	-0.06673107
benzene	phenyl	-694.0292552	-694.0566796	164.794	8.776	-33.7487911	-0.06374212	-0.082231703
benzene	3-pyridine	-726.0906785	-726.110944	149.461	8.696	-33.8913068	-0.071693622	-0.091367281
benzene	2-thiophene	-1335.544469	-1335.612718	123.177	8.264	-32.1626331	-0.064749294	-0.063432807
benzene	2-pyrrole	-649.9050798	-649.9703343	143.394	7.79	-30.614042	-0.071527153	-0.069596639
benzene	3-pyridine	-726.0906785	-726.110944	149.461	8.696	-33.8913068	-0.071693622	-0.091367281
benzene	3-thiophene	-1335.575165	-1335.636226	123.741	8.179	-32.0582806	-0.066922445	-0.064864903
benzene	3-pyrrole	-649.9247249	-649.9826145	143.661	7.769	-30.58094735	-0.072232918	-0.069811544
benzene	phenyl/2-methoxyphenyl	-808.5693877	-808.6018609	185.286	10.379	-37.256824	-0.060974154	-0.059355449

M<sub>5</sub>=M<sub>6</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_G (Hartree)
ethene	phenyl	-1000.78806	-1000.839361	132.516	7.922	-32.22912055	-0.026670742	-0.025624889
pyrrole	phenyl	-1132.368325	-1132.40018	151.904	9.255	-35.16351285	-0.039428648	-0.036438373
thiophene	phenyl	-1475.185839	-1475.236956	140.636	9.277	-35.15218315	-0.024476093	-0.022423046
benzene	phenyl	-1154.438821	-1154.468756	163.128	9.703	-36.08897045	-0.034010137	-0.032435024
benzene	3-pyridine	-1186.476436	-1186.512179	146.827	9.302	-35.169774	-0.04194948	-0.063011468
benzene	2-thiophene	-1795.955462	-1796.009139	119.908	9.204	-35.4393016	-0.024782256	-0.022958386
benzene	2-pyrrole	-1110.300054	-1110.358426	139.336	8.964	-34.2562424	-0.032299832	-0.030096307
benzene	3-pyridine	-1186.476436	-1186.512179	146.827	9.302	-35.169774	-0.04194948	-0.063011468
benzene	3-thiophene	-1795.982273	-1796.026784	120.146	9.25	-35.4691166	-0.027477662	-0.026091699
benzene	3-pyrrole	-1110.322539	-1110.369466	140.02	8.901	-34.32034465	-0.038440439	-0.034886653
benzene	phenyl/2-methoxyphenyl	-1268.957213	-1268.994954	183.344	11.218	-39.5245529	-0.032036083	-0.02931753

M<sub>7</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_X (Hartree)
ethene	phenyl	-1000.79817	-1000.876749	132.536	9.014	-36.1220651	-0.009183712	-0.008995311
pyrrole	phenyl	-1132.353944	-1132.44545	151.207	10.34	-38.9729754	-0.015518894	-0.015051395
thiophene	phenyl	-1475.187142	-1475.2751	141.308	10.468	-39.4207967	-0.010850388	-0.010762293
benzene	phenyl	-1154.436471	-1154.524429	162.584	10.591	-39.05138885	-0.0104366	-0.010564946
benzene	3-pyridine	-1186.522043	-1186.573451	148.003	9.965	-37.6014854	-0.014371403	-0.052802401
benzene	2-thiophene	-1795.95585	-1796.037352	120.394	10.356	-38.8578895	-0.011302854	-0.011221123
benzene	2-pyrrole	-1110.293668	-1110.375878	140.531	9.729	-36.93512015	-0.017302715	-0.016911855
benzene	3-pyridine	-1186.522043	-1186.573451	148.003	9.965	-37.6014854	-0.014371403	-0.052802401
benzene	3-thiophene	-1795.963565	-1796.049448	120.567	10.376	-39.12234855	-0.011419743	-0.011560372
benzene	3-pyrrole	-1110.289261	-1110.382154	140.636	9.764	-36.9318405	-0.019320571	-0.018220966
benzene	phenyl/2-methoxyphenyl	-1268.955854	-1269.043731	183.055	12.198	-42.58744785	-0.011865153	-0.01192554

M<sub>8</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol (Hartree)
ethene	phenyl	-539.7622939	-539.8273811	128.807	6.781	-28.986143	-0.066198452	-0.108856224
pyrrole	phenyl	-671.3782944	-671.4469804	147.688	8.031	-31.925902	-0.06139385	-0.075976981
thiophene	phenyl	-1014.200703	-1014.265753	137.261	8.267	-32.66441955	-0.05705109	-0.072216431
benzene	phenyl	-693.4387426	-693.4892257	158.534	8.487	-33.0374052	-0.058117368	-0.095338482
benzene	3-pyridine	-725.5022572	-725.5528965	143.128	8.383	-32.91784705	-0.058709591	-0.093608564
benzene	2-thiophene	-1334.952103	-1335.041975	116.308	8.023	-32.0517213	-0.06358869	-0.064585008
benzene	2-pyrrole	-649.3114406	-649.3927529	136.892	7.56	-30.64117365	-0.06850342	-0.082010725
benzene	3-pyridine	-725.5022572	-725.5528965	143.128	8.383	-32.91784705	-0.058709591	-0.093608564
benzene	3-thiophene	-1334.971126	-1335.049329	116.816	7.999	-32.0892882	-0.06171559	-0.065904164
benzene	3-pyrrole	-649.3232056	-649.3925838	137.064	7.623	-30.79442275	-0.0677067	-0.082873261
benzene	phenyl/2- methoxyphenyl	-807.9625478	-808.0399689	179.108	10.104	-36.6158015	-0.055308356	-0.06719489

M<sub>9</sub>

## Energies &amp; thermochemical data:

R1	R2=R3	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_G (Hartree)
ethene	phenyl	-539.4061658	-539.5545665	122.099	6.517	-28.3755318	-0.006270942	-0.006467846
pyrrole	phenyl	-670.9758164	-671.1214265	140.498	7.87	-31.42530815	-0.01796811	-0.013200534
thiophene	phenyl	-1013.800507	-1013.951808	130.449	8.056	-32.12476805	-0.00968114	-0.008354125
benzene	phenyl	-693.0522621	-693.2002024	151.342	8.363	-33.0719906	-0.00782665	-0.00813524
benzene	3-pyridine	-725.1230569	-725.2483137	136.621	8.104	-32.34003235	-0.011854589	-0.036781507
benzene	2-thiophene	-1334.576175	-1334.717814	109.551	7.834	-31.5615627	-0.00795307	-0.007858693
benzene	2-pyrrole	-648.9079798	-649.0517601	129.262	7.567	-30.4923968	-0.01509626	-0.016106302
benzene	3-pyridine	-725.1230569	-725.2483137	136.621	8.104	-32.34003235	-0.011854589	-0.036781507
benzene	3-thiophene	-1334.567945	-1334.716315	109.538	7.846	-31.60717965	-0.01019549	-0.008068084
benzene	3-pyrrole	-648.8953924	-649.0483365	129.081	7.681	-30.7297242	-0.02322568	-0.018239623
benzene	phenyl/2- methoxyphenyl	-807.5726194	-807.7173566	172.026	10.013	-37.5382776	-0.010024728	-0.009754335

Energies & thermochemical data for 1-(2-methoxyphenyl)-2-phenylbenzene:

Geometry	E_X (Hartree)	E_G (Hartree)	ZPVE (kcal/mol)	H (kcal/mol)	-TS (kcal/mol)	Gsol_X (Hartree)	Gsol_G (Hartree)
M <sub>1e</sub>	-808.7377264	-808.9021119	185.129	10.736	-38.4273609	-0.011370762	-0.00972967
M <sub>2e</sub>	-808.7202076	-808.7832959	183.873	10.02	-35.9580826	-0.012359474	-0.009604674
M <sub>3e</sub>	-808.7170554	-808.7043539	183.857	10.579	-37.6891415	-0.01569891	-0.103429943
M <sub>4e</sub>	-808.7104584	-808.7799225	182.572	10.505	-37.232972	-0.017348284	-0.01397875
M <sub>5e</sub>	-808.7804884	-808.9281102	184.22	11.186	-41.41154425	-0.011987689	-0.012433589

Ground state coordinates for: [FeCl3(H2O)3]

Fe	0.0000003157	-0.0171307376	0.0669921556
Cl	2.2825762222	0.4144574717	-0.0416216307
Cl	-2.2825743707	0.4144570636	-0.0416702918
Cl	-0.0000012572	-2.2453417827	0.2264896814
O	-0.0000212781	0.5003222825	2.1187726330
H	-0.7906485599	0.9820987028	2.4037212470
O	0.0000168264	-0.1794784567	-2.1086568919
H	-0.7800495393	-0.6928278966	-2.3727795837
O	0.0000023642	2.1986997701	-0.3275051435
H	-0.7900919977	2.4507076046	-0.8284474169
H	0.7800779606	-0.6928399714	-2.3727712548
H	0.7900950642	2.4507061714	-0.8284510256
H	0.7906030406	0.9820950154	2.4037357369

Ground state coordinates for: [FeCl3(H2O)3]-

Fe	0.6149960487	-0.2138430453	0.1221448857
Cl	2.6099507986	1.1770338049	0.3485304950
Cl	-2.3587034179	1.5051653373	-2.3061049471
Cl	0.5319000238	-2.5006750468	0.4652180066
O	0.3330165487	0.4564762841	2.2472657219
H	-0.2018063136	1.2210194721	1.9728766213
O	-0.1361842466	-0.4669658786	-1.8190630298
H	-0.8994274915	0.1109055923	-2.1168881771
O	-0.4253982347	1.7265065010	-0.0201121712
H	-1.1631472590	1.7725421643	-0.6978272684
H	-0.3935268037	-1.3924971484	-1.9308936583
H	0.2567433385	2.3503439024	-0.3128892258
H	1.2315717996	0.8199132977	2.3455509622

Ground state coordinates for: [FeCl2(H2O)4]

Fe	0.2066814611	0.0707652904	0.0690031427
Cl	2.5625277152	-0.1697152077	-0.0433763368
Cl	-2.0730355175	-0.5884088269	0.0953304062
O	0.2788865810	1.7520862235	-1.3406121579
H	1.1258831656	2.2076486772	-1.2282147952
H	0.3388541891	1.2810133742	-2.1865815566
O	0.1174117026	-0.8850189553	-2.0272059084
H	0.7850462595	-1.5649862984	-2.1900784624
H	-0.7541449084	-1.3129876491	-2.0163383678
O	-0.1367488283	1.4358642271	1.7518573138
H	-0.1077055034	0.8230048390	2.5031668913
H	-1.0483656779	1.7588091310	1.7055065537
O	0.4828002291	-1.2181695175	1.9565548655
H	-0.0639192370	-2.0152995614	1.9773761376
H	1.4121483693	-1.4903457458	1.8870022740

Ground state coordinates for: HCL

Cl	0.0000000000	0.0000000000	-0.0525386768
H	0.0000000000	0.0000000000	1.2347608990

Ground state coordinates for: H2O

O	0.0000008238	-0.1359439512	0.0000000000
H	-0.7593010324	0.4600006855	0.0000000000
H	0.7593101558	0.4599911720	0.0000000000

R1 : ethene, R2=R3 : phenyl

Ground state coordinates for: S1

C	0.6750754351	-1.8256233399	0.0032886232
C	-0.6739466582	-1.8266179586	-0.0016285411
C	1.6441364221	-0.7154551852	-0.0647892327

C	-1.6440242762	-0.7170591837	0.0651216168
H	1.1435797173	-2.8086107811	0.0475173777
H	-1.1411810750	-2.8102681482	-0.0444408094
C	1.4168276168	0.4595513630	-0.8047296873
C	2.8900202198	-0.8658686198	0.5702495773
C	2.3895623148	1.4533443306	-0.8801766263
C	3.6124373477	1.2989173275	-0.2223298059
C	3.8596988126	0.1326318583	0.5029354808
H	2.1958715678	2.3495768589	-1.4629751056
H	4.3687128843	2.0759938693	-0.2843883363
H	4.8104735343	-0.0033667748	1.0104848809
C	-2.8864416964	-0.8646916987	-0.5771484385
C	-1.4204207027	0.4545780363	0.8114268045
C	-2.3935178167	1.4480887029	0.8863843707
C	-3.6129758804	1.2965260066	0.2215895939
C	-3.8564363790	0.1335705163	-0.5102905533
H	-3.0853370577	-1.7733092809	-1.1399703239
H	-4.8045511229	-0.0000441634	-1.0234286201
H	-2.2028387238	2.3417230075	1.4741445047
H	-4.3696428336	2.0732489408	0.2833276720
H	-0.4838471194	0.5762480593	1.3445654830
H	0.4777619946	0.5837547732	-1.3328105489
H	3.0918403398	-1.7770536546	1.1278599502

Ground state coordinates for: S2

C	0.6919173244	-1.7235144380	0.0875088739
C	-0.6919897315	-1.7235174271	-0.0876134723
C	1.6642237522	-0.6818987326	-0.0124516168
C	-1.6642669913	-0.6818844983	0.0123881856
H	1.1118262026	-2.7089825859	0.2867302625
H	-1.1119045747	-2.7089863652	-0.2868108230
C	1.4385114969	0.5532767110	-0.6903159936
C	2.9647320075	-0.9407294145	0.5126978088
C	2.4503228215	1.4904076486	-0.7879226201
C	3.7084273633	1.2315857022	-0.2184215448
C	3.9622591672	0.0132033821	0.4318947288
H	2.2805271843	2.4192818051	-1.3219631902
H	4.4979199897	1.9721307914	-0.3008681403
H	4.9406765994	-0.1824115942	0.8570457531
C	-2.9648538159	-0.9407205456	-0.5125663770
C	-1.4384030166	0.5533337525	0.6901159998
C	-2.4501760762	1.4904930415	0.7878148251
C	-3.7083798697	1.2316501219	0.2185368794
C	-3.9623451283	0.0132391881	-0.4316758752
H	-3.1556585136	-1.8910731947	-1.0018965119
H	-4.9408304970	-0.1823718976	-0.8566713144
H	-2.2802730236	2.4194188285	1.3217351067
H	-4.4978416293	1.9722161748	0.3010736569
H	-0.4852715245	0.7361697908	1.1716057223
H	0.4854923785	0.7361154644	-1.1720264753
H	3.1554615868	-1.8910541671	1.0021071435

Ground state coordinates for: S3

C	0.6716449624	-2.1739923320	-0.0827457015
C	-0.6716515527	-2.1739917458	0.0827436139
C	1.4244850292	-0.9261541956	-0.1562473209
C	-1.4244884349	-0.9261522497	0.1562469661
H	1.2209208689	-3.1102236775	-0.1190247194
H	-1.2209292582	-3.1102220757	0.1190211667
C	0.6764069825	0.3104147954	-0.5072916300
C	2.7464445382	-0.8554085761	0.2377560214
C	1.4513558807	1.5507073128	-0.4604990761
C	2.7641678871	1.5757942497	-0.0477582014
C	3.4204373314	0.3805442792	0.3004759340
H	0.9690929620	2.4672028277	-0.7860757568
H	3.3089609262	2.5139713648	-0.0271112583
H	4.4581942586	0.4076544364	0.6164571067
C	-2.7464481675	-0.8554016024	-0.2377551741
C	-0.6764058255	0.3104131435	0.5072917821
C	-1.4513493491	1.5507088153	0.4605007748

C	-2.7641615807	1.5758014455	0.0477608762
C	-3.4204357947	0.3805540428	-0.3004734399
H	-3.2688838241	-1.7639985727	-0.5211809195
H	-4.4581928449	0.4076685644	-0.6164540272
H	-0.9690820322	2.4672020765	0.7860773376
H	-3.3089509105	2.5139807173	0.0271143946
H	-0.1732511674	0.2192455220	1.4759346793
H	0.1732533379	0.2192498637	-1.4759353049
H	3.2688763963	-1.7640078725	0.5211812825

Ground state coordinates for: S4

C	0.6978572854	0.0078028408	2.1072110752
C	-0.6978572854	-0.0078028408	2.1072110752
C	1.4317057605	-0.0714030146	0.9174906437
C	-1.4317057605	0.0714030146	0.9174906437
H	1.2335866230	0.0657303317	3.0501982997
H	-1.2335866230	-0.0657303317	3.0501982997
C	0.6967215428	-0.3501089239	-0.3795921527
C	2.8389790227	0.0418238178	0.9095692036
C	1.5293848543	-0.1463443478	-1.6101270244
C	2.8740606936	0.0111771965	-1.5444191493
C	3.5426076849	0.0765717071	-0.2763764524
H	1.0442529256	-0.2272016999	-2.5767554129
H	3.4611038851	0.0892439598	-2.4534958897
H	4.6221251959	0.1883740283	-0.2556812554
C	-2.8389790227	-0.0418238178	0.9095692036
C	-0.6967215428	0.3501089239	-0.3795921527
C	-1.5293848543	0.1463443478	-1.6101270244
C	-2.8740606936	-0.0111771965	-1.5444191493
C	-3.5426076849	-0.0765717071	-0.2763764524
H	-3.3608880082	-0.1569214078	1.8549667229
H	-4.6221251959	-0.1883740283	-0.2556812554
H	-1.0442529256	0.2272016999	-2.5767554129
H	-3.4611038851	-0.0892439598	-2.4534958897
H	-0.4832234486	1.4410788513	-0.3617688697
H	0.4832234486	-1.4410788513	-0.3617688697
H	3.3608880082	0.1569214078	1.8549667229

Ground state coordinates for: S5=S6

C	1.0701864298	-1.8026937293	1.2121515090
C	-0.2877822171	-2.0725977960	1.1123576525
C	1.7042856326	-0.8470771529	0.4086162009
C	-1.1343925075	-1.3071887690	0.2728601864
H	1.6641263016	-2.3288314760	1.9556338811
H	-0.7359257462	-2.8395443505	1.7369937425
C	0.9318354155	-0.2357027500	-0.7498944419
C	3.0565385401	-0.4916525051	0.6006143211
C	1.5583476719	1.0309451737	-1.2696347845
C	2.8446567738	1.3487514199	-0.9936858241
C	3.6311002488	0.5522251484	-0.0911585233
H	0.9823572915	1.6572560204	-1.9419983504
H	3.2897783117	2.2365384942	-1.4332864113
H	4.6654230104	0.8238887125	0.0945922866
C	-2.5264897385	-1.5509358998	0.2183914021
C	-0.5883606860	-0.1645900571	-0.4621794411
C	-1.4568737680	0.4358923473	-1.4541146163
C	-2.7997380135	0.1576805972	-1.4939139304
C	-3.3400029870	-0.8293338843	-0.6313985042
H	-2.9445862031	-2.3381057782	0.8394961391
H	-4.4058644953	-1.0371710534	-0.6599489645
H	-1.0533145048	1.2041542894	-2.1045415778
H	-3.4492041131	0.6827500626	-2.1867090030
H	-0.6322814621	0.6918919222	0.3914069129
H	1.0272949606	-0.9747490919	-1.5785350548
H	3.6276605989	-1.0223231804	1.3581555433
Cl	-0.4989635581	1.9041279693	1.5657803238

Ground state coordinates for: S7

C	1.1547000530	-1.9901417737	1.1123552021
C	-0.1841028410	-2.2592677575	0.9924051243

C	1.7834685983	-0.9752077203	0.3497659098
C	-1.0497920105	-1.4451982892	0.1656366037
H	1.7501102046	-2.5287975755	1.8462571767
H	-0.6436806961	-3.0303266618	1.6043000508
C	1.0304978088	-0.4074401829	-0.8462372330
C	3.0859861361	-0.5358119409	0.6204754552
C	1.6166334186	0.8912904866	-1.3419451646
C	2.8607671041	1.2949043847	-0.9792258016
C	3.6409642952	0.5556850003	-0.0314679105
H	1.0589510032	1.4656054471	-2.0734982483
H	3.2738405024	2.2070494539	-1.4018831677
H	4.6419743794	0.8916235783	0.2190990273
C	-2.4497312889	-1.5858404491	0.2314510771
C	-0.4917953332	-0.4516302736	-0.6834430246
C	-1.3543245376	0.3647264431	-1.4218796554
C	-2.7454209917	0.2146261573	-1.3409084142
C	-3.2924457449	-0.7678566689	-0.5138552456
H	-2.8682536008	-2.3433486035	0.8891987281
H	-4.3693416493	-0.8904440815	-0.4474153226
H	-0.9521132124	1.1213822320	-2.0869262173
H	-3.3909099991	0.8629545939	-1.9256253486
H	-1.3254160975	1.7349946897	0.5771913582
H	1.2198849297	-1.1477308329	-1.6611978335
H	3.6470390105	-1.0397060231	1.4043945748
Cl	-1.4476782541	2.6775110506	1.4590289731

Ground state coordinates for: S8

C	0.6972361568	-2.0714226015	0.0600983064
C	-0.6790854236	-2.1073690187	0.0860871337
C	1.4481834375	-0.8558396049	0.0550884650
C	-1.4268324038	-0.9139974139	0.1054483658
H	1.2481588048	-3.0069082726	0.0081315412
H	-1.2024728063	-3.0563367074	0.0324057226
C	0.7760335460	0.3961640810	0.1383893870
C	2.8572096139	-0.8897098304	-0.0638740964
C	1.5282172020	1.5692743400	0.1169874099
C	2.9167661237	1.5147476122	-0.0145927828
C	3.5858054776	0.2857287156	-0.1015128421
H	1.0521992527	2.5404146432	0.1883270947
H	3.4824845878	2.4400940812	-0.0542772423
H	4.6658113380	0.2591540786	-0.1965634003
C	-2.8305728942	-0.9095363207	-0.0499242486
C	-0.7240942334	0.3874384305	0.3535527651
C	-1.5225368536	1.6124903447	0.0566530982
C	-2.8613160072	1.5430197532	-0.1554565970
C	-3.5216596848	0.2750040124	-0.1840610713
H	-3.3525043649	-1.8581238857	-0.1268905870
H	-4.5961205843	0.2479706077	-0.3398368455
H	-1.0275374533	2.5751976660	0.1071996116
H	-3.4388332620	2.4473491527	-0.3136640221
H	-0.7872284673	0.4004818091	1.4761342448
H	3.3575980960	-1.8514325623	-0.1242998513

Ground state coordinates for: S9

C	0.6796942699	-2.0940979775	-0.0001421111
C	-0.6797064490	-2.0940946035	0.0001429160
C	1.4229560432	-0.8664222849	-0.0001957672
C	-1.4229585548	-0.8664140445	0.0001517477
H	1.2319664606	-3.0301067027	-0.0002232487
H	-1.2319841897	-3.0300972999	0.0003700421
C	0.7286977914	0.3804425750	0.0000157533
C	2.8371085962	-0.8789187866	-0.0002698944
C	1.4992359208	1.5667230164	0.0003846006
C	2.8815641062	1.5295280904	0.0002988094
C	3.5605444747	0.2969458840	-0.0000924411
H	1.0056152231	2.5320699554	0.0009386461
H	3.4449896076	2.4580075417	0.0005361102
H	4.6462265807	0.2728188569	-0.0001566994
C	-2.8371148519	-0.8789156676	0.0002739576
C	-0.7286978903	0.3804451723	-0.0000752975



C	-1.4992318920	1.5667344666	-0.0003678063
C	-2.8815531685	1.5295320416	-0.0002814474
C	-3.5605400067	0.2969476383	0.0000914066
H	-3.3485076559	-1.8381150254	0.0004996796
H	-4.6462223500	0.2728306279	0.0002175553
H	-1.0056051556	2.5320784471	-0.0008017081
H	-3.4449835162	2.4580107819	-0.0005839340
H	3.3485146607	-1.8381103032	-0.0004030001

R1 : pyrrole, R2=R3 : phenyl

Ground state coordinates for: S1

C	1.4013011673	0.9600969229	0.9242273462
C	-1.3990145441	0.9632630734	-0.9281886706
H	0.4832069154	0.9910865799	1.5013312657
H	-0.4810423353	0.9926320623	-1.5055679932
C	1.6573389357	-0.1482238075	0.0977673891
C	2.8609215594	-0.1671162242	-0.6285005385
C	3.7804933953	0.8757030155	-0.5252391203
C	3.5113421813	1.9701464989	0.2976542373
C	2.3159451021	2.0072965708	1.0185760696
C	-1.6571494884	-0.1449779857	-0.1022944071
C	-2.8603867866	-0.1616193590	0.6246027567
C	-3.7777697180	0.8832207756	0.5222741593
C	-2.3114478278	2.0124779533	-1.0215961397
C	-3.5066302358	1.9774872686	-0.3002055546
C	0.7217001574	-1.2877353703	0.0171735679
C	-0.7236815388	-1.2863472066	-0.0224045931
C	1.1176086845	-2.6136598914	0.0270347968
C	-1.1221335143	-2.6114974341	-0.0332401046
N	-0.0030107951	-3.4027721120	-0.0034887061
H	3.0634394290	-1.0034835337	-1.2914799263
H	4.7033466871	0.8373919215	-1.0975070289
H	4.2233416658	2.7867156684	0.3748068905
H	2.0970448798	2.8526123688	1.6651541799
H	-3.0643082098	-0.9978797909	1.2872796705
H	-4.7004339757	0.8466371461	1.0949547449
H	-2.0909841082	2.8576889903	-1.6677757433
H	-4.2169034949	2.7956296993	-0.3766015880
H	2.1059923368	-3.0409122033	0.1061754714
H	-2.1113242863	-3.0368045750	-0.1128149845
H	-0.0039727520	-4.4094929212	-0.0039424097

Ground state coordinates for: S2

C	1.4355217699	1.0653085820	0.8054519273
C	-1.4384076494	1.0630959669	-0.8093197987
H	0.4922433951	1.1752674206	1.3282963762
H	-0.4970016685	1.1719793405	-1.3358199260
C	1.6866367545	-0.0992123687	0.0478210359
C	2.9343165564	-0.2302474132	-0.6042083187
C	3.8922171603	0.7715638711	-0.5091411361
C	3.6306905855	1.9171869913	0.2488260676
C	2.4011409109	2.0569419667	0.9078663922
C	-1.6866765377	-0.0995275420	-0.0481970102
C	-2.9319077989	-0.2293171654	0.6082944872
C	-3.8904721629	0.7720935794	0.5140654026
C	-2.4045477719	2.0544844049	-0.9106373750
C	-3.6318039367	1.9160325681	-0.2472512462
C	0.7107299364	-1.1874936240	-0.0225063264
C	-0.7101331732	-1.1878144168	0.0212658029
C	1.1074448513	-2.5480719883	-0.0306007540
C	-1.1058876563	-2.5480780494	0.0285618290
N	0.0011174134	-3.3452069018	-0.0010296563
H	3.1385325382	-1.1090317580	-1.2087069134
H	4.8408393987	0.6631714304	-1.0241748870
H	4.3800182945	2.6980734988	0.3286760079
H	2.2041652323	2.9408070531	1.5055825889
H	-3.1338326373	-1.1068143314	1.2154582735

H	-4.8373507100	0.6645720330	1.0324927293
H	-2.2096872414	2.9370203821	-1.5110178850
H	-4.3815549747	2.6965862416	-0.3263503711
H	2.1034532611	-2.9676303644	-0.0036883512
H	-2.1017020860	-2.9680822758	0.0014261136
H	0.0012779828	-4.3559338175	-0.0010438917

Ground state coordinates for: S3

C	0.7010976552	0.9297520236	0.3960309753
C	-0.7012238952	0.9303197079	-0.3949150585
H	0.3773484176	0.8225256902	1.4410827301
H	-0.3774924334	0.8244559709	-1.4401085326
C	1.4762285314	-0.2953749063	0.0007627307
C	2.7841031041	-0.1872851534	-0.4454398780
C	3.4265839711	1.0545888660	-0.5137535015
C	2.7543914561	2.2445796749	-0.1408885476
C	1.4607813267	2.1990810768	0.2956213513
C	-1.4761639851	-0.2954305386	-0.0011476472
C	-2.7840118136	-0.1880804209	0.4452880969
C	-3.4266846796	1.0536126711	0.5152327765
C	-1.4611100500	2.1993996642	-0.2928661220
C	-2.7546967732	2.2441566155	0.1437987140
C	0.7223906170	-1.5272665103	-0.0017409804
C	-0.7222259762	-1.5272970998	-0.0003506925
C	1.1270550592	-2.8508046878	0.0023049715
C	-1.1268040787	-2.8508422622	-0.0063105346
N	0.0001512701	-3.6309744935	-0.0025605680
H	3.3133370284	-1.0772364159	-0.7717374879
H	4.4514671295	1.1065729900	-0.8665510137
H	3.2811978211	3.1921732756	-0.1861163278
H	0.9672555530	3.1088041147	0.6215138984
H	-3.3130939217	-1.0785345899	0.7704587765
H	-4.4515481485	1.1049982981	0.8681716167
H	-0.9677667619	3.1096052614	-0.6176805936
H	-3.2816365810	3.1916185229	0.1902325868
H	2.1110900820	-3.2922242841	0.0545185247
H	-2.1108141807	-3.2922403339	-0.0591656006
H	0.0001742932	-4.6409294137	-0.0032934746

Ground state coordinates for: S4

C	0.7004028410	-1.0245871088	-0.3404919948
C	-0.7004380261	-1.0244752344	0.3404124655
H	0.5029288939	-1.0049649196	-1.4375397697
H	-0.5029930044	-1.0047768014	1.4374720379
C	1.4751013538	0.2563113908	-0.0642117376
C	2.8785856600	0.2129009141	0.0261298779
C	3.5568696016	-0.9876884587	0.0524811105
C	2.8565225485	-2.2395016992	0.0146877639
C	1.5106491903	-2.2726993881	-0.1187231851
C	-1.4750024245	0.2564880635	0.0640934123
C	-2.8785312388	0.2132219251	-0.0259013402
C	-3.5569354837	-0.9872919563	-0.0520184575
C	-1.5108317095	-2.2725213166	0.1188177330
C	-2.8567247770	-2.2391921894	-0.0143264246
C	0.7295825827	1.4520935020	-0.0010233096
C	-0.7293680904	1.4521583270	0.0005629875
C	1.1322045917	2.7932213296	0.0071799107
C	-1.1318757895	2.7933372749	-0.0079559623
N	0.0001902299	3.5503186033	-0.0004152808
H	3.4332043607	1.1396405871	0.1349788704
H	4.6382832772	-0.9899849571	0.1445800537
H	3.4205766106	-3.1619919553	0.1049555094
H	1.0030192634	-3.2288492905	-0.1675725507
H	-3.4330837116	1.1400095332	-0.1346736328
H	-4.6383734686	-0.9894764343	-0.1438494093
H	-1.0032747862	-3.2287133333	0.1675824426
H	-3.4209024411	-3.1616189366	-0.1044624044
H	2.1096460529	3.2489876621	-0.0113808604
H	-2.1092808949	3.2491889932	0.0104308572
H	0.0002403672	4.5623711982	-0.0005234245

## Ground state coordinates for: S5=S6

C	0.6776103911	-0.8828392546	0.3201834844
C	-0.7625798896	-0.7186407342	0.9526771936
H	-0.5320756322	-0.4932207886	2.0151576461
C	1.4807810893	0.3419835821	0.3140322966
C	2.8810132304	0.2478123067	0.3058437422
C	3.5103886923	-0.9815671340	0.4273314060
C	2.7672540201	-2.1725587738	0.5774500941
C	1.3958478142	-2.1173359464	0.5778723644
C	-1.4853079387	0.4984577675	0.3986155559
C	-2.8381514781	0.4563599456	0.1161224839
C	-3.5857899617	-0.7215043363	0.2431127434
C	-1.6116293727	-1.9581643632	0.9405790863
C	-2.9392697926	-1.9258234787	0.6376752338
C	0.7807953412	1.5904973998	0.2171199430
C	-0.6629229399	1.6713234421	0.2235445691
C	1.2690667436	2.8794937296	0.0184883871
C	-0.9858244491	3.0021864606	0.0296022470
N	0.1952186943	3.7080728456	-0.0887965136
H	3.4800518046	1.1495865227	0.2264185232
H	4.5959891552	-1.0266613498	0.4204516752
H	3.2811427816	-3.1213535943	0.6923184978
H	0.8244779315	-3.0357047408	0.6526999896
H	-3.3235950219	1.3532362577	-0.2604033220
H	-4.6412467427	-0.7273152044	-0.0065889088
H	-1.1613262993	-2.8910142322	1.2633199061
H	-3.5194011758	-2.8433310292	0.6904054970
H	2.2769702127	3.2552034649	-0.0707401671
H	-1.9391033304	3.5046075716	-0.0214689473
H	0.2531455168	4.7032757591	-0.2399822772
H	0.4331581374	-1.0099806950	-0.7726144399
Cl	-0.0567072758	-1.1887036110	-2.4735066137

## Ground state coordinates for: S7

C	-0.6864782493	0.2658068046	-0.9005730748
C	0.2054229969	-0.9680543312	-1.1531373860
H	0.6816725502	-0.7313016986	-2.1322346075
C	-0.0843719215	1.4650542158	-0.4416846617
C	-0.8698754408	2.6215612831	-0.3105584610
C	-2.2257879557	2.6133260631	-0.6271487742
C	-2.8248741371	1.4324226917	-1.0647529207
C	-2.0556389103	0.2699590267	-1.1948531615
C	1.3631918751	-1.0743343868	-0.1666164416
C	1.7483554891	-2.2970082516	0.3515026524
C	1.0565070336	-3.4821235246	0.0578105876
C	-0.5248906531	-2.2726341990	-1.3393819142
C	-0.0908171294	-3.4382924620	-0.7833715154
C	1.3267883617	1.4304431438	-0.0694310211
C	2.0172752739	0.1800739891	0.1183239450
C	2.2018453499	2.4401430839	0.2837607678
C	3.2879060559	0.4828632969	0.5856785596
N	3.3798678366	1.8503740152	0.6761592583
H	-0.4127601334	3.5334530285	0.0634732857
H	-2.8143974238	3.5195381081	-0.5183329179
H	-3.8842043626	1.4072212840	-1.3022292206
H	-2.5366036991	-0.6376252037	-1.5427891462
H	2.5942133794	-2.3317350625	1.0344092751
H	1.3742151057	-4.4222164591	0.4962556397
H	-1.3784777626	-2.2849291491	-2.0094196982
H	-0.6337453460	-4.3587537222	-0.9835652073
H	2.0882214647	3.5136761611	0.2927750724
H	4.1274774959	-0.1521338576	0.8243554759
H	4.2079622590	2.3526967554	0.9531432184
H	-2.4718190844	-0.2200079537	1.1223285247
Cl	-2.9443767640	-0.5463476673	2.2854167997

## Ground state coordinates for: S8

C	0.6977822518	-1.0860908605	0.1315822608
C	-0.8094771619	-0.9496392428	0.3738084783

H	-0.8831397728	-0.8946167866	1.4915103874
C	1.4970344663	0.0751255603	0.0036696777
C	2.8879658331	-0.0556590525	-0.1526493799
C	3.4877436283	-1.3060295068	-0.1715524361
C	2.6996509452	-2.4519469400	-0.0344234019
C	1.3206332013	-2.3386657220	0.1227347725
C	-1.4395910596	0.3776075929	0.0423029494
C	-2.8362720138	0.4394831890	-0.1630624833
C	-3.5871663331	-0.7099482663	-0.2535846759
C	-1.6784430006	-2.1374620296	0.1182722863
C	-3.0037023561	-2.0101872314	-0.1363238431
C	0.8472224112	1.3748857482	0.0141104070
C	-0.5964464881	1.4994181822	0.0193620852
C	1.3518526616	2.6521722657	-0.0403006278
C	-0.8989493940	2.8747929193	-0.0403877865
N	0.2751886631	3.5269612818	-0.0674614919
H	3.4976896996	0.8354114141	-0.2620404538
H	4.5623208428	-1.3921985324	-0.2931525429
H	3.1568850661	-3.4356424401	-0.0546776258
H	0.7437881236	-3.2492675373	0.23111223127
H	-3.3098192027	1.4027428654	-0.3192256639
H	-4.6532903755	-0.6301540933	-0.4457651027
H	-1.2437800033	-3.1229669787	0.2315551857
H	-3.6285281657	-2.8876667366	-0.2610817564
H	2.3626187612	3.0276485619	-0.0657299561
H	-1.8417727502	3.4001650992	-0.0372112077
H	0.3662815001	4.5340696278	-0.0984497418

Ground state coordinates for: S9

C	0.7400231941	-1.0295119465	0.0008015139
C	-0.7384619993	-1.0308875245	0.0007707539
C	1.4629998915	0.1973524598	0.0010283884
C	2.8704919203	0.1779179205	0.0016045230
C	3.5742593310	-1.0151560861	0.0017227327
C	2.8730439858	-2.2277884070	0.0011566317
C	1.4863456516	-2.2269940134	0.0006868328
C	-1.4635393682	0.1947250229	0.0005119305
C	-2.8710586318	0.1728044658	0.0006472606
C	-3.5727115438	-1.0215398296	0.0008482536
C	-1.4826327699	-2.2297219889	0.0010326058
C	-2.8693835227	-2.2329567263	0.0010652678
C	0.7159312373	1.4386410437	0.0007316297
C	-0.7187177665	1.4373479774	0.0002207780
C	1.1269590138	2.7626515537	0.0004780614
C	-1.1322422560	2.7605602797	-0.0007005473
N	-0.0033464677	3.5395394506	-0.0000884548
H	3.4107260342	1.1204143846	0.0018897876
H	4.6603717600	-1.0084874030	0.0022001141
H	3.4113751362	-3.1709834499	0.0011933298
H	0.9755971343	-3.1828392505	0.0001331095
H	-3.4130450226	1.1142781331	0.0005382991
H	-4.6588367583	-1.0167798107	0.0010794163
H	-0.9702049544	-3.1846541621	0.0011477005
H	-3.4061775856	-3.1770245927	0.0012155798
H	2.1088913340	3.2099267353	0.0004895421
H	-2.1149691706	3.2060754411	-0.0016406119
H	-0.0042960730	4.5469208509	0.0001182440

R1: thiophene, R2=R3 : phenyl

Ground state coordinates for: S1

C	1.3282325733	1.0965176387	1.0107955640
C	-1.3226354458	1.1030352174	-1.0194483692
H	0.4405218737	1.0477822604	1.6323880252
H	-0.4357788771	1.0500578664	-1.6419231501
C	1.6047483652	0.0481816241	0.1171317928
C	2.7671666753	0.1295115563	-0.6672384576
C	3.6292965888	1.2202492662	-0.5588373212

C	3.3425776813	2.2548951420	0.3324236613
C	2.1883721623	2.1877846594	1.1154952185
C	-1.6034923903	0.0559166995	-0.1256441582
C	-2.7649119020	0.1427890666	0.6595931883
C	-3.6218793518	1.2377165434	0.5519481431
C	-2.1775778783	2.1984209837	-1.1234058359
C	-3.3308766211	2.2710065384	-0.3394538533
C	0.7232452918	-1.1419898701	0.0272602823
C	-0.7276523965	-1.1385569998	-0.0367530031
C	1.2279480699	-2.4191947464	0.0453110677
C	-1.2383257475	-2.4133805627	-0.0547967871
S	-0.0079503870	-3.6283147930	-0.0067411985
H	2.9821393683	-0.6638431679	-1.3771287259
H	4.5211662979	1.2642691847	-1.1774724885
H	4.0107894826	3.1070552560	0.4151229036
H	1.9580698863	2.9860374583	1.8152986921
H	-2.9832160199	-0.6495916628	1.3695675168
H	-4.5130774632	1.2859275276	1.1712445224
H	-1.9440639270	2.9955692412	-1.8234070888
H	-3.9950347906	3.1263874897	-0.4215520644
H	2.2650129949	-2.7079817950	0.1424757490
H	-2.2767729787	-2.6971893729	-0.1518029158

Ground state coordinates for: S2

C	1.2501597442	1.1890034326	0.9033571240
C	-1.2505157879	1.1902152181	-0.9052282731
H	0.3447829270	1.1383126855	1.4960698911
H	-0.3462317884	1.1389920287	-1.4995315228
C	1.5971564556	0.0973343698	0.0573699629
C	2.8341879522	0.1417593497	-0.6342032227
C	3.6676695053	1.2389698759	-0.5094905900
C	3.3064004205	2.3121751050	0.3274709472
C	2.1009734095	2.2784381747	1.0339820997
C	-1.5968617239	0.0986241860	-0.0588477258
C	-2.8328208635	0.1437442722	0.6345718450
C	-3.6657857731	1.2415212125	0.5113393005
C	-2.1008025177	2.2802533469	-1.0343165044
C	-3.3050914675	2.3146701256	-0.3259261489
C	0.7384308056	-1.0737744341	-0.0446208926
C	-0.7388725338	-1.0732011377	0.0417583893
C	1.2358476389	-2.3618527015	-0.1145155005
C	-1.2371546361	-2.3607999547	0.1135518970
S	-0.0014294736	-3.5409098703	-0.0035814837
H	3.1021305467	-0.6716178578	-1.3002998828
H	4.5996301424	1.2765267312	-1.0636986342
H	3.9723378117	3.1629976033	0.4298278259
H	1.8359255088	3.0937678946	1.6985914126
H	-3.1002600986	-0.6695728360	1.3009456710
H	-4.5968698752	1.2795824443	1.0669855213
H	-1.8363011925	3.0954920484	-1.6992568609
H	-3.9706333297	3.1659438864	-0.4271020377
H	2.2723602514	-2.6680766130	-0.1243207955
H	-2.2739238220	-2.6660680171	0.1253137075

Ground state coordinates for: S3

C	0.7325767076	1.1672640747	0.5137560118
C	-0.7318914577	1.1679311955	-0.5137915796
H	0.2319979414	1.0419897388	1.4753539529
H	-0.2314037916	1.0427314180	-1.47544454365
C	1.4639295234	-0.0364678822	0.0644742261
C	2.7377376884	0.0971367602	-0.4783397758
C	3.3618118867	1.3450796631	-0.5544509009
C	2.7138918381	2.5145916303	-0.0908585571
C	1.4564719041	2.4330351366	0.4465568816
C	-1.4639570899	-0.0355281077	-0.0649624669
C	-2.7376608544	0.0986435926	0.4779575309
C	-3.3609532690	1.3469443075	0.5546174824
C	-1.4550031294	2.4341219939	-0.4460607760
C	-2.7123384112	2.5162445619	0.0914669720
C	0.7253858497	-1.2901289542	0.0418644219

C	-0.7261922150	-1.2896584484	-0.0429048760
C	1.2377178744	-2.5651798400	0.0768040935
C	-1.2393267531	-2.5643683296	-0.0784040978
S	-0.0011834189	-3.7658191105	-0.0010831892
H	3.2425344416	-0.7772997601	-0.8762324186
H	4.3554988100	1.4186442729	-0.9847502975
H	3.2298588415	3.4679501453	-0.1357936741
H	0.9723145361	3.3184992141	0.8464163892
H	-3.2429881086	-0.7756410790	0.8755099414
H	-4.3545712372	1.4209476524	0.9850008671
H	-0.9703073075	3.3194416246	-0.8455876769
H	-3.2277118359	3.4699046903	0.1368252349
H	2.2699602621	-2.8650452993	0.1947715237
H	-2.2717609894	-2.8635142924	-0.1965142869

Ground state coordinates for: S4

C	1.2788976464	-0.6915985869	0.3560556878
C	1.2791352851	0.6907161697	-0.3568749562
H	1.2277177987	-0.4694203940	1.4479479989
H	1.2268053691	0.4685485558	-1.4486919269
C	0.0082520730	-1.4674571588	0.0527274876
C	0.0634125838	-2.8642748306	-0.0667120150
C	1.2692613055	-3.5406181865	-0.0651368639
C	2.5151449283	-2.8422196241	0.0394190821
C	2.5373231545	-1.4969167442	0.1909232746
C	0.0093717913	1.4675181428	-0.0522060583
C	0.0657154526	2.8641794345	0.0680941991
C	1.2720963478	3.5396145837	0.0658388962
C	2.5383243829	1.4950441190	-0.1926496901
C	2.5173089997	2.8402842843	-0.0403667580
C	-1.2089156605	-0.7298679328	-0.0077938137
C	-1.2083651338	0.7308494456	0.0087834684
C	-2.5047871265	-1.2412369355	-0.0260421523
C	-2.5038108724	1.2431895118	0.0276915809
S	-3.6755405815	0.0014110488	0.0009986337
H	-0.8532645496	-3.4249363462	-0.2156854082
H	1.2755733339	-4.6201023311	-0.1773770011
H	3.4421275143	-3.4037259697	-0.0110737139
H	3.4872720660	-0.9869399864	0.3000089001
H	-0.8504120770	3.4254157969	0.2182813687
H	1.2793697575	4.6190145535	0.1787989295
H	3.4877952283	0.9844418489	-0.3029922954
H	3.4447840710	3.4010375185	0.0094921709
H	-2.8226535202	-2.2736004857	-0.0160618361
H	-2.8208783859	2.2757979347	0.0177731715

Ground state coordinates for: S5=S6

C	1.1037808765	0.1986729954	-0.6903006077
C	0.0932073025	1.3805887131	-0.8870950404
H	-0.1961351992	1.2617983721	-1.9536181867
C	0.5465536487	-1.1332426144	-0.6537289254
C	1.3983155525	-2.2278427086	-0.8562482169
C	2.7341334467	-2.0480418147	-1.1970013012
C	3.2605517173	-0.7592507490	-1.3681660635
C	2.4447991019	0.3384205649	-1.1693750063
C	-1.1779666139	1.1960779593	-0.0786742481
C	-1.8011486110	2.2824977092	0.5113928624
C	-1.2517082071	3.5689874013	0.4734951714
C	0.6787949278	2.7614318256	-0.7586549954
C	0.0092026162	3.7789910539	-0.1524408771
C	-0.8626492711	-1.2961888935	-0.3168749507
C	-1.7044530732	-0.1522195020	-0.0180436428
C	-1.5398469692	-2.4890455978	-0.1966703682
C	-2.9841183226	-0.5391835537	0.3183241880
S	-3.1815209849	-2.2579401949	0.2735499050
H	1.0100903711	-3.2363292292	-0.7581906047
H	3.3690767479	-2.9166618570	-1.3447828763
H	4.2979734589	-0.6240556379	-1.6568122377
H	2.8635763770	1.3329527230	-1.2654628169
H	-2.7231236214	2.1219145069	1.0637484490

H	-1.7605295310	4.3918294515	0.9638597026
H	1.6267659488	2.9638228025	-1.2448336835
H	0.4520309044	4.7711840495	-0.1325079966
H	-1.1674888071	-3.4919616044	-0.3470075938
H	-3.8281489159	0.0886934813	0.5641672899
H	1.3804599965	0.3394210279	0.5401468046
Cl	1.5978420082	0.6276425609	2.0646915167

Ground state coordinates for: S7

C	-0.7782902225	0.4050116687	-0.9584535335
C	-0.3206695280	-1.0470486500	-1.1956721945
H	0.2257126026	-0.9903194153	-2.1632039159
C	0.1692989142	1.3520795456	-0.5014593414
C	-0.2178957529	2.6937622586	-0.3548264088
C	-1.5113839864	3.1090554253	-0.6584773379
C	-2.4497720838	2.1755908159	-1.0988197756
C	-2.0812308797	0.8335431316	-1.2417783981
C	0.7098225401	-1.4858105266	-0.1659660457
C	0.6371720692	-2.7293008800	0.4332872658
C	-0.4047595497	-3.6278731452	0.1573892489
C	-1.4255687966	-2.0526690967	-1.3876175327
C	-1.4313901341	-3.2602721979	-0.7582011641
C	1.5174674151	0.8889010543	-0.1411990942
C	1.7642339147	-0.5209369183	0.0854097552
C	2.6254760680	1.6569808702	0.1126725144
C	3.0506446605	-0.7577315012	0.5181106352
S	3.9714063587	0.7022110177	0.6370433858
H	0.4990570851	3.4155803783	0.0244804237
H	-1.7900323334	4.1513279695	-0.5360868088
H	-3.4664414004	2.4826394081	-1.3257599899
H	-2.8214372594	0.1199143936	-1.5865844807
H	1.3949580082	-3.0028488826	1.1633804758
H	-0.4422695898	-4.5886719204	0.6595044834
H	-2.2005514358	-1.8195720975	-2.1110816917
H	-2.2370744004	-3.9623209612	-0.9566967160
H	2.7330979855	2.7292759765	0.0306724265
H	3.5176806974	-1.7090838560	0.7298899178
H	-2.6301254392	0.5075505448	1.0951465740
Cl	-3.1295973571	0.3018463409	2.2726317596

Ground state coordinates for: S8

C	1.2250464751	-0.8784776278	-0.1419223567
C	1.3205024745	0.6287975354	-0.3972870617
H	1.2151575637	0.7105502838	-1.5119058715
C	-0.0457103343	-1.4764356857	0.0188174543
C	-0.1290479413	-2.8676470586	0.2033176966
C	1.0110251615	-3.6577058856	0.2110949356
C	2.2640656540	-3.0649209223	0.0382772438
C	2.3654926818	-1.6879832823	-0.1415875077
C	0.1326132413	1.4552766472	0.0039947727
C	0.3118657849	2.8252846093	0.2698535619
C	1.5753833828	3.3804317996	0.3143699856
C	2.6439157772	1.2907637171	-0.2230435056
C	2.7515060454	2.6103712593	0.0775907826
C	-1.2421870773	-0.6347839276	0.0113541179
C	-1.1345609306	0.8133329914	0.0302074139
C	-2.5533779568	-1.0357102190	0.0393472610
C	-2.3815877172	1.4399063740	0.0862756045
S	-3.6460664697	0.3092765276	0.0923398377
H	-1.0987716831	-3.3313563123	0.3487590624
H	0.9270496728	-4.7296681579	0.3549656188
H	3.1635400233	-3.6712848533	0.0529275274
H	3.3530803434	-1.2611953693	-0.2679508444
H	-0.5470327927	3.4428257607	0.5063043943
H	1.6786841692	4.4349451652	0.5539286138
H	3.5358504125	0.7127662897	-0.4306428544
H	3.7243967223	3.0840557599	0.1489935487
H	-2.9576688839	-2.0374930967	0.0339264672
H	-2.6005806755	2.4982351815	0.0854279167

Ground state coordinates for: S9

C	1.3010852255	-0.7338806713	0.0008144104
C	1.2954004252	0.7439683707	0.0011648765
C	0.0795339764	-1.4599432754	0.0006281521
C	0.1084920764	-2.8666469843	0.0004699653
C	1.3051536961	-3.5647506969	0.0003536897
C	2.5131372495	-2.8577258438	0.0000284191
C	2.5035075067	-1.4712516803	0.0002043485
C	0.0681387772	1.4604355222	-0.0003132983
C	0.0859972432	2.8674227517	-0.0005324973
C	1.2771902988	3.5748673982	0.0013652919
C	2.4920126057	1.4906874420	0.0033020058
C	2.4906604985	2.8772829111	0.0035104712
C	-1.1825730947	-0.7262298390	0.0001109147
C	-1.1882075340	0.7168932052	-0.0010094156
C	-2.4565156395	-1.2505947458	-0.0001820306
C	-2.4662234852	1.2313075951	-0.0023243443
S	-3.6575314512	-0.0143352566	-0.0005861961
H	-0.8269715317	-3.4170682677	0.0003123768
H	1.3028720582	-4.6506086643	0.0003142746
H	3.4595416253	-3.3901672761	-0.0005021613
H	3.4556707013	-0.9545553713	-0.0005644774
H	-0.8537253896	3.4105071337	-0.0018148657
H	1.2663323710	4.6607034114	0.0014501767
H	3.4482024296	0.9813991888	0.0052679561
H	3.4326922630	3.4174563006	0.0055073128
H	-2.7607204450	-2.2867129284	0.0003830025
H	-2.7787364400	2.2649870659	-0.0033659084

R1: benzene, R2=R3 : phenyl

Ground state coordinates for: S1

C	1.3852919663	0.8966428930	1.0693196395
C	-1.2177343895	1.1568619279	-1.0113208200
H	0.5617490231	0.8216475896	1.7716954101
H	-0.4148714340	0.9834682473	-1.7202603436
C	2.2896096929	1.9520257193	1.1700030222
C	3.3565520566	2.0551533596	0.2748419374
C	3.5134951466	1.0907841390	-0.7208966379
C	2.6106495366	0.0319342814	-0.8185214455
C	1.5307695177	-0.0812172842	0.0717995095
C	0.6076836142	-1.2507837741	-0.0183578226
C	-0.8051340784	-1.1370206515	-0.0323087920
C	-1.5266038059	0.1687760950	-0.0621454051
C	-1.9368972704	2.3493181958	-1.0594455918
C	-2.9789362441	2.5816602501	-0.1594815788
C	-2.5811250954	0.4127247771	0.8326093265
C	-3.2988850534	1.6081489996	0.7871872248
C	1.1805404601	-2.5332990566	-0.0541920438
C	-1.5747766518	-2.3124369758	-0.0562230759
C	0.4010171943	-3.6864515201	-0.0885148928
C	-0.9883249102	-3.5751118886	-0.0827038478
H	2.1626295801	2.6942556600	1.9529247107
H	4.0586001613	2.8801054551	0.3536057606
H	4.3373049071	1.1625742067	-1.4254311980
H	-1.6849588523	3.0978643831	-1.8052689405
H	-3.5366912252	3.5128482583	-0.1969665706
H	-2.8264996768	-0.3380034351	1.5784729496
H	-4.1056730370	1.7787243749	1.4944123263
H	2.2628025486	-2.6171739578	-0.0228075731
H	-2.6565630472	-2.2216154538	-0.0860456253
H	0.8763923361	-4.6627260723	-0.1092364030
H	-1.6132743586	-4.4629957885	-0.1087125169
H	2.7300618998	-0.7102178511	-1.6025484691

Ground state coordinates for: S2

C	1.1586273715	-1.0456557587	-1.0048998500
C	-1.1589648392	-1.0442177124	1.0036826163



H	0.2942954249	-0.9041839810	-1.6426002566
H	-0.2933598755	-0.9041179064	1.6399826964
C	1.9515489871	-2.1741822520	-1.1621370169
C	3.1063679277	-2.3282254229	-0.3904608554
C	3.4775256868	-1.3347940517	0.5346338644
C	2.7079835898	-0.1934662770	0.6787438930
C	1.5158359783	-0.0290309346	-0.0729332251
C	0.7228728017	1.1925899685	0.0493628584
C	-0.7215326060	1.1935793160	-0.0504753668
C	-1.5161457801	-0.0268965742	0.0725325712
C	-1.9531947979	-2.1717116360	1.1617339522
C	-3.1092948369	-2.3239950332	0.3916128059
C	-2.7094724448	-0.1895086895	-0.6776263088
C	-3.4803610542	-1.3298475284	-0.5327505137
C	1.3926372125	2.4300945246	0.1663804339
C	-1.3896381794	2.4319447645	-0.1674655123
C	0.7024126744	3.6258140652	0.0898643375
C	-0.6977700648	3.6267457451	-0.0911870436
H	1.6806691528	-2.9268697622	-1.8948258433
H	3.7264221527	-3.2109953795	-0.5102279369
H	4.3690595322	-1.4658914925	1.1390678727
H	-1.6822474027	-2.9250003148	1.8937756277
H	-3.7303602559	-3.2059675796	0.5119895726
H	-2.9911802645	0.5633919547	-1.4061178563
H	-4.3728963698	-1.4595820996	-1.1359968146
H	2.4747280681	2.4401314610	0.2321415274
H	-2.4717317583	2.4434042606	-0.2330919587
H	1.2412808396	4.5662504569	0.1407036656
H	-1.2353689857	4.5679066115	-0.1420654116
H	2.9897394651	0.5587807030	1.4078856204

Ground state coordinates for: S3

C	1.1927393699	-0.6026698965	0.4737635689
C	1.1623155165	0.6677038183	-0.4482592803
H	1.0787547099	-0.1859623054	1.4846641279
H	1.0855372122	0.2428649252	-1.4594487845
C	2.4796007620	-1.3423403451	0.4485258627
C	2.5678820145	-2.6508576537	0.0635922797
C	1.4033683807	-3.3548925531	-0.3174926189
C	0.1423099203	-2.7380117029	-0.2814802945
C	-0.0127727256	-1.4277647577	0.1346485176
C	-1.3121277020	-0.7450316636	0.0941420025
C	-1.3507176559	0.6676878380	-0.0971250695
C	-0.0928996818	1.4226759944	-0.1304494156
C	2.4039864924	1.4802208687	-0.4128628472
C	2.4110671606	2.7970459683	-0.0477313357
C	-0.0198339260	2.7470441193	0.2670289729
C	1.2014283800	3.4367693518	0.3063383689
C	-2.5173089701	-1.4471441120	0.2148642527
C	-2.5927091817	1.3020525105	-0.2267660045
C	-3.7463705724	-0.7922512874	0.1074998171
C	-3.7839308031	0.5800423742	-0.1298010696
H	3.3689396348	-0.8110032489	0.7717635436
H	3.5272861220	-3.1578034574	0.0625049260
H	1.4815202260	-4.3864959414	-0.6450058386
H	-0.7227200534	-3.3024291596	-0.6116751297
H	3.3277704983	0.9963294362	-0.7134779487
H	3.3393201946	3.3588494745	-0.0405398150
H	-0.9201561452	3.2650085437	0.5783908785
H	1.2150252572	4.4761483441	0.6182592851
H	-2.5007608965	-2.5114006513	0.4237885984
H	-2.6350567530	2.3654634907	-0.4362473737
H	-4.6675381745	-1.3567163566	0.2065051827
H	-4.7341767601	1.0924053386	-0.2367569475

Ground state coordinates for: S4

C	1.2081652776	-0.6735827214	0.3870719787
C	1.2081883124	0.6735254914	-0.3870997207
H	1.1206941930	-0.4036270891	1.4629331444
H	1.1206748003	0.4035738595	-1.4629574285

C	2.4792579370	-1.4674023700	0.2955403074
C	2.4782640017	-2.8072531883	0.1106058052
C	1.2423057869	-3.5033151530	-0.0889837119
C	0.0316184241	-2.8400813411	-0.1169445220
C	-0.0551030399	-1.4443233690	0.0534047593
C	-1.2875005315	-0.7239027506	-0.0141269077
C	-1.2874659358	0.7239626190	0.0141396082
C	-0.0550331041	1.4443241525	-0.0533882157
C	2.4793214658	1.4672831344	-0.2955934040
C	2.4783983528	2.8071281520	-0.1106156616
C	0.0317616900	2.8400702203	0.1170124789
C	1.2424819165	3.5032450000	0.0890419544
C	-2.5406435833	-1.3974074336	-0.0470087836
C	-2.5405750238	1.3975290392	0.0470202121
C	-3.7302118836	-0.7058894825	-0.0252878548
C	-3.7301774504	0.7060692887	0.0252981829
H	3.4126284530	-0.9482461227	0.4813925314
H	3.4086149552	-3.3653698207	0.1087924120
H	1.2611630225	-4.5774668744	-0.2440481800
H	3.4126610660	0.9480884291	-0.4814937394
H	3.4087766686	3.3651993682	-0.1088173741
H	-0.8604042827	3.4162302826	0.3279897281
H	1.2613987886	4.5773892952	0.2441498958
H	-2.5716215414	-2.4794322559	-0.0511007816
H	-2.5714972325	2.4795555888	0.0511038222
H	-4.6705573542	-1.2467962377	-0.0371725589
H	-4.6704963827	1.2470223330	0.0371784991
H	-0.8605810059	-3.4162077906	-0.3278714665

Ground state coordinates for: S5=S6

C	-0.9312477470	0.7439291850	-0.5011210610
C	-0.8209342331	-0.6806568372	-1.1352248973
H	-0.4022586726	-0.4890849253	-2.1456055656
C	-2.0517210801	1.5809441140	-0.9019918462
C	-1.9871388038	2.9480771220	-0.8477615825
C	-0.7647409494	3.5588413869	-0.4955055040
C	0.3762933268	2.8109962534	-0.2466577562
C	0.3639745815	1.4069015785	-0.3213324976
C	1.5561302331	0.5984304700	-0.1075966193
C	1.4600361710	-0.8323690726	-0.0727520450
C	0.2074555061	-1.4931092699	-0.3748695070
C	-2.1293114552	-1.3928302953	-1.3359017532
C	-2.3150128182	-2.6863291294	-0.9666696625
C	-0.0633589312	-2.8116581648	-0.0248475208
C	-1.2851428551	-3.4203678290	-0.3081905349
C	2.8132723534	1.2007159337	0.1321373374
C	2.6263248418	-1.5706588313	0.2366967717
C	3.9383329587	0.4497597082	0.4202187115
C	3.8379134682	-0.9496501392	0.4810421465
H	-2.9960606406	1.0939857199	-1.1160918715
H	-2.8595447901	3.5551881322	-1.0655561741
H	-0.7087270698	4.6418534148	-0.4286749352
H	-2.9191239470	-0.8650469683	-1.8606254097
H	-3.2666123334	-3.1713079398	-1.1657086203
H	0.6748840186	-3.3745134992	0.5367390682
H	-1.4668710896	-4.4417273491	0.0083502613
H	2.9127515807	2.2788396673	0.0934101859
H	2.5794119906	-2.6534273339	0.2471302875
H	4.8896033522	0.9409409736	0.5985484373
H	4.7161315014	-1.5492063421	0.7020826902
H	1.2899747415	3.3398626252	-0.0060986915
H	-1.2253899797	0.5263267661	0.5362456639
Cl	-1.7138954052	0.0327120216	2.2105516457

Ground state coordinates for: S7

C	-0.6712916079	0.3637061013	-0.9954324882
C	-0.1162335185	-1.0530771841	-1.2076371300
H	0.4968281448	-0.9681614044	-2.1317011789
C	-1.9888750813	0.7138899308	-1.3115259298
C	-2.4452320111	2.0262174455	-1.1468019992

C	-1.5800236631	2.9986241490	-0.6469361704
C	-0.2706112182	2.6562002898	-0.3172565953
C	0.2113782016	1.3479742612	-0.4931791422
C	1.5887732083	0.9673514768	-0.1072020340
C	1.8733336800	-0.3975948042	0.1779574156
C	0.8496112127	-1.4013021304	-0.0909384312
C	-1.1471854741	-2.1190653331	-1.4637160417
C	-1.1754699887	-3.2881507787	-0.7664393589
C	0.7543251096	-2.6083168512	0.5776292737
C	-0.2351647784	-3.5550682795	0.2688892336
C	2.6041804556	1.9207458737	0.0646800082
C	3.1461182608	-0.7385450143	0.6751315108
C	3.8611870698	1.5613806280	0.5419849478
C	4.1283462397	0.2261686995	0.8622362142
H	-2.6698527889	-0.0386766088	-1.6945947706
H	-3.4712965752	2.2775313038	-1.3986691071
H	-1.9270594110	4.0165058367	-0.4968254322
H	-1.8496471462	-1.9552699338	-2.2750590945
H	-1.9282260057	-4.0359271408	-1.0021233948
H	1.4490069359	-2.8190646565	1.3863397356
H	-0.2924031361	-4.4825235201	0.8286535881
H	2.4139110249	2.9589475768	-0.1879710210
H	3.3731951871	-1.7812462345	0.8747508122
H	4.6318464960	2.3175884829	0.6584027277
H	5.1085367733	-0.0628448742	1.2301921236
H	0.3775186370	3.4120591837	0.1133760436
H	-2.6068646024	0.2715587518	0.9859822141
Cl	-3.1478137947	-0.0453139809	2.1199892019

Ground state coordinates for: S8

C	1.3228956181	-0.5866336942	-0.1687612341
C	1.0795238201	0.8922803229	-0.4429144676
H	0.9211887552	0.9255883791	-1.5530550317
C	2.6126583583	-1.1225267379	-0.1362270580
C	2.8132569753	-2.4816718022	0.0897735488
C	1.7169476883	-3.3259683930	0.2802154720
C	0.4326830718	-2.8058050839	0.2375561312
C	0.2037351785	-1.4346604110	-0.0006725770
C	-1.1568490952	-0.8842059092	-0.0495167538
C	-1.3726961194	0.5330247219	0.0016067088
C	-0.2488392655	1.4207720653	0.0081716341
C	2.2327026621	1.8267190562	-0.3232979521
C	2.0678206003	3.1281317606	0.0229880752
C	-0.3451406211	2.7854424462	0.3441375874
C	0.7679159595	3.6029210257	0.3617693267
C	-2.2880559021	-1.7164515722	-0.1094473246
C	-2.7011827343	1.0386057194	0.0327241633
C	-3.5738946967	-1.1952648739	-0.0869950534
C	-3.7872825899	0.1912736882	-0.0088290018
H	3.4829727692	-0.4899846622	-0.2595893711
H	3.8234103107	-2.8749896576	0.1357718041
H	1.8660581809	-4.3835686757	0.4697243815
H	-0.4033162868	-3.4719929939	0.4104526329
H	3.2131001331	1.4619715010	-0.6045043383
H	2.9138826386	3.8055030709	0.0575677494
H	-1.2960700097	3.1989060781	0.6546299987
H	0.6494662894	4.6420223148	0.6555038861
H	-2.1681816456	-2.7891459268	-0.1896541482
H	-2.8714357434	2.1081671497	0.0430198488
H	-4.4229633045	-1.8695961083	-0.1380337910
H	-4.7952086761	0.5912410647	-0.0032933236

Ground state coordinates for: S9

C	0.6921574484	-1.2674293906	0.0006669154
C	-0.7738786869	-1.2196545224	0.0005351956
C	1.3919198796	-2.4951232634	0.0022170814
C	2.7737096794	-2.5498540875	0.0010895760
C	3.5133000967	-1.3603698834	-0.0017905778
C	2.8530406936	-0.1451013787	-0.0029021197
C	1.4427427701	-0.0605306835	-0.0013689239

C	0.7514178103	1.2334322965	-0.0010828626
C	-0.6689730721	1.2797151368	0.0004960233
C	-1.4437624357	0.0340744148	-0.0002619145
C	-1.5525146212	-2.3989313651	0.0002353135
C	-2.9349729318	-2.3625077520	-0.0012912123
C	-2.8566518817	0.0424007217	-0.0022026305
C	-3.5950289905	-1.1270167297	-0.0027531379
C	1.4649390275	2.4530560086	-0.0014875798
C	-1.3010104577	2.5435472708	0.0028518735
C	0.8212044281	3.6771117284	0.0001482068
C	-0.5786516804	3.7228915065	0.0026634876
H	0.8440972684	-3.4291236606	0.0044582041
H	3.2779582510	-3.5115743916	0.0023609363
H	4.5988577460	-1.3876029565	-0.0030056740
H	-1.0675096349	-3.3672468106	0.0010402554
H	-3.5021681613	-3.2885015898	-0.0018780468
H	-3.3917710882	0.9839610139	-0.0037932960
H	-4.6800502767	-1.0828928434	-0.0045004094
H	2.5479095177	2.4454031241	-0.0027848527
H	-2.3821290249	2.6070937938	0.0053974249
H	1.4019842074	4.5946507878	-0.0002056506
H	-1.0978025431	4.6766287479	0.0046541394
H	3.4488511155	0.7592118595	-0.0050585420

R1 : benzene, R2=R3 : 3-pyridine

Ground state coordinates for: S1

C	1.2987337719	1.0002301603	1.0783745296
C	-1.2985025929	1.0008919004	-1.0791760597
H	0.4951801814	0.8545211355	1.7967840930
H	-0.4950164413	0.8546985762	-1.7975639974
N	2.0224302070	2.1121809925	1.2260443763
C	3.0274554505	2.3141191183	0.3638060731
C	3.3515833681	1.4206996614	-0.6562822020
C	2.5894836266	0.2629970625	-0.7946124844
C	1.5224665343	0.0320889030	0.0835890054
C	0.7078928848	-1.2126923159	0.0096246368
C	-0.7089261921	-1.2122911356	-0.0102429332
C	-1.5227820366	0.0329486165	-0.0843175891
N	-2.0215809084	2.1132348113	-1.2269294593
C	-3.0264763282	2.3158279451	-0.3646897562
C	-2.5896764988	0.2645318586	0.7938563425
C	-3.3511137246	1.4226630747	0.6554560608
C	1.3828080911	-2.4445835261	0.0047034591
C	-1.3845354528	-2.4438014584	-0.0051587707
C	0.6958342088	-3.6556891411	-0.0019424831
C	-0.6982442528	-3.6552943288	0.0016320783
H	3.5988135344	3.2306991873	0.4977624247
H	4.1772777350	1.6303980233	-1.3290650251
H	-3.5972787022	3.2327488550	-0.4986856385
H	-2.8052270048	-0.4498448825	1.5835707624
H	-4.1766772115	1.6328813752	1.3282370524
H	2.4684010899	-2.4427212608	0.0387231246
H	-2.4701278785	-2.4413293918	-0.0391667885
H	1.2467696303	-4.5914116418	0.0010321968
H	-1.2497108916	-4.5907042986	-0.0012168781
H	2.8046242910	-0.4515694534	-1.5842651772

Ground state coordinates for: S2

C	1.1582519105	-1.0454819641	-0.9710445897
C	-1.1577139834	-1.0467531957	0.9717129293
H	0.3312209769	-0.8910038626	-1.6589357615
H	-0.3314813452	-0.8912679102	1.6603313056
N	1.8484712369	-2.1661379168	-1.1269340280
C	2.9449079337	-2.3417781247	-0.3816786583
C	3.4286537702	-1.3685274462	0.5136969755
C	2.7037388645	-0.2040103462	0.6879953967
C	1.5041934581	-0.0187994152	-0.0398859395

C	0.7216085770	1.2084674634	0.0514150280
C	-0.7228766175	1.2076602766	-0.0506700138
C	-1.5041197178	-0.0204973764	0.0402419292
N	-1.8469826374	-2.1680298190	1.1273853208
C	-2.9427759967	-2.3448573060	0.3814709344
C	-2.7030474826	-0.2069978639	-0.6883246724
C	-3.4269116356	-1.3722134198	-0.5143467181
C	1.3923775351	2.4458685264	0.1520178150
C	-1.3950247697	2.4443097423	-0.1513624990
C	0.6993003200	3.6407647702	0.0827415495
C	-0.7032965590	3.6399819918	-0.0820246870
H	3.4534462349	-3.2967988628	-0.4871488060
H	4.3299700913	-1.5586158652	1.0863091740
H	-3.4504560740	-3.3003510526	0.4867884001
H	-3.0214111311	0.5350065747	-1.4135079884
H	-4.3276840842	-1.5632627232	-1.0874936401
H	2.4748693068	2.4572270689	0.2149985800
H	-2.4775201823	2.4544447351	-0.2144686557
H	1.2364020631	4.5822394988	0.1322001787
H	-1.2414510045	4.5808530371	-0.1315302405
H	3.0217831781	0.5384013158	1.4129019414

Ground state coordinates for: S3

C	1.1437449468	-0.6979043279	0.6192208617
C	1.1437513580	0.6978821111	-0.6192204434
H	1.0243860456	-0.0500383347	1.4875678577
H	1.0243756775	0.0500170428	-1.4875656493
N	2.3858134283	-1.2943828903	0.6112057686
C	2.4965217928	-2.5054908085	0.1189261789
C	1.3875373111	-3.2708047329	-0.3362698404
C	0.1157708708	-2.7155222639	-0.3035132186
C	-0.0547914629	-1.4153902341	0.1857814957
C	-1.3307710355	-0.7067871118	0.1119036986
C	-1.3307609290	0.7067997321	-0.1118907912
C	-0.0547705462	1.4153836735	-0.1857690654
N	2.3858285801	1.2943426310	-0.6112139568
C	2.4965596039	2.5054432931	-0.1189212298
C	0.1158154966	2.7155067900	0.3035407817
C	1.3875913912	3.2707679635	0.3362960250
C	-2.5555690691	-1.3790742534	0.2320060986
C	-2.5555483459	1.3791060846	-0.2319906768
C	-3.7597627411	-0.6887294707	0.1217110979
C	-3.7597525595	0.6887798160	-0.1216935366
H	3.4967785960	-2.9325901663	0.0892026965
H	1.5470689068	-4.2725678003	-0.7211939911
H	3.4968227444	2.9325283414	-0.0892050078
H	-0.7333007615	3.2700520692	0.6887396740
H	1.5471424830	4.2725225020	0.7212343028
H	-2.5659717892	-2.4425598592	0.4463435551
H	-2.5659341123	2.4425921198	-0.4463270393
H	-4.6983197460	-1.2229191343	0.2253616423
H	-4.6983016259	1.2229838319	-0.2253420422
H	-0.7333563334	-3.2700584764	-0.6887008596

Ground state coordinates for: S4

C	1.2426407462	-0.7112908070	0.3017753780
C	1.2426589930	0.7112580930	-0.3017697582
H	1.3138258916	-0.5733657393	1.4029227646
H	1.3138416397	0.5733314030	-1.4029170629
N	2.4738649064	-1.3874932731	-0.0529699062
C	2.4510455538	-2.6684215796	-0.1735860395
C	1.2480981361	-3.4692250637	-0.0689819607
C	0.0230695865	-2.8571459867	0.0129539636
C	-0.0605630077	-1.4437157423	0.0790631714
C	-1.2875544761	-0.7255481153	0.0297870988
C	-1.2875360653	0.7255798055	-0.0297831944
C	-0.0605261365	1.4437161071	-0.0790583179
N	2.4739001260	1.3874286683	0.0529773978
C	2.4511133401	2.6683572823	0.1735960311
C	0.0231424731	2.8571442403	-0.0129480889

C	1.2481865624	3.4691918268	0.0689913236
C	-2.5423588852	-1.3982766551	0.0583705220
C	-2.5423232740	1.3983403836	-0.0583666565
C	-3.7315692419	-0.7059890711	0.0310261337
C	-3.7315512746	0.7060830960	-0.0310221840
H	3.3944047796	-3.1648726826	-0.3992034279
H	1.3227551607	-4.5501558577	-0.1314470418
H	3.3944849723	3.1647837457	0.3992157388
H	-0.8712226387	3.4660127086	0.0362339248
H	1.3228712365	4.5501206036	0.1314580268
H	-2.5750349012	-2.4782062281	0.1225244431
H	-2.5749714742	2.4782708158	-0.1225205297
H	-4.6723105072	-1.2455082030	0.0603063151
H	-4.6722787223	1.2456263349	-0.0603022877
H	-0.8713107768	-3.4659920081	-0.0362296082

Ground state coordinates for: S5=S6

C	0.9395154591	-0.7944640276	-0.5213917682
C	0.9393613478	0.6777881833	-1.0144823564
H	0.6972385404	0.5785236464	-2.0948588337
N	2.0472816173	-1.5234752896	-0.8633504921
C	2.0086118604	-2.8324456012	-0.7162148613
C	0.8463395369	-3.5234334278	-0.3204160600
C	-0.3286533579	-2.8149495023	-0.1457538465
C	-0.3384825883	-1.4160646432	-0.3096043311
C	-1.5518468036	-0.6038178553	-0.1691679387
C	-1.4660394847	0.8223815888	-0.1910025030
C	-0.1860716805	1.4748969266	-0.3875904600
N	2.2743589822	1.2426526146	-0.9823037333
C	2.3987617848	2.4895528406	-0.6585944875
C	0.0567211148	2.8112423681	-0.0871472861
C	1.3271289037	3.3528471278	-0.2532159207
C	-2.8123076688	-1.2055201441	0.0105404039
C	-2.6547224675	1.5675619708	-0.0200318218
C	-3.9641323101	-0.4494655176	0.1733344199
C	-3.8809470266	0.9490158453	0.1610449830
H	2.9238215674	-3.3771063854	-0.9412990040
H	0.8689753227	-4.6008191484	-0.1891948162
H	3.4134762672	2.8918948314	-0.6724729107
H	-0.7297134728	3.4265146338	0.3383888681
H	1.5335444864	4.3866460305	0.0013152164
H	-2.9013929454	-2.2856493066	0.0155936389
H	-2.6124484567	2.6501173287	-0.0606366517
H	-4.9222337360	-0.9421637189	0.3054994832
H	-4.7772766767	1.5506710461	0.2791672075
H	-1.2358134485	-3.3496195203	0.1091452475
H	1.2259886132	-0.5730957227	0.7063419494
Cl	1.5753586654	-0.2365838027	2.1454925677

Ground state coordinates for: S7

C	-0.7166145450	0.5643367540	-0.4944294643
C	-0.4569279512	-0.9179791383	-0.7664832584
H	-0.1543856806	-0.9478624502	-1.8379988467
N	-1.9687186237	1.0149595822	-0.5983011586
C	-2.2207246747	2.3157327389	-0.4037401676
C	-1.2197695638	3.2283787537	-0.0859083857
C	0.0855870522	2.7635855167	0.0283845595
C	0.3740079933	1.4077668142	-0.1914624571
C	1.7359345579	0.8464296830	-0.0767861444
C	1.9017342550	-0.5586527476	0.0896294810
C	0.7391146121	-1.4263097903	0.0151709385
N	-1.6869882208	-1.6855108009	-0.7028186563
C	-1.6451919398	-2.8679422296	-0.1755283950
C	0.6792932670	-2.7104276296	0.5387382923
C	-0.4884303170	-3.4648385944	0.4263121458
C	2.8729515124	1.6692115551	-0.0695013631
C	3.2009828301	-1.0675250185	0.3000470081
C	4.1460626127	1.1442797549	0.1285703072
C	4.3083446689	-0.2317348967	0.3251942692
H	-3.2612120471	2.6159906039	-0.5000679832

H	-1.4597363955	4.2731987778	0.0802852212
H	-2.5834604739	-3.4250603461	-0.1731681146
H	1.5291919952	-3.1169434522	1.0795069214
H	-0.5548028947	-4.4624409429	0.8467358410
H	2.7665314910	2.7363649941	-0.2344746919
H	3.3407962009	-2.1384137458	0.4058813829
H	5.0094497275	1.8024992253	0.1214592852
H	5.2994360777	-0.6502382000	0.4725707466
H	0.8759895822	3.4514391805	0.3092633075
H	-3.4476537240	0.1650252095	-0.9139799201
Cl	-4.7687341997	-0.0419402891	-1.0999408733

Ground state coordinates for: S8

C	1.3999638014	0.3625452602	-0.1435944383
C	0.2937148091	1.3853725689	-0.3887161028
H	0.2383704621	1.3625399406	-1.5078591436
N	2.6449044907	0.8211093631	-0.1656807267
C	3.6387161854	-0.0487445591	0.0239744921
C	3.4242123316	-1.4171629299	0.2331666675
C	2.1248574315	-1.8923147192	0.2187275336
C	1.0528636171	-0.9973698821	0.0118589553
C	-0.3475402568	-1.4199420518	-0.0256919717
C	-1.4083025744	-0.4454354428	-0.0565752008
C	-1.0901944178	0.9421159929	-0.0447069653
N	0.6931974437	2.7426563822	-0.1465011543
C	-0.2185261036	3.6015883659	0.1571010518
C	-2.0361690952	1.9669867791	0.2280526388
C	-1.6147852098	3.2651987169	0.3293854723
C	-0.7075330209	-2.7779537140	-0.0057489250
C	-2.7633893038	-0.8859876076	-0.0602814112
C	-2.0369623281	-3.1747219599	-0.0160326701
C	-3.0759440975	-2.2260201038	-0.0442201125
H	4.6453179222	0.3612689759	0.0073031759
H	4.2623825310	-2.0870972031	0.3894793860
H	1.9455761150	-2.9500837041	0.3698081710
H	0.0984925049	4.6329789146	0.3042832949
H	-3.0719428674	1.7238772640	0.4297395592
H	-2.3203133160	4.0539925066	0.5728703138
H	0.0581235115	-3.5431008734	0.0027837878
H	-3.5657228913	-0.1606453107	-0.1142272511
H	-2.2761793977	-4.2335850582	-0.0101745144
H	-4.1107419162	-2.5493028633	-0.0653645782

Ground state coordinates for: S9

C	0.7339059361	-1.2317427043	0.0000454572
C	-0.7343774222	-1.2314939181	0.0000856560
N	1.3530295633	-2.4313327736	0.0004014910
C	2.6766512674	-2.4600776706	-0.0000349066
C	3.4748946579	-1.3059056026	-0.0009891340
C	2.8460278633	-0.0758948713	-0.0012462713
C	1.4377430966	0.0001212647	-0.0005842241
C	0.7107997647	1.2716758696	-0.0003713405
C	-0.7104241624	1.2719143980	0.0000864512
C	-1.4377975331	0.0006092411	-0.0001981531
N	-1.3539076857	-2.4308734218	0.0001511992
C	-2.6775396551	-2.4591697249	-0.0002175718
C	-2.8461077186	-0.0749288846	-0.0008903174
C	-3.4753910678	-1.3047252306	-0.0008769191
C	1.3866483707	2.5111135487	-0.0003737647
C	-1.3858524260	2.5115817299	0.0008647579
C	0.7011510141	3.7130033726	0.0001685465
C	-0.6999482376	3.7132392517	0.0008859454
H	3.1379908924	-3.4468556699	0.0003602475
H	4.5575458633	-1.3823283245	-0.0015137901
H	-3.1392167196	-3.4457896830	-0.0000683667
H	-3.4475632437	0.8267039373	-0.0016024856
H	-4.5580682541	-1.3807828047	-0.0014425534
H	2.4700574284	2.5357494243	-0.0007138178
H	-2.4692527908	2.5365887434	0.0016510978
H	1.2499935210	4.6498290143	0.0001409087

H -1.2484726105 4.6502510285 0.0015350346  
H 3.4477854269 0.8255353479 -0.0020004589

R1 : benzene, R2=R3 : 2-thiophene

Ground state coordinates for: S1

C 1.2827631631 -1.0568715306 1.2686384138  
C -1.2827631631 1.0568715306 1.2686384138  
H 0.4175117649 -1.7044184211 1.3413881893  
H -0.4175117649 1.7044184211 1.3413881893  
C 1.4995425312 -0.2317888530 0.1917647885  
S 2.9975400185 0.6596612034 0.4115633339  
C 3.2955036028 -0.0993850330 1.9410458789  
C 2.3021224086 -0.9833263467 2.2614365146  
C 0.7066490710 -0.0773732796 -1.0445399734  
C -0.7066490710 0.0773732796 -1.0445399734  
C -1.4995425312 0.2317888530 0.1917647885  
S -2.9975400185 -0.6596612034 0.4115633339  
C -3.2955036028 0.0993850330 1.9410458789  
C -2.3021224086 0.9833263467 2.2614365146  
C 1.3771579606 -0.1240638599 -2.2794970032  
C 0.6947145517 -0.0554066569 -3.4903568346  
C -0.6947145517 0.0554066569 -3.4903568346  
C -1.3771579606 0.1240638599 -2.2794970032  
H 4.1802293060 0.1542187527 2.5082845508  
H 2.2969833405 -1.5690646114 3.1736215754  
H -4.1802293060 -0.1542187527 2.5082845508  
H -2.2969833405 1.5690646114 3.1736215754  
H 2.4552369153 -0.2516028792 -2.2784179128  
H 1.2453727516 -0.1028840122 -4.4249596738  
H -1.2453727516 0.1028840122 -4.4249596738  
H -2.4552369153 0.2516028792 -2.2784179128

Ground state coordinates for: S2

C 1.1870626950 -0.9799105203 1.2895555197  
C -1.1870626950 0.9799105203 1.2895555197  
H 0.2901168684 -1.5833033077 1.3394731824  
H -0.2901168684 1.5833033077 1.3394731824  
C 1.4865391993 -0.1606092265 0.1866234740  
S 3.0753116536 0.5642971528 0.3898979446  
C 3.2780821883 -0.2083651007 1.9198512493  
C 2.2007565596 -1.0031110183 2.2612208381  
C 0.7224852296 0.0177940932 -1.0259406026  
C -0.7224852296 -0.0177940932 -1.0259406026  
C -1.4865391993 0.1606092265 0.1866234740  
S -3.0753116536 -0.5642971528 0.3898979446  
C -3.2780821883 0.2083651007 1.9198512493  
C -2.2007565596 1.0031110183 2.2612208381  
C 1.3945736774 0.1255471287 -2.2656973197  
C 0.7008339844 0.0768670442 -3.4597807604  
C -0.7008339844 -0.0768670442 -3.4597807604  
C -1.3945736774 -0.1255471287 -2.2656973197  
H 4.1795843782 -0.0329978786 2.4928464612  
H 2.1594776600 -1.5876404162 3.1719546565  
H -4.1795843782 0.0329978786 2.4928464612  
H -2.1594776600 1.5876404162 3.1719546565  
H 2.4785850664 0.1650720148 -2.2779007948  
H 1.2403952253 0.1250686416 -4.3997350089  
H -1.2403952253 -0.1250686416 -4.3997350089  
H -2.4785850664 -0.1650720148 -2.2779007948

Ground state coordinates for: S3

C 0.6493769637 -0.6078811102 1.3223162182  
C -0.6493769637 0.6078811102 1.3223162182  
H 0.0476337512 -1.5179930164 1.3132161384  
H -0.0476337512 1.5179930164 1.3132161384  
C 1.3628173519 -0.2964414431 0.0862883911  
S 2.9451891258 0.3024658644 0.4000006773



C	2.7802900977	0.0180914846	2.1267387401
C	1.5661727842	-0.4631189536	2.4643758316
C	0.6996414074	-0.1609752575	-1.2003703092
C	-0.6996414074	0.1609752575	-1.2003703092
C	-1.3628173519	0.2964414431	0.0862883911
S	-2.9451891258	-0.3024658644	0.4000006773
C	-2.7802900977	-0.0180914846	2.1267387401
C	-1.5661727842	0.4631189536	2.4643758316
C	1.3622435379	-0.3198201161	-2.4202026333
C	0.6784512069	-0.1585752544	-3.6293183189
C	-0.6784512069	0.1585752544	-3.6293183189
C	-1.3622435379	0.3198201161	-2.4202026333
H	3.6259068482	0.2164559767	2.7725843478
H	1.2868038742	-0.7252631281	3.4780047560
H	-3.6259068482	-0.2164559767	2.7725843478
H	-1.2868038742	0.7252631281	3.4780047560
H	2.4102569313	-0.6034062099	-2.4272247588
H	1.2089966668	-0.2875856565	-4.5666281494
H	-1.2089966668	0.2875856565	-4.5666281494
H	-2.4102569313	0.6034062099	-2.4272247588

Ground state coordinates for: S4

C	0.6589331789	-0.3989623159	1.3715908866
C	-0.6589331789	0.3989623159	1.3715908866
H	0.3877356945	-1.4728285016	1.3400934854
H	-0.3877356945	1.4728285016	1.3400934854
C	1.4003720241	-0.0991939240	0.0839251919
S	3.0967744927	0.0788243689	0.3471444599
C	2.8912054195	-0.0074472407	2.1135168672
C	1.6276722127	-0.2024461967	2.5025449862
C	0.7299377717	0.0096314193	-1.1412877437
C	-0.7299377717	-0.0096314193	-1.1412877437
C	-1.4003720241	0.0991939240	0.0839251919
S	-3.0967744927	-0.0788243689	0.3471444599
C	-2.8912054195	0.0074472407	2.1135168672
C	-1.6276722127	0.2024461967	2.5025449862
C	1.4082637993	0.0802748056	-2.3931047908
C	0.7089529848	0.0495306454	-3.5754970439
C	-0.7089529848	-0.0495306454	-3.5754970439
C	-1.4082637993	-0.0802748056	-2.3931047908
H	3.7750702648	0.0898735505	2.7310731102
H	1.3355891388	-0.3057753023	3.5413234144
H	-3.7750702648	-0.0898735505	2.7310731102
H	-1.3355891388	0.3057753023	3.5413234144
H	2.4928731577	0.1228153603	-2.4089578934
H	1.2418962367	0.0865084654	-4.5196279942
H	-1.2418962367	-0.0865084654	-4.5196279942
H	-2.4928731577	-0.1228153603	-2.4089578934

Ground state coordinates for: S5=S6

C	1.1398750413	0.5564016377	-0.5460735764
C	-0.1192799352	1.2861766524	-1.0177692087
H	1.1811965017	0.8831356686	0.6794463311
H	-0.1725951399	1.1258793305	-2.1172610630
C	1.0135050971	-0.8641328213	-0.4516339877
S	2.5653761114	-1.6337832053	-0.5649063563
C	3.3548330384	-0.1149121703	-0.9519915836
C	2.4929333778	0.9253863087	-0.9566617808
C	-0.2255171406	-1.5319998080	-0.2031802956
C	-1.4231924993	-0.7213330701	-0.1128431876
C	-1.3466060149	0.6493449054	-0.4042766098
S	-2.5939591236	1.8364990337	-0.0859574501
C	-1.4566035935	3.1651071547	-0.4009527705
C	-0.2444944608	2.7712451232	-0.7989163349
C	-0.3153242329	-2.9218112837	0.0215987099
C	-1.5164961828	-3.5175304728	0.3590986697
C	-2.6779413223	-2.7250743521	0.4988680912
C	-2.6332847780	-1.3664781656	0.2765493040
H	4.4234366252	-0.1046222091	-1.1165925164
H	2.7977511539	1.9507397933	-1.1290912171

H	-1.8021755094	4.1789247249	-0.2455135068
H	0.5567807361	3.4617988576	-1.0349458539
H	0.5813603866	-3.5304455387	-0.0564030447
H	-1.5643589430	-4.5876408459	0.5311017333
H	-3.6168612049	-3.1929342617	0.7789847649
H	-3.5369125037	-0.7727971098	0.3760503627
Cl	1.2046866623	1.4740427767	2.1548204218

Ground state coordinates for: S7

C	1.0769659612	0.4947999980	-0.9149759226
C	-0.1914032251	1.2656330886	-1.1985423945
H	1.3407102444	0.8817073154	1.4785835734
H	-0.3629597760	1.1770720859	-2.2971873009
C	0.9909629031	-0.8369607531	-0.5408682817
S	2.5857268683	-1.5493536839	-0.4272598609
C	3.3387836299	-0.0594624392	-0.9019597353
C	2.4214313524	0.9295575541	-1.1288391088
C	-0.2528874362	-1.5328321866	-0.2570909730
C	-1.4547628763	-0.7389860778	-0.1909581685
C	-1.3775854429	0.6384901270	-0.5000336337
S	-2.5781144368	1.8492145689	-0.0687364530
C	-1.4155671766	3.1543206559	-0.3870543100
C	-0.2490118126	2.7464065969	-0.8968918976
C	-0.3197578783	-2.9028810444	0.0241105079
C	-1.5195702901	-3.5076616496	0.3903261959
C	-2.6871822932	-2.7343508870	0.4959071244
C	-2.6557726108	-1.3789359579	0.2164768386
H	4.4159992509	-0.0003767043	-0.9709146516
H	2.6945517779	1.9334834568	-1.4331553803
H	-1.7143961217	4.1708524172	-0.1631734529
H	0.5532613050	3.4249887197	-1.1650970677
H	0.5846684727	-3.5028826977	-0.0344153118
H	-1.5472037677	-4.5718989604	0.6016815305
H	-3.6222320166	-3.2012469502	0.7910119319
H	-3.5674528834	-0.7922206975	0.2863660889
Cl	1.5789304252	1.3227107584	2.6742381579

Ground state coordinates for: S8

C	0.7943971434	-1.3528190210	0.1396843695
C	-0.6743511633	-1.4016109146	0.4302643405
H	-0.71139861127	-1.3746912846	1.5478580943
C	1.3982218334	-0.1041801748	0.0368127383
S	3.1234896010	-0.2727571909	-0.1795517399
C	2.9994524005	-1.9935622029	-0.1083910924
C	1.7103397461	-2.4307539118	0.0718188411
C	0.6797103725	1.1406229995	0.0730592889
C	-0.7660352685	1.1195875468	0.1038019262
C	-1.4102685027	-0.1336420566	0.1200279136
S	-3.0604157703	-0.4449797458	-0.2206110393
C	-2.8168746694	-2.2040978851	-0.1933955452
C	-1.5589737022	-2.5620460354	0.0887567867
C	1.3209850987	2.3937549382	0.0261401131
C	0.5879544321	3.5675277901	-0.0019661077
C	-0.8249923588	3.5494385931	0.0107070088
C	-1.4880985722	2.3464065270	0.0568342537
H	3.8908327070	-2.5962311792	-0.2197287372
H	1.4437092571	-3.4785130747	0.1353710437
H	-3.6698849693	-2.8387713893	-0.3961648586
H	-1.2280648862	-3.5906077610	0.1658414107
H	2.4048709016	2.4402376411	0.0098572305
H	1.1087825612	4.5191686855	-0.0368307617
H	-1.3795555108	4.4808535294	-0.0090354443
H	-2.5733914483	2.3259271633	0.0848987568

Ground state coordinates for: S9

C	0.7176301222	-1.3692842487	0.0013936957
C	-0.7167097511	-1.3696898134	0.0016677431
C	1.3886639341	-0.1428368367	0.0009793473
S	3.1261792410	-0.3822715533	0.0005004466
C	2.9246753144	-2.1139529422	0.0011332670

C	1.6165155163	-2.4886446036	0.0014436292
C	0.7162434782	1.1222480772	0.0008711784
C	-0.7167590921	1.1218508244	0.0012088923
C	-1.3884585746	-0.1436168630	0.0015316276
S	-3.1258454210	-0.3840768023	0.0021099377
C	-2.9233440762	-2.1156417262	0.0020452657
C	-1.6149599053	-2.4895746292	0.0016736220
C	1.3965461228	2.3627873540	0.0004596784
C	0.7037109047	3.5566796018	0.0004539407
C	-0.7055729274	3.5562864860	0.0009233749
C	-1.3977501576	2.3620093126	0.0013124446
H	3.7990257863	-2.7499707877	0.0011130915
H	1.2948276590	-3.5234523041	0.0017745728
H	-3.7973188000	-2.7521753238	0.0022462795
H	-1.2926760010	-3.5241929796	0.0016493390
H	2.4829390587	2.3697124069	0.0001520984
H	1.2457012682	4.4974124978	0.0001221742
H	-1.2480843507	4.4967176678	0.0010074786
H	-2.4841482633	2.3683254655	0.0016962674

R1: benzene, R2=R3 : 2-pyrrole

Ground state coordinates for: S1

C	1.3799360683	1.5545382674	0.8720522437
C	-1.3799234878	1.5545498426	-0.8720519678
H	0.5201449030	1.8183390205	1.4686501442
H	-0.5201304780	1.8183426702	-1.4686507218
C	1.5275321952	0.3713549442	0.1623081210
N	2.7769166416	0.4260243477	-0.4335417561
C	3.3985380081	1.6119559791	-0.1358324323
C	2.5548065686	2.3293510448	0.6871257692
C	0.7088579661	-0.8476111303	0.0602695793
C	-0.7088660391	-0.8476049998	-0.0602685911
C	-1.5275294948	0.3713683063	-0.1623069501
N	-2.7769137554	0.4260485161	0.4335424442
C	-3.3985234180	1.6119869374	0.1358357340
C	-2.5547862771	2.3293739330	-0.6871236657
C	1.3741776328	-2.0874142729	0.1078464495
C	0.6948309942	-3.3009205460	0.0501645339
C	-0.6948603907	-3.3009145051	-0.0501641198
C	-1.3741965010	-2.0874023076	-0.1078457430
H	4.3735051478	1.8478074559	-0.5353098569
H	2.7606270694	3.3020520794	1.1111757173
H	-4.3734877419	1.8478477017	0.5353145508
H	-2.7605980041	3.3020770876	-1.1111730176
H	2.4521672741	-2.0913196826	0.2420488251
H	1.2470341300	-4.2347264854	0.0991245349
H	-1.2470716544	-4.2347156357	-0.0991243119
H	-2.4521861880	-2.0912981565	-0.2420479927
H	-3.1226737630	-0.2659348921	1.0789521174
H	3.1226674121	-0.2659586106	-1.0789568566

Ground state coordinates for: S2

C	1.2786323505	0.8666690284	-1.4744482455
C	-1.2786323505	-0.8666690284	-1.4744482455
H	0.4357523763	1.5220529292	-1.6292415289
H	-0.4357523763	-1.5220529292	-1.6292415289
C	1.4873577001	0.0727095722	-0.3163412965
N	2.7301056703	-0.5114439996	-0.4709249719
C	3.2719931528	-0.1511830910	-1.6707987328
C	2.3909009191	0.7222457814	-2.3071312322
C	0.7165356049	-0.0479996409	0.8968300312
C	-0.7165356049	0.0479996409	0.8968300312
C	-1.4873577001	-0.0727095722	-0.3163412965
N	-2.7301056703	0.5114439996	-0.4709249719
C	-3.2719931528	0.1511830910	-1.6707987328
C	-2.3909009191	-0.7222457814	-2.3071312322
C	1.3874255928	-0.1614032450	2.1372927934

C	0.6980746624	-0.0915571475	3.3332058968
C	-0.6980746624	0.0915571475	3.3332058968
C	-1.3874255928	0.1614032450	2.1372927934
H	4.2307344811	-0.5343427553	-1.9893274857
H	2.5625516784	1.2062650509	-3.2571238272
H	-4.2307344811	0.5343427553	-1.9893274857
H	-2.5625516784	-1.2062650509	-3.2571238272
H	2.4709630517	-0.2186819285	2.1528663191
H	1.2375732777	-0.1493150509	4.2726535888
H	-1.2375732777	0.1493150509	4.2726535888
H	-2.4709630517	0.2186819285	2.1528663191
H	-3.1260224112	1.1984830088	0.1542002015
H	3.1260224112	-1.1984830088	0.1542002015

Ground state coordinates for: S3

C	-0.5765933983	-0.6845183152	1.4816588310
C	0.5765933983	0.6845183152	1.4816588310
H	-1.5142791521	-0.1348688983	1.5322696610
H	1.5142791521	0.1348688983	1.5322696610
C	-0.2340483588	-1.3534378151	0.2250500029
N	0.2814605191	-2.5637172702	0.5407318680
C	0.2312170670	-2.7835871455	1.9170334170
C	-0.3168377888	-1.6952247827	2.5171501635
C	-0.1264395682	-0.7040235126	-1.0724848337
C	0.1264395682	0.7040235126	-1.0724848337
C	0.2340483588	1.3534378151	0.2250500029
N	-0.2814605191	2.5637172702	0.5407318680
C	-0.2312170670	2.7835871455	1.9170334170
C	0.3168377888	1.6952247827	2.5171501635
C	-0.2551163805	-1.3767321234	-2.2889314830
C	-0.1255682991	-0.6848996332	-3.4986810659
C	0.1255682991	0.6848996332	-3.4986810659
C	0.2551163805	1.3767321234	-2.2889314830
H	0.5770057628	-3.7194700901	2.3311189128
H	-0.5263943694	-1.5871164412	3.5711641564
H	-0.5770057628	3.7194700901	2.3311189128
H	0.5263943694	1.5871164412	3.5711641564
H	-0.4961515974	-2.4357296223	-2.2988290583
H	-0.2299179487	-1.2200617810	-4.4364924034
H	0.2299179487	1.2200617810	-4.4364924034
H	0.4961515974	2.4357296223	-2.2988290583
H	-0.7404947134	3.1780144629	-0.1188629874
H	0.7404947134	-3.1780144629	-0.1188629874

Ground state coordinates for: S4

C	-0.3978177586	-0.6544832687	1.5034458932
C	0.3978177586	0.6544832687	1.5034458932
H	-1.4736406127	-0.3914751968	1.5008038994
H	1.4736406127	0.3914751968	1.5008038994
C	-0.1052979834	-1.3808923305	0.2029153924
N	0.0473077917	-2.6880098807	0.5070401371
C	0.0335510397	-2.8886517468	1.9049968994
C	-0.1642922971	-1.7238913607	2.5417943438
C	0.0014064246	-0.7281629964	-1.0354785386
C	-0.0014064246	0.7281629964	-1.0354785386
C	0.1052979834	1.3808923305	0.2029153924
N	-0.0473077917	2.6880098807	0.5070401371
C	-0.0335510397	2.8886517468	1.9049968994
C	0.1642922971	1.7238913607	2.5417943438
C	0.0529961853	-1.4087134170	-2.2851488874
C	0.0338711834	-0.7100444624	-3.4682354191
C	-0.0338711834	0.7100444624	-3.4682354191
C	-0.0529961853	1.4087134170	-2.2851488874
H	0.1633162176	-3.8873756315	2.2974257277
H	-0.2591683994	-1.5900914044	3.6095905335
H	-0.1633162176	3.8873756315	2.2974257277
H	0.2591683994	1.5900914044	3.6095905335
H	0.0676853354	-2.4943956543	-2.3090439043
H	0.0574352270	-1.2438380184	-4.4122095087
H	-0.0574352270	1.2438380184	-4.4122095087

H	-0.0676853354	2.4943956543	-2.3090439043
H	-0.2819054463	3.4128435906	-0.1567294324
H	0.2819054463	-3.4128435906	-0.1567294324

Ground state coordinates for: S5=S6

C	-1.0535592427	0.3322808012	-0.9356018178
C	-0.6475624332	-1.0997195824	-1.2541146344
H	-0.3031063035	-1.1130311642	-2.3103160919
C	0.0280588342	1.2286934673	-0.6640157603
N	-0.4216580299	2.4856650122	-0.9133385947
C	-1.7139240423	2.4466257552	-1.4349202165
C	-2.1028259363	1.1453772342	-1.5357405169
C	1.3110356652	0.8313487474	-0.1550797370
C	1.5104062316	-0.5860429726	0.0659232025
C	0.5116047936	-1.4781298057	-0.3536754035
N	0.3396498342	-2.7963773363	0.0209797170
C	-0.9550376743	-3.2120059964	-0.3496562976
C	-1.5895765447	-2.2683070894	-1.0622654590
C	2.3212209385	1.7371365235	0.2069125522
C	3.4963327664	1.3038950142	0.8053630957
C	3.6776172612	-0.0708741274	1.0687893946
C	2.7123921735	-0.9920520902	0.7155753434
H	-2.2382535078	3.3628425909	-1.6623310760
H	-3.0648100879	0.7938908654	-1.8796292637
H	-1.2909968102	-4.2007112641	-0.0669860013
H	-2.5639409918	-2.3631566804	-1.5196368468
H	2.1807273859	2.8009474825	0.0288326495
H	4.2660000805	2.0185914512	1.0774329088
H	4.5938450001	-0.4099049628	1.5436078303
H	2.8897191057	-2.0491402545	0.8934142921
H	0.7774161150	-3.1586882398	0.8571207941
H	0.0659066784	3.3337307653	-0.6671648470
H	-1.5363735083	0.2259417149	0.3206157688
Cl	-2.1288502061	0.0104369197	1.7575284438

Ground state coordinates for: S7

C	-0.9010924477	-0.0136904542	-1.0542620211
C	-0.3116037566	-1.3951104949	-1.1056838371
H	-0.0256560381	-1.5888332729	-2.1652878238
C	-0.0947762305	1.0628468070	-0.7048154906
N	-0.8581066748	2.2066010067	-0.8403624251
C	-2.1228507331	1.8778009374	-1.2568340454
C	-2.1819324790	0.4998088438	-1.4082813979
C	1.2764379987	0.9734720547	-0.2409028845
C	1.7723773135	-0.3545684124	0.0380041011
C	0.9366409980	-1.4531138605	-0.2499474291
N	1.0072700686	-2.7271260075	0.3012445818
C	-0.2435828670	-3.3543268578	0.1389884855
C	-1.0679567008	-2.6240906885	-0.6305386666
C	2.0903771903	2.0776961617	0.0240668513
C	3.3611092242	1.9257468521	0.5828695957
C	3.8344792679	0.6412701172	0.8938483867
C	3.0584817780	-0.4767218670	0.6300197089
H	-2.8751514958	2.6358363366	-1.4166706075
H	-3.0319856249	-0.0567271389	-1.7796276038
H	-0.4088137259	-4.3240529860	0.5904781141
H	-2.0477072743	-2.9227297711	-0.9762223189
H	1.7307565392	3.0794310147	-0.2016384418
H	3.9765984727	2.7985207238	0.7770369322
H	4.8219893964	0.5195818270	1.3300368484
H	3.4557739403	-1.4668620433	0.8384280294
H	1.5521181283	-2.8875781203	1.1379973456
H	-0.5674798188	3.1314532880	-0.5662694364
H	-2.9453806121	0.4477466163	0.6708426307
Cl	-3.4983760383	0.3177308084	1.8479778456

Ground state coordinates for: S8

C	1.5171870267	-0.7399392886	-0.0860191143
C	1.5174117727	0.7236814431	-0.3815932982
H	1.5237800580	0.7934461560	-1.4955819463

C	0.2796759009	-1.3829259791	0.0168989306
N	0.5440087780	-2.7280499528	0.1628427814
C	1.8943847790	-2.9334268602	0.1480154802
C	2.5326758675	-1.7141910555	-0.0213680752
C	-0.9998143370	-0.7300674493	-0.0212817651
C	-1.0364727348	0.7090856190	-0.0529881580
C	0.2134704159	1.3865066237	-0.0527944995
N	0.4922841783	2.6464294729	0.2794930281
C	1.8895649398	2.8765861517	0.3371548214
C	2.5433420942	1.7465408329	0.0244189962
C	-2.2299076739	-1.4158980016	0.0161548016
C	-3.4309566293	-0.7254928022	0.0343892111
C	-3.4633003437	0.6831447114	0.0168236349
C	-2.2785851372	1.3882418127	-0.0218311729
H	2.3088903008	-3.9222076045	0.2759275363
H	3.6010477359	-1.5644963423	-0.0722483020
H	2.2559136411	3.8579028869	0.6016009589
H	3.6138315621	1.6199098254	-0.0433433610
H	-2.2458763190	-2.5009402514	0.0251600365
H	-4.3632144798	-1.2807398912	0.0598411968
H	-4.4128753315	1.2061502843	0.0226362592
H	-2.3037684659	2.4736267380	-0.0650423448
H	-0.1984868910	3.3398689039	0.5385948508
H	-0.1408495513	-3.4536142910	0.3091530730

Ground state coordinates for: S9

C	1.5124134843	-0.7111575323	0.0002988024
C	1.5087699067	0.7191921912	0.0002579954
C	0.2735973731	-1.3769829064	-0.0003251696
N	0.5409052606	-2.7322022572	0.0000133632
C	1.9032552406	-2.9318229916	0.0004240060
C	2.5337560797	-1.7092697032	0.0008506766
C	-0.9992766806	-0.7203851239	-0.0013392016
C	-1.0029219676	0.7158126512	-0.0015867162
C	0.2666405370	1.3787889951	-0.0005712523
N	0.5270984126	2.7353521799	-0.0004839422
C	1.8883546350	2.9418080109	0.0006907024
C	2.5250787499	1.7224475657	0.0011652030
C	-2.2374232649	-1.4006842377	-0.0020896345
C	-3.4370131997	-0.7120159225	-0.0031726221
C	-3.4405720165	0.6951445593	-0.0036132390
C	-2.2444707104	1.3898574188	-0.0028429835
H	2.3141531117	-3.9307975284	0.0005096497
H	3.6021820229	-1.5488939483	0.0013610008
H	2.2942763548	3.9428241067	0.0014808454
H	3.5943109243	1.5675728535	0.0017553916
H	-2.2521485816	-2.4880859132	-0.0018929532
H	-4.3756994921	-1.2578928746	-0.0037246514
H	-4.3820160457	1.2362471283	-0.0045875039
H	-2.2647609981	2.4771706299	-0.0034004807
H	-0.1660039672	3.4643823344	-0.0003397790
H	-0.1484679616	-3.4647662620	0.0004676446

R1 : benzene, R2=R3 : 3-pyridine

Ground state coordinates for: S1

C	1.2987337719	1.0002301603	1.0783745296
C	-1.2985025929	1.0008919004	-1.0791760597
H	0.4951801814	0.8545211355	1.7967840930
H	-0.4950164413	0.8546985762	-1.7975639974
N	2.0224302070	2.1121809925	1.2260443763
C	3.0274554505	2.3141191183	0.3638060731
C	3.3515833681	1.4206996614	-0.6562822020
C	2.5894836266	0.2629970625	-0.7946124844
C	1.5224665343	0.0320889030	0.0835890054
C	0.7078928848	-1.2126923159	0.0096246368
C	-0.7089261921	-1.2122911356	-0.0102429332
C	-1.5227820366	0.0329486165	-0.0843175891

N	-2.0215809084	2.1132348113	-1.2269294593
C	-3.0264763282	2.3158279451	-0.3646897562
C	-2.5896764988	0.2645318586	0.7938563425
C	-3.3511137246	1.4226630747	0.6554560608
C	1.3828080911	-2.4445835261	0.0047034591
C	-1.3845354528	-2.4438014584	-0.0051587707
C	0.6958342088	-3.6556891411	-0.0019424831
C	-0.6982442528	-3.6552943288	0.0016320783
H	3.5988135344	3.2306991873	0.4977624247
H	4.1772777350	1.6303980233	-1.3290650251
H	-3.5972787022	3.2327488550	-0.4986856385
H	-2.8052270048	-0.4498448825	1.5835707624
H	-4.1766772115	1.6328813752	1.3282370524
H	2.4684010899	-2.4427212608	0.0387231246
H	-2.4701278785	-2.4413293918	-0.0391667885
H	1.2467696303	-4.5914116418	0.0010321968
H	-1.2497108916	-4.5907042986	-0.0012168781
H	2.8046242910	-0.4515694534	-1.5842651772

Ground state coordinates for: S2

C	1.1582519105	-1.0454819641	-0.9710445897
C	-1.1577139834	-1.0467531957	0.9717129293
H	0.3312209769	-0.8910038626	-1.6589357615
H	-0.3314813452	-0.8912679102	1.6603313056
N	1.8484712369	-2.1661379168	-1.1269340280
C	2.9449079337	-2.3417781247	-0.3816786583
C	3.4286537702	-1.3685274462	0.5136969755
C	2.7037388645	-0.2040103462	0.6879953967
C	1.5041934581	-0.0187994152	-0.0398859395
C	0.7216085770	1.2084674634	0.0514150280
C	-0.7228766175	1.2076602766	-0.0506700138
C	-1.5041197178	-0.0204973764	0.0402419292
N	-1.8469826374	-2.1680298190	1.1273853208
C	-2.9427759967	-2.3448573060	0.3814709344
C	-2.7030474826	-0.2069978639	-0.6883246724
C	-3.4269116356	-1.3722134198	-0.5143467181
C	1.3923775351	2.4458685264	0.1520178150
C	-1.3950247697	2.4443097423	-0.1513624990
C	0.6993003200	3.6407647702	0.0827415495
C	-0.7032965590	3.6399819918	-0.0820246870
H	3.4534462349	-3.2967988628	-0.4871488060
H	4.3299700913	-1.5586158652	1.0863091740
H	-3.4504560740	-3.3003510526	0.4867884001
H	-3.0214111311	0.5350065747	-1.4135079884
H	-4.3276840842	-1.5632627232	-1.0874936401
H	2.4748693068	2.4572270689	0.2149985800
H	-2.4775201823	2.4544447351	-0.2144686557
H	1.2364020631	4.5822394988	0.1322001787
H	-1.2414510045	4.5808530371	-0.1315302405
H	3.0217831781	0.5384013158	1.4129019414

Ground state coordinates for: S3

C	1.1437449468	-0.6979043279	0.6192208617
C	1.1437513580	0.6978821111	-0.6192204434
H	1.0243860456	-0.0500383347	1.4875678577
H	1.0243756775	0.0500170428	-1.4875656493
N	2.3858134283	-1.2943828903	0.6112057686
C	2.4965217928	-2.5054908085	0.1189261789
C	1.3875373111	-3.2708047329	-0.3362698404
C	0.1157708708	-2.7155222639	-0.3035132186
C	-0.0547914629	-1.4153902341	0.1857814957
C	-1.3307710355	-0.7067871118	0.1119036986
C	-1.3307609290	0.7067997321	-0.1118907912
C	-0.0547705462	1.4153836735	-0.1857690654
N	2.3858285801	1.2943426310	-0.6112139568
C	2.4965596039	2.5054432931	-0.1189212298
C	0.1158154966	2.7155067900	0.3035407817
C	1.3875913912	3.2707679635	0.3362960250
C	-2.5555690691	-1.3790742534	0.2320060986
C	-2.5555483459	1.3791060846	-0.2319906768

C	-3.7597627411	-0.6887294707	0.1217110979
C	-3.7597525595	0.6887798160	-0.1216935366
H	3.4967785960	-2.9325901663	0.0892026965
H	1.5470689068	-4.2725678003	-0.7211939911
H	3.4968227444	2.9325283414	-0.0892050078
H	-0.7333007615	3.2700520692	0.6887396740
H	1.5471424830	4.2725225020	0.7212343028
H	-2.5659717892	-2.4425598592	0.4463435551
H	-2.5659341123	2.4425921198	-0.4463270393
H	-4.6983197460	-1.2229191343	0.2253616423
H	-4.6983016259	1.2229838319	-0.2253420422
H	-0.7333563334	-3.2700584764	-0.6887008596

Ground state coordinates for: S4

C	1.2426407462	-0.7112908070	0.3017753780
C	1.2426589930	0.7112580930	-0.3017697582
H	1.3138258916	-0.5733657393	1.4029227646
H	1.3138416397	0.5733314030	-1.4029170629
N	2.4738649064	-1.3874932731	-0.0529699062
C	2.4510455538	-2.6684215796	-0.1735860395
C	1.2480981361	-3.4692250637	-0.0689819607
C	0.0230695865	-2.8571459867	0.0129539636
C	-0.0605630077	-1.4437157423	0.0790631714
C	-1.2875544761	-0.7255481153	0.0297870988
C	-1.2875360653	0.7255798055	-0.0297831944
C	-0.0605261365	1.4437161071	-0.0790583179
N	2.4739001260	1.3874286683	0.0529773978
C	2.4511133401	2.6683572823	0.1735960311
C	0.0231424731	2.8571442403	-0.0129480889
C	1.2481865624	3.4691918268	0.0689913236
C	-2.5423588852	-1.3982766551	0.0583705220
C	-2.5423232740	1.3983403836	-0.0583666565
C	-3.7315692419	-0.7059890711	0.0310261337
C	-3.7315512746	0.7060830960	-0.0310221840
H	3.3944047796	-3.1648726826	-0.3992034279
H	1.3227551607	-4.5501558577	-0.1314470418
H	3.3944849723	3.1647837457	0.3992157388
H	-0.8712226387	3.4660127086	0.0362339248
H	1.3228712365	4.5501206036	0.1314580268
H	-2.5750349012	-2.4782062281	0.1225244431
H	-2.5749714742	2.4782708158	-0.1225205297
H	-4.6723105072	-1.2455082030	0.0603063151
H	-4.6722787223	1.2456263349	-0.0603022877
H	-0.8713107768	-3.4659920081	-0.0362296082

Ground state coordinates for: S5=S6

C	0.9395154591	-0.7944640276	-0.5213917682
C	0.9393613478	0.6777881833	-1.0144823564
H	0.6972385404	0.5785236464	-2.0948588337
N	2.0472816173	-1.5234752896	-0.8633504921
C	2.0086118604	-2.8324456012	-0.7162148613
C	0.8463395369	-3.5234334278	-0.3204160600
C	-0.3286533579	-2.8149495023	-0.1457538465
C	-0.3384825883	-1.4160646432	-0.3096043311
C	-1.5518468036	-0.6038178553	-0.1691679387
C	-1.4660394847	0.8223815888	-0.1910025030
C	-0.1860716805	1.4748969266	-0.3875904600
N	2.2743589822	1.2426526146	-0.9823037333
C	2.3987617848	2.4895528406	-0.6585944875
C	0.0567211148	2.8112423681	-0.0871472861
C	1.3271289037	3.3528471278	-0.2532159207
C	-2.8123076688	-1.2055201441	0.0105404039
C	-2.6547224675	1.5675619708	-0.0200318218
C	-3.9641323101	-0.4494655176	0.1733344199
C	-3.8809470266	0.9490158453	0.1610449830
H	2.9238215674	-3.3771063854	-0.9412990040
H	0.8689753227	-4.6008191484	-0.1891948162
H	3.4134762672	2.8918948314	-0.6724729107
H	-0.7297134728	3.4265146338	0.3383888681
H	1.5335444864	4.3866460305	0.0013152164



H	-2.9013929454	-2.2856493066	0.0155936389
H	-2.6124484567	2.6501173287	-0.0606366517
H	-4.9222337360	-0.9421637189	0.3054994832
H	-4.7772766767	1.5506710461	0.2791672075
H	-1.2358134485	-3.3496195203	0.1091452475
H	1.2259886132	-0.5730957227	0.7063419494
Cl	1.5753586654	-0.2365838027	2.1454925677

Ground state coordinates for: S7

C	-0.7166145450	0.5643367540	-0.4944294643
C	-0.4569279512	-0.9179791383	-0.7664832584
H	-0.1543856806	-0.9478624502	-1.8379988467
N	-1.9687186237	1.0149595822	-0.5983011586
C	-2.2207246747	2.3157327389	-0.4037401676
C	-1.2197695638	3.2283787537	-0.0859083857
C	0.0855870522	2.7635855167	0.0283845595
C	0.3740079933	1.4077668142	-0.1914624571
C	1.7359345579	0.8464296830	-0.0767861444
C	1.9017342550	-0.5586527476	0.0896294810
C	0.7391146121	-1.4263097903	0.0151709385
N	-1.6869882208	-1.6855108009	-0.7028186563
C	-1.6451919398	-2.8679422296	-0.1755283950
C	0.6792932670	-2.7104276296	0.5387382923
C	-0.4884303170	-3.4648385944	0.4263121458
C	2.8729515124	1.6692115551	-0.0695013631
C	3.2009828301	-1.0675250185	0.3000470081
C	4.1460626127	1.1442797549	0.1285703072
C	4.3083446689	-0.2317348967	0.3251942692
H	-3.2612120471	2.6159906039	-0.5000679832
H	-1.4597363955	4.2731987778	0.0802852212
H	-2.5834604739	-3.4250603461	-0.1731681146
H	1.5291919952	-3.1169434522	1.0795069214
H	-0.5548028947	-4.4624409429	0.8467358410
H	2.7665314910	2.7363649941	-0.2344746919
H	3.3407962009	-2.1384137458	0.4058813829
H	5.0094497275	1.8024992253	0.1214592852
H	5.2994360777	-0.6502382000	0.4725707466
H	0.8759895822	3.4514391805	0.3092633075
H	-3.4476537240	0.1650252095	-0.9139799201
Cl	-4.7687341997	-0.0419402891	-1.0999408733

Ground state coordinates for: S8

C	1.3999638014	0.3625452602	-0.1435944383
C	0.2937148091	1.3853725689	-0.3887161028
H	0.2383704621	1.3625399406	-1.5078591436
N	2.6449044907	0.8211093631	-0.1656807267
C	3.6387161854	-0.0487445591	0.0239744921
C	3.4242123316	-1.4171629299	0.2331666675
C	2.1248574315	-1.8923147192	0.2187275336
C	1.0528636171	-0.9973698821	0.0118589553
C	-0.3475402568	-1.4199420518	-0.0256919717
C	-1.4083025744	-0.4454354428	-0.0565752008
C	-1.0901944178	0.9421159929	-0.0447069653
N	0.6931974437	2.7426563822	-0.1465011543
C	-0.2185261036	3.6015883659	0.1571010518
C	-2.0361690952	1.9669867791	0.2280526388
C	-1.6147852098	3.2651987169	0.3293854723
C	-0.7075330209	-2.7779537140	-0.0057489250
C	-2.7633893038	-0.8859876076	-0.0602814112
C	-2.0369623281	-3.1747219599	-0.0160326701
C	-3.0759440975	-2.2260201038	-0.0442201125
H	4.6453179222	0.3612689759	0.0073031759
H	4.2623825310	-2.0870972031	0.3894793860
H	1.9455761150	-2.9500837041	0.3698081710
H	0.0984925049	4.6329789146	0.3042832949
H	-3.0719428674	1.7238772640	0.4297395592
H	-2.3203133160	4.0539925066	0.5728703138
H	0.0581235115	-3.5431008734	0.0027837878
H	-3.5657228913	-0.1606453107	-0.1142272511
H	-2.2761793977	-4.2335850582	-0.0101745144

H -4.1107419162 -2.5493028633 -0.0653645782

Ground state coordinates for: S9

C 0.7339059361 -1.2317427043 0.0000454572  
C -0.7343774222 -1.2314939181 0.0000856560  
N 1.3530295633 -2.4313327736 0.0004014910  
C 2.6766512674 -2.4600776706 -0.0000349066  
C 3.4748946579 -1.3059056026 -0.0009891340  
C 2.8460278633 -0.0758948713 -0.0012462713  
C 1.4377430966 0.0001212647 -0.0005842241  
C 0.7107997647 1.2716758696 -0.0003713405  
C -0.7104241624 1.2719143980 0.0000864512  
C -1.4377975331 0.0006092411 -0.0001981531  
N -1.3539076857 -2.4308734218 0.0001511992  
C -2.6775396551 -2.4591697249 -0.0002175718  
C -2.8461077186 -0.0749288846 -0.0008903174  
C -3.4753910678 -1.3047252306 -0.0008769191  
C 1.3866483707 2.5111135487 -0.0003737647  
C -1.3858524260 2.5115817299 0.0008647579  
C 0.7011510141 3.7130033726 0.0001685465  
C -0.6999482376 3.7132392517 0.0008859454  
H 3.1379908924 -3.4468556699 0.0003602475  
H 4.5575458633 -1.3823283245 -0.0015137901  
H -3.1392167196 -3.4457896830 -0.0000683667  
H -3.4475632437 0.8267039373 -0.0016024856  
H -4.5580682541 -1.3807828047 -0.0014425534  
H 2.4700574284 2.5357494243 -0.0007138178  
H -2.4692527908 2.5365887434 0.0016510978  
H 1.2499935210 4.6498290143 0.0001409087  
H -1.2484726105 4.6502510285 0.0015350346  
H 3.4477854269 0.8255353479 -0.0020004589

R1: benzene R2=R3 : 3-thiophene

Ground state coordinates for: S1

C 1.3826829572 0.9028395843 -0.9793897452  
C -1.3826829572 -0.9028395843 -0.9793897452  
H 0.6368217390 1.6778085196 -1.0799149852  
H -0.6368217390 -1.6778085196 -1.0799149852  
C 1.5355619995 0.0116248320 0.0549086085  
C 2.6546853270 -0.8640611357 -0.1697352127  
C 3.3029586654 -0.6257344909 -1.3474669291  
S 2.5711672040 0.6847532383 -2.2178048304  
C 0.7085658786 -0.0180620236 1.2894503527  
C -0.7085658786 0.0180620236 1.2894503527  
C -1.5355619995 -0.0116248320 0.0549086085  
C -2.6546853270 0.8640611357 -0.1697352127  
C -3.3029586654 0.6257344909 -1.3474669291  
S -2.5711672040 -0.6847532383 -2.2178048304  
C 1.3810526127 -0.0534865939 2.5226704834  
C 0.6962447039 -0.0318049659 3.7346630242  
C -0.6962447039 0.0318049659 3.7346630242  
C -1.3810526127 0.0534865939 2.5226704834  
H 4.1572076635 -1.1438646345 -1.7598035805  
H -4.1572076635 1.1438646345 -1.7598035805  
H 2.4670542371 -0.0678805234 2.5208698130  
H 1.2480906708 -0.0534566429 4.6697537344  
H -1.2480906708 0.0534566429 4.6697537344  
H -2.4670542371 0.0678805234 2.5208698130  
H 2.9399190280 -1.6503840192 0.5200845631  
H -2.9399190280 1.6503840192 0.5200845631

Ground state coordinates for: S2

C 1.2191625291 0.8324921508 -0.9962348954  
C -1.2191625291 -0.8324921508 -0.9962348954  
H 0.4407589768 1.5801295970 -1.0436022347  
H -0.4407589768 -1.5801295970 -1.0436022347  
C 1.5021590240 -0.0289982564 0.0819414653

C	2.7102804751	-0.7655757762	-0.1514471572
C	3.2795437001	-0.4836632077	-1.3582527825
S	2.3877000836	0.7321897706	-2.2410296153
C	0.7144750855	-0.0878261573	1.3053569650
C	-0.7144750855	0.0878261573	1.3053569650
C	-1.5021590240	0.0289982564	0.0819414653
C	-2.7102804751	0.7655757762	-0.1514471572
C	-3.2795437001	0.4836632077	-1.3582527825
S	-2.3877000836	-0.7321897706	-2.2410296153
C	1.3804956331	-0.2347010399	2.5395290445
C	0.6929664569	-0.1253270156	3.7364326435
C	-0.6929664569	0.1253270156	3.7364326435
C	-1.3804956331	0.2347010399	2.5395290445
H	4.1666759682	-0.9213814174	-1.7961249154
H	-4.1666759682	0.9213814174	-1.7961249154
H	2.4569760564	-0.3659298566	2.5475630622
H	1.2277304406	-0.2099127901	4.6767127508
H	-1.2277304406	0.2099127901	4.6767127508
H	-2.4569760564	0.3659298566	2.5475630622
H	3.1064257829	-1.5068395227	0.5315367901
H	-3.1064257829	1.5068395227	0.5315367901

Ground state coordinates for: S3

C	-0.6098492745	-0.7607292116	1.0356961134
C	0.6098492745	0.7607292116	1.0356961134
H	-1.5394974348	-0.2001444381	1.0429596825
H	1.5394974348	0.2001444381	1.0429596825
C	-0.1413740648	-1.4218043133	-0.1699352374
C	0.4348309483	-2.6733821800	0.1005926446
C	0.3774021337	-3.0275330026	1.4368285114
S	-0.4196591105	-1.8556717546	2.4216113647
C	-0.0815037138	-0.7098171183	-1.4469420132
C	0.0815037138	0.7098171183	-1.4469420132
C	0.1413740648	1.4218043133	-0.1699352374
C	-0.4348309483	2.6733821800	0.1005926446
C	-0.3774021337	3.0275330026	1.4368285114
S	0.4196591105	1.8556717546	2.4216113647
C	-0.1606780429	-1.3886814991	-2.6681498949
C	-0.0821603882	-0.6931015682	-3.8753660463
C	0.0821603882	0.6931015682	-3.8753660463
C	0.1606780429	1.3886814991	-2.6681498949
H	0.7962343223	-3.9166486116	1.8914566002
H	-0.7962343223	3.9166486116	1.8914566002
H	-0.3174635679	-2.4624791225	-2.6745392646
H	-0.1522859513	-1.2339085574	-4.8132095834
H	0.1522859513	1.2339085574	-4.8132095834
H	0.3174635679	2.4624791225	-2.6745392646
H	0.9313976930	-3.2830051267	-0.6447677334
H	-0.9313976930	3.2830051267	-0.6447677334

Ground state coordinates for: S4

C	-0.3787504929	-0.6579763901	1.0652599682
C	0.3787504929	0.6579763901	1.0652599682
H	-1.4617589001	-0.4560396787	1.0807276466
H	1.4617589001	0.4560396787	1.0807276466
C	-0.0462436344	-1.4246085538	-0.2008221775
C	0.1491532242	-2.7947036461	0.0504827154
C	0.1595998001	-3.1188559200	1.3894452635
S	-0.0628803551	-1.8010204314	2.4835562509
C	0.0156900499	-0.7251720008	-1.4329273649
C	-0.0156900499	0.7251720008	-1.4329273649
C	0.0462436344	1.4246085538	-0.2008221775
C	-0.1491532242	2.7947036461	0.0504827154
C	-0.1595998001	3.1188559200	1.3894452635
S	0.0628803551	1.8010204314	2.4835562509
C	0.0652633858	-1.4045998769	-2.6802485254
C	0.0375060344	-0.7069827366	-3.8674243312
C	-0.0375060344	0.7069827366	-3.8674243312
C	-0.0652633858	1.4045998769	-2.6802485254
H	0.3068223635	-4.1136350199	1.7942875202

H	-0.3068223635	4.1136350199	1.7942875202
H	0.0923861204	-2.4882701863	-2.6983544460
H	0.0627120911	-1.2432700443	-4.8101259508
H	-0.0627120911	1.2432700443	-4.8101259508
H	-0.0923861204	2.4882701863	-2.6983544460
H	0.3299479898	-3.5381529621	-0.7160086551
H	-0.3299479898	3.5381529621	-0.7160086551

Ground state coordinates for: S5=S6

C	0.9474270616	-0.5734615284	-0.2681218691
C	0.8540173357	0.8462434811	-0.7843185882
H	1.0521834599	-0.4532747159	1.0079573232
H	0.8239153962	0.8287310525	-1.8858845694
C	-0.2555243710	-1.3516883814	-0.4005173759
C	0.0210763247	-2.7371423067	-0.5362023151
C	1.3584645056	-3.0046724587	-0.6824350028
S	2.3565836944	-1.6022552327	-0.6756183024
C	-1.5459797506	-0.7143593568	-0.2985733224
C	-1.6083098275	0.7181452916	-0.1731657705
C	-0.4118255181	1.4925513983	-0.2550158174
C	-0.2045289858	2.8288364345	0.1316121744
C	1.1087559909	3.2322152113	0.1189718492
S	2.2483443581	2.0051336495	-0.3734892176
C	-2.7411798815	-1.4624145769	-0.2599330938
C	-3.9675852900	-0.8475489503	-0.0810514973
C	-4.0295752144	0.5506159500	0.0765476699
C	-2.8787679642	1.3131459534	0.0352289516
H	1.8133895826	-3.9847079390	-0.7525404555
H	1.4816329061	4.2016141541	0.4230290068
H	-2.6976467389	-2.5420280423	-0.3578823765
H	-4.8755969577	-1.4409046318	-0.0518639095
H	-4.9902398219	1.0349198628	0.2240177683
H	-2.9484235034	2.3907497405	0.1386201571
H	-0.7279863524	-3.5185797984	-0.5202913380
H	-0.9944760599	3.4811508862	0.4857473195
Cl	1.1891896878	-0.2122324171	2.5873309249

Ground state coordinates for: S7

C	0.8925730630	-0.5392741653	-0.7600101998
C	0.7920778199	0.9260514714	-1.0435137792
H	0.9660825949	-0.6081926035	1.7238209688
H	0.7090883723	1.0722172303	-2.1344137836
C	-0.2340412652	-1.3070505299	-0.5144985355
C	0.0844619311	-2.7075924326	-0.4412739689
C	1.4060462561	-2.9666389232	-0.6543267797
S	2.3175282160	-1.5177469530	-0.9525628112
C	-1.5552870806	-0.6848281099	-0.3671973668
C	-1.6335337403	0.7405280973	-0.2655834001
C	-0.4261114467	1.5208108061	-0.3646190799
C	-0.1771346008	2.8031107269	0.1488774276
C	1.1427374125	3.1983042246	0.1157392853
S	2.2375089790	2.0069774657	-0.5606704136
C	-2.7290716980	-1.4428911297	-0.2689139538
C	-3.9648369680	-0.8357756113	-0.0584578228
C	-4.0434123429	0.5569740363	0.0670692098
C	-2.8955002189	1.3305919957	-0.0321500402
H	1.9133968467	-3.9206004016	-0.6159030471
H	1.5487294577	4.1192243616	0.5131378621
H	-2.6762123065	-2.5236439901	-0.3564023429
H	-4.8620024973	-1.4432777310	0.0101168374
H	-5.0041214601	1.0362156067	0.2311126212
H	-2.9692733052	2.4113771819	0.0420597551
H	-0.6353107394	-3.4841005679	-0.2131103848
H	-0.9417045467	3.4164204236	0.6136060260
Cl	1.1146573337	-0.6784077496	3.0102260402

Ground state coordinates for: S8

C	1.0674482041	-0.7320177923	-0.1238681015
C	1.0627964291	0.7142698169	-0.4551371509
H	1.1188127082	0.8072957977	-1.5586687142

C	-0.1244801885	-1.4254753999	0.0174575974
C	0.1044654944	-2.8321597248	0.2029623979
C	1.4262948986	-3.1557756439	0.1831093182
S	2.4452505943	-1.7661422447	-0.0670510639
C	-1.4030308574	-0.7303818172	-0.0283950790
C	-1.4378197538	0.7082834118	-0.0913716420
C	-0.2114141549	1.4282097262	-0.1055724942
C	0.0172447614	2.7823970607	0.1875166045
C	1.3581952361	3.0988672769	0.2936230621
S	2.4636612698	1.8183523863	0.0421485267
C	-2.6246516528	-1.4177526685	0.0315636197
C	-3.8323125415	-0.7314772673	0.0337774844
C	-3.8691352277	0.6748306558	-0.0164355195
C	-2.6877654568	1.3830727181	-0.0693349830
H	1.8816730041	-4.1268762262	0.3191606381
H	1.7471935745	4.0866111808	0.5186006857
H	-2.6312085248	-2.5004854339	0.0744604303
H	-4.7618220851	-1.2904479932	0.0764261494
H	-4.8204912636	1.1950124678	-0.0191830055
H	-2.7128446646	2.4658192689	-0.1268697158
H	-0.6742579763	-3.5675325555	0.3584913943
H	-0.7602214957	3.5104860192	0.3805423577

Ground state coordinates for: S9

C	1.0606232636	-0.7075168650	0.0004063629
C	1.0616746599	0.7061750787	-0.0008651542
C	-0.1452212242	-1.4205715239	0.0014119756
C	0.0836042553	-2.8402727084	0.0021370646
C	1.4025195980	-3.1720131257	0.0018791475
S	2.4471008895	-1.7730723065	0.0002247034
C	-1.4041786053	-0.7142188904	0.0012238061
C	-1.4030526701	0.7166753476	-0.0002014184
C	-0.1430029016	1.4210918115	-0.0010847488
C	0.0880130902	2.8405051870	-0.0021741373
C	1.4074165392	3.1703442096	-0.0029772819
S	2.4497017696	1.7697159321	-0.0022696306
C	-2.6453898473	-1.3926635533	0.0024569108
C	-3.8406496023	-0.7007926542	0.0020478363
C	-3.8396356853	0.7068057591	0.0003358850
C	-2.6433670245	1.3968955479	-0.0006355852
H	1.8401701649	-4.1605293049	0.0025854124
H	1.8465338869	4.1582234355	-0.0035523408
H	-2.6571608623	-2.4778503663	0.0037840026
H	-4.7812358771	-1.2434242015	0.0030841239
H	-4.7794476969	1.2507865997	-0.0001952699
H	-2.6536387584	2.4820768293	-0.0020014936
H	-0.7044275432	-3.5834290547	0.0030603793
H	-0.6988087103	3.5849372504	-0.0022878039

R1: benzene, R2=R3 : 3-pyrrole

Ground state coordinates for: S1

C	1.3609018806	1.3697579310	0.8947016411
C	-1.3608952210	1.3697623048	-0.8947052051
H	0.5843837653	1.5876219252	1.6109537507
H	-0.5843775119	1.5876226959	-1.6109583546
C	1.5367197333	0.2721249533	0.0693500467
C	2.7448356532	0.5097782080	-0.6655800202
C	3.2497818807	1.7282699275	-0.2736444372
N	2.3986344586	2.2409818609	0.6777921653
C	0.7099215717	-0.9538910917	0.0097436568
C	-0.7099283184	-0.9538867201	-0.0097412335
C	-1.5367197142	0.2721354767	-0.0693472197
C	-2.7448345065	0.5097960892	0.6655779285
C	-3.2497692583	1.7282949045	0.2736470505
N	-2.3986156403	2.2410027169	-0.6777849275
C	1.3802790159	-2.1896122275	-0.0010077070
C	0.6969365498	-3.4025853074	-0.0065860440

C	-0.6969575899	-3.4025794906	0.0065848566
C	-1.3802935747	-2.1896044318	0.0010089178
H	4.1279610764	2.2698909641	-0.5915466449
H	-4.1279412703	2.2699246415	0.5915538418
H	2.4659794240	-2.1857753729	0.0279482919
H	1.2501590455	-4.3374967168	-0.0082535764
H	-1.2501845078	-4.3374891052	0.0082509740
H	-2.4659937904	-2.1857601568	-0.0279465497
H	3.1717285277	-0.1420920736	-1.4150232093
H	-3.1717392006	-0.1420698377	1.4150180646
H	-2.5241751236	3.1169399713	-1.1577998848
H	2.5241972209	3.1169219613	1.1578011968

Ground state coordinates for: S2

C	1.1947004845	0.8698157139	-1.3545730618
C	-1.1947004845	-0.8698157139	-1.3545730618
H	0.4068270218	1.5955856385	-1.4814156237
H	-0.4068270218	-1.5955856385	-1.4814156237
C	1.4926586710	0.0335002238	-0.2460847271
C	2.7461564451	-0.5851495768	-0.5379338537
C	3.1494979945	-0.1465987006	-1.7751014723
N	2.1992023482	0.7419774673	-2.2511076663
C	0.7156904172	-0.0604267344	0.9756418752
C	-0.7156904172	0.0604267344	0.9756418752
C	-1.4926586710	-0.0335002238	-0.2460847271
C	-2.7461564451	0.5851495768	-0.5379338537
C	-3.1494979945	0.1465987006	-1.7751014723
N	-2.1992023482	-0.7419774673	-2.2511076663
C	1.3870368943	-0.1863748357	2.2100099827
C	0.6964338790	-0.1037541002	3.4066058140
C	-0.6964338790	0.1037541002	3.4066058140
C	-1.3870368943	0.1863748357	2.2100099827
H	4.0204474360	-0.3963681918	-2.3625900663
H	-4.0204474360	0.3963681918	-2.3625900663
H	2.4674661033	-0.2824603710	2.2145650198
H	1.2332539899	-0.1743526277	4.3469236899
H	-1.2332539899	0.1743526277	4.3469236899
H	-2.4674661033	0.2824603710	2.2145650198
H	3.2659164226	-1.3056726524	0.0759624746
H	-3.2659164226	1.3056726524	0.0759624746
H	-2.2757390507	-1.2631526806	-3.1128525151
H	2.2757390507	1.2631526806	-3.1128525151

Ground state coordinates for: S3

C	0.7494668696	0.5438522048	-1.3950658607
C	-0.7494668696	-0.5438522048	-1.3950658607
H	0.2636150315	1.5151418294	-1.4563948906
H	-0.2636150315	-1.5151418294	-1.4563948906
C	1.4065803357	0.0818037580	-0.1664094291
C	2.6092460519	-0.5249142888	-0.5354320478
C	2.7492008102	-0.4008634111	-1.9195970374
N	1.6706478596	0.2624102489	-2.4178770230
C	0.7119905156	0.0488598603	1.1171613555
C	-0.7119905156	-0.0488598603	1.1171613555
C	-1.4065803357	-0.0818037580	-0.1664094291
C	-2.6092460519	0.5249142888	-0.5354320478
C	-2.7492008102	0.4008634111	-1.9195970374
N	-1.6706478596	-0.2624102489	-2.4178770230
C	1.3953789839	0.0949947013	2.3367425267
C	0.6962046371	0.0475314265	3.5437979045
C	-0.6962046371	-0.0475314265	3.5437979045
C	-1.3953789839	-0.0949947013	2.3367425267
H	3.5355250821	-0.7629627416	-2.5672523658
H	-3.5355250821	0.7629627416	-2.5672523658
H	2.4759456969	0.1973273899	2.3411849060
H	1.2392661777	0.0889105104	4.4821403912
H	-1.2392661777	-0.0889105104	4.4821403912
H	-2.4759456969	-0.1973273899	2.3411849060
H	3.2909008266	-1.0566982935	0.1127526478
H	-3.2909008266	1.0566982935	0.1127526478

H -1.5910103945 -0.5943612014 -3.3677012076  
H 1.5910103945 0.5943612014 -3.3677012076

Ground state coordinates for: S4

C -0.4003511543 -0.6439701350 1.4372573658  
C 0.4003511543 0.6439701350 1.4372573658  
H -1.4760881472 -0.3937631922 1.4572815659  
H 1.4760881472 0.3937631922 1.4572815659  
C -0.0851512170 -1.4075461542 0.1581171511  
C 0.0897039000 -2.7551743398 0.5111247485  
C 0.0378039775 -2.8491523672 1.8939119145  
N -0.1087332782 -1.6308344606 2.4792924298  
C 0.0055111704 -0.7245179401 -1.0775029312  
C -0.0055111704 0.7245179401 -1.0775029312  
C 0.0851512170 1.4075461542 0.1581171511  
C -0.0897039000 2.7551743398 0.5111247485  
C -0.0378039775 2.8491523672 1.8939119145  
N 0.1087332782 1.6308344606 2.4792924298  
C 0.0556420238 -1.4071887590 -2.3220907184  
C 0.0345070705 -0.7079719855 -3.5082296293  
C -0.0345070705 0.7079719855 -3.5082296293  
C -0.0556420238 1.4071887590 -2.3220907184  
H 0.1198309727 -3.7418893005 2.5016700004  
H -0.1198309727 3.7418893005 2.5016700004  
H 0.0763478703 -2.4919023013 -2.3340090811  
H 0.0588602036 -1.2429194167 -4.4517851338  
H -0.0588602036 1.2429194167 -4.4517851338  
H -0.0763478703 2.4919023013 -2.3340090811  
H 0.2947396342 -3.5835898595 -0.1512998504  
H -0.2947396342 3.5835898595 -0.1512998504  
H 0.4793554393 1.5392697269 3.4156221019  
H -0.4793554393 -1.5392697269 3.4156221019

Ground state coordinates for: S5=S6

C 1.2295938586 0.0575881233 -0.5207103233  
C 0.6478030098 1.4365841388 -0.7406061417  
H 0.5091764864 1.5952905349 -1.8312267506  
C 0.2879479411 -1.0270558959 -0.7407852063  
C 1.0067655501 -2.1111295850 -1.2841040634  
C 2.3066110809 -1.6748616377 -1.4995206934  
N 2.4262656986 -0.3617468703 -1.1937592778  
C -1.1070169468 -0.8864760340 -0.4147812502  
C -1.5855921511 0.4095721656 -0.0070586568  
C -0.6989265982 1.5197957700 -0.0351780501  
C -0.7678900314 2.7894811578 0.5755573156  
C 0.4590679492 3.4067563438 0.4440150410  
N 1.3680553727 2.5876000194 -0.1887679568  
C -1.9923054733 -1.9822564412 -0.4211063126  
C -3.3119547743 -1.8386000514 -0.0263403011  
C -3.7803609250 -0.5768664176 0.3943027842  
C -2.9387868391 0.5185288164 0.4100154240  
H 3.1641344334 -2.2451404615 -1.8327904149  
H 0.7689418776 4.3740888499 0.8176755403  
H -1.6216516816 -2.9594440211 -0.7177982372  
H -3.9782188093 -2.6948666732 -0.0272188408  
H -4.8151787153 -0.4639912580 0.7047101207  
H -3.3192838253 1.4864185245 0.7215718922  
H 0.6354344435 -3.0998301909 -1.5115797720  
H -1.5976193871 3.1818641427 1.1465295169  
H 2.1422810613 2.9874066790 -0.6982791816  
H 3.3239059251 0.0379684441 -0.9482220249  
H 1.5921756128 -0.0216868688 0.7189212673  
Cl 2.3890147472 -0.1073960392 2.1906235061

Ground state coordinates for: S7

C 1.1069565030 -0.3130210018 -0.9237916083  
C 0.8557444593 1.1449272123 -1.1231591775  
H 0.6881374031 1.3292098864 -2.2077693604  
C 0.0850117988 -1.2160119785 -0.6421353813  
C 0.6526897816 -2.5280795062 -0.7476357510

C	1.9753240510	-2.3774070013	-1.0932828735
N	2.2382544261	-1.0297704139	-1.2309208566
C	-1.2713856300	-0.7633583724	-0.3331851258
C	-1.4870214241	0.6435387657	-0.1555820319
C	-0.3887713926	1.5481440515	-0.3481604031
C	-0.1391168432	2.8309693935	0.1811823111
C	1.1793155841	3.1624236359	-0.0434528222
N	1.8725422948	2.1101231969	-0.6522433103
C	-2.3371594285	-1.6488824931	-0.1407112326
C	-3.5988918811	-1.1893742074	0.2349435914
C	-3.8090523287	0.1811171267	0.4364247576
C	-2.7685394733	1.0810174246	0.2479368664
H	2.7565623665	-3.1113987316	-1.2229825526
H	1.7133867676	4.0519540656	0.2638111146
H	-2.1724715429	-2.7139940933	-0.2780049511
H	-4.4126430597	-1.8943847153	0.3761916417
H	-4.7891476546	0.5438042318	0.7331192274
H	-2.9429206326	2.1442441920	0.3876516261
H	0.1545802882	-3.4702606633	-0.5697419528
H	-0.8290905319	3.4228933613	0.7682399994
H	2.5810748042	2.3728166777	-1.3268462908
H	3.1549209663	-0.6324498640	-1.3635766493
H	1.3530016450	-0.6480305509	1.3665218270
Cl	1.9776271657	-0.7296161460	2.5081759705

Ground state coordinates for: S8

C	1.4235993670	-0.7241835618	-0.0760921603
C	1.4484772898	0.7082124290	-0.4798164823
H	1.4842861976	0.7477265726	-1.5870148619
C	0.2142854341	-1.4017997760	0.0448607338
C	0.5328647540	-2.7894668301	0.1862188979
C	1.8989948072	-2.9014448734	0.1257606390
N	2.4351230480	-1.6409772412	-0.0637294587
C	-1.0610645676	-0.7085509060	-0.0159859075
C	-1.0808385477	0.7252684339	-0.1007186538
C	0.1655084995	1.4203605083	-0.1108972086
C	0.5002224908	2.7167178772	0.2700583456
C	1.8968227128	2.8081231642	0.2980224701
N	2.4766999586	1.6511256161	-0.0296099424
C	-2.2891624031	-1.3818470625	0.0565140089
C	-3.4885497708	-0.6797469106	0.0473313806
C	-3.5076707055	0.7247735727	-0.0230949679
C	-2.3149269088	1.4186057960	-0.0846691215
H	2.5402264004	-3.7640431542	0.2239870219
H	2.4967745189	3.6765994072	0.5455456135
H	-2.3021627006	-2.4642080190	0.1221301501
H	-4.4252931250	-1.2259079033	0.0985701529
H	-4.4522091009	1.2572460287	-0.0331420807
H	-2.3197295256	2.5017626936	-0.1552982347
H	-0.1561822399	-3.6094891466	0.3221583013
H	-0.1720140206	3.5039210851	0.5783923764
H	3.4633675726	1.5574148403	-0.2283465410
H	3.4243167582	-1.4450650594	-0.0796877827

Ground state coordinates for: S9

C	1.4259005979	-0.7093532826	-0.0025487736
C	1.4279694379	0.7052792362	-0.0021436694
C	0.2096966455	-1.4142050904	-0.0012287453
C	0.5459317884	-2.8074647505	-0.0016195456
C	1.9140980540	-2.9048948663	-0.0018811988
N	2.4515053170	-1.6293293131	-0.0042561628
C	-1.0518041177	-0.7147473188	0.0001882285
C	-1.0497942129	0.7178697401	0.0008055421
C	0.2137814746	1.4136835627	-0.0008160925
C	0.5541979346	2.8060117741	-0.0024779374
C	1.9226421545	2.8993364282	-0.0046651414
N	2.4562119230	1.6222281683	-0.0040025870
C	-2.2914233263	-1.3916744130	0.0012126928
C	-3.4882263270	-0.6983788254	0.0028998643
C	-3.4861949208	0.7086359156	0.0036540583



C	-2.2873635610	1.3984572444	0.0025925343
H	2.5568402236	-3.7725596158	-0.0020328317
H	2.5679501356	3.7650988208	-0.0053383807
H	-2.2980345306	-2.4780101480	0.0006345723
H	-4.4294699992	-1.2405501089	0.0035961607
H	-4.4258455211	1.2535661028	0.0051153598
H	-2.2907479414	2.4848026751	0.0032743647
H	-0.1389955897	-3.6429795152	-0.0018056325
H	-0.1282686860	3.6435341696	-0.0020278967
H	3.4398048803	1.4122720505	-0.0082487726
H	3.4357159354	-1.4223395037	0.0006119977

R1 : benzene, R2 : Phenyl, R3 : 2-methoxyphenyl

Ground state coordinates for: S1

C	0.6829049444	-0.9405777424	-1.6869595335
C	-1.4606330886	-0.9516951919	1.1479964205
H	-0.1679397325	-0.6525561948	-2.2967653284
H	-0.5258550827	-0.8049743130	1.6798120378
C	1.3784682301	-2.1164209219	-1.9736227016
C	2.4701232952	-2.4711359087	-1.1869879162
C	2.8622818632	-1.6634633296	-0.1171421931
C	2.1582758784	-0.4882285569	0.1656334404
C	1.0526617165	-0.1063145945	-0.6275576607
C	0.3250438366	1.1763076257	-0.3802633541
C	-1.0533010778	1.2214581442	-0.0656079044
C	-1.8660508373	-0.0007619610	0.1975284750
C	-2.2509741288	-2.0657361574	1.4238237728
C	-3.4621688029	-2.2532929600	0.7547854467
C	-3.0894141302	-0.1974229380	-0.4622321016
C	-3.8790883675	-1.3146274955	-0.1891134643
C	1.0221965741	2.3831887050	-0.5462461440
C	-1.6822198569	2.4742140971	0.0368010422
C	0.3861641669	3.6155354989	-0.4296053466
C	-0.9784390546	3.6610756999	-0.1435059056
H	1.0696233116	-2.7427859352	-2.8044951475
H	3.0254643824	-3.3809320750	-1.3966553766
H	3.7099113775	-1.9592887734	0.4890676471
O	2.4600430859	0.3435290046	1.2099535123
H	-1.9220571596	-2.7875269213	2.1662476742
H	-4.0762383679	-3.1233591240	0.9689435368
H	-3.4141309449	0.5257938694	-1.2052292295
H	-4.8187802058	-1.4521831330	-0.7168651381
H	2.0800621881	2.3421494148	-0.7856833668
H	-2.7374789043	2.5067064062	0.2917391974
H	0.9508866449	4.5330692633	-0.5676531344
H	-1.4900675573	4.6146099397	-0.0488714272
C	3.5620607101	0.0163531755	2.0398172896
H	3.6178505112	0.8071991011	2.7892647162
H	4.5029264572	-0.0125461699	1.4751366474
H	3.4201791825	-0.9484838180	2.5438875942

Ground state coordinates for: S2

C	0.4137134761	-1.1293756129	-1.4008510223
C	-1.5280264943	-0.9048706588	1.1021054134
H	-0.5227898866	-0.8684031430	-1.8780542275
H	-0.5685642700	-0.8199308483	1.5997179030
C	1.0472553449	-2.3107900086	-1.7268233769
C	2.2876751334	-2.6272181773	-1.1360440497
C	2.8920442029	-1.7633191192	-0.2323778677
C	2.2677511239	-0.5517509948	0.0925812792
C	0.9977838755	-0.1976067424	-0.5027707360
C	0.3736013466	1.1033283080	-0.2735444773
C	-1.0549459104	1.2406944869	-0.1186183769
C	-1.9279293467	0.0978373391	0.1832214887
C	-2.3810699634	-1.9541069026	1.4224564100
C	-3.6438110328	-2.0342745526	0.8300334698
C	-3.2203301362	0.0142998948	-0.3850194155

C	-4.0583077157	-1.0477333914	-0.0775863783
C	1.1653346067	2.2763264566	-0.3445676488
C	-1.6161747806	2.5298251106	-0.1563936305
C	0.5820255552	3.5281584858	-0.3607682352
C	-0.8179659438	3.6572063289	-0.2726765509
H	0.6028280001	-2.9868919792	-2.4486763388
H	2.7823004870	-3.5592158412	-1.3907311195
H	3.8391525091	-2.0290719207	0.2186383861
O	2.7465599707	0.3152112067	0.9924639432
H	-2.0703323106	-2.7017351510	2.1448779357
H	-4.3101494321	-2.8539955192	1.0791030232
H	-3.5402236660	0.7644316115	-1.1010817159
H	-5.0363686553	-1.1159017924	-0.5426053506
H	2.2373131253	2.1821125071	-0.4568307214
H	-2.6861079382	2.6411520085	-0.0197939385
H	1.2021717282	4.4125611626	-0.4631914867
H	-1.2712540590	4.6432844050	-0.2696959100
C	3.9774014475	0.0339449305	1.6815814226
H	4.1343202048	0.8808550566	2.3470555282
H	4.8080838934	-0.0452566637	0.9741136201
H	3.8875661135	-0.8870106167	2.2650417493

Ground state coordinates for: S3

C	-0.2059209452	-1.2304981738	-0.7214848748
C	-1.3747673420	-0.9325131945	0.5738543272
H	-0.8162910957	-0.9048347859	-1.5647592442
H	-0.6855023149	-0.9992944883	1.4165956766
C	0.1206708057	-2.6454337081	-0.8109586289
C	1.3574419715	-3.1002863944	-0.4435490780
C	2.3546565866	-2.1978640958	-0.0195984469
C	2.1302094282	-0.8106598545	0.0002190368
C	0.8792739372	-0.2868830963	-0.3935367822
C	0.5277015137	1.1348365434	-0.2729803021
C	-0.8079185583	1.4861486773	0.1043765237
C	-1.8200650517	0.4368260164	0.2614641836
C	-2.4081357887	-1.9593503889	0.6427859993
C	-3.7117361227	-1.6947684208	0.3127370991
C	-3.1520838900	0.6533402402	-0.0807280022
C	-4.0887653446	-0.3838538927	-0.0554973819
C	1.4457854482	2.1666975010	-0.5226533122
C	-1.1409364855	2.8366277657	0.2750077704
C	1.0821657441	3.5045126300	-0.3750756725
C	-0.2045456296	3.8419881814	0.0440698510
H	-0.6436299543	-3.3302753564	-1.1624857783
H	1.5937121539	-4.1581053017	-0.4969577150
H	3.3148440792	-2.5909069202	0.2891651613
O	3.0692775668	0.0748869372	0.3988896494
H	-2.1151113675	-2.9533223574	0.9656231546
H	-4.4604652227	-2.4786262340	0.3604550513
H	-3.4660632491	1.6388707518	-0.4062881996
H	-5.1184264210	-0.1782956184	-0.3304419625
H	2.4461941365	1.9184499343	-0.8479633324
H	-2.1345115448	3.1020412442	0.6201767494
H	1.8102253600	4.2823059502	-0.5809255837
H	-0.4798692500	4.8813696569	0.1888088950
C	4.3492324182	-0.3921977308	0.8399142260
H	4.9049178597	0.5037311711	1.1133328840
H	4.8773690738	-0.9187874358	0.0379250087
H	4.2531355999	-1.0419142677	1.7163889471

Ground state coordinates for: S4

C	-0.1292917676	-1.2617550674	-0.5914816789
C	-1.3592713923	-1.0417232383	0.3313659828
H	-0.4698244359	-0.9957907098	-1.6132329360
H	-0.9577416860	-1.0487386845	1.3704029107
C	0.3313602373	-2.6808620450	-0.6839759891
C	1.6303500997	-3.0127149898	-0.5033091505
C	2.5925764783	-2.0271660912	-0.1408744548
C	2.2598144196	-0.6800395134	0.0116047131
C	0.9229533354	-0.2292628870	-0.2038645294

C	0.4725720572	1.1276302716	-0.1271329198
C	-0.9563293346	1.4110200910	-0.0728086975
C	-1.8945336646	0.3559056710	0.1163661249
C	-2.3865122012	-2.1347900092	0.3308750436
C	-3.7112230697	-1.8687205764	0.3487022076
C	-3.2943997746	0.5495922622	0.1697917191
C	-4.1667661545	-0.5104374143	0.2804442117
C	1.3602368910	2.2411069520	-0.1846359605
C	-1.3869106972	2.7675989832	-0.1343094729
C	0.8932880990	3.5364025151	-0.2338976562
C	-0.4915740946	3.8071263737	-0.2110904047
H	-0.3923069030	-3.4293558085	-0.9857731252
H	1.9615298506	-4.0386344978	-0.6281324493
H	3.6129184845	-2.3466354403	0.0268043313
O	3.1667536748	0.2351194188	0.4151428347
H	-2.0304076930	-3.1547795896	0.4204751786
H	-4.4383781640	-2.6711424501	0.4142930541
H	-3.7106738127	1.5442302499	0.0783416268
H	-5.2345049314	-0.3143566778	0.2981176540
H	2.4213798650	2.0614746955	-0.2359163937
H	-2.4437162356	2.9980507582	-0.1029546238
H	1.6012852334	4.3557706369	-0.3059888698
H	-0.8483951465	4.8308531905	-0.2505295309
C	4.4959167723	-0.1703689464	0.7667095659
H	4.9930155099	0.7372727026	1.1063407729
H	5.0279744022	-0.5761451148	-0.0996747444
H	4.4806723677	-0.9048594536	1.5783750795

Ground state coordinates for: S5=S6

C	-0.0812153131	-1.2626500430	-0.6880530683
C	-1.3630000068	-1.0587068864	0.1858187827
H	-0.4154339409	-0.9808966739	-1.7068707170
C	0.3986072159	-2.6773988875	-0.7636764972
C	1.6806871176	-3.0071579572	-0.4691751134
C	2.6211494303	-2.0322790681	-0.0371207780
C	2.2598222159	-0.6814811069	0.0616428054
C	0.9629658017	-0.2462633617	-0.2646365404
C	0.4955837739	1.1278923411	-0.2222392988
C	-0.9069789757	1.4004105569	-0.0654687178
C	-1.8427009407	0.3149530651	0.2085525893
C	-2.3524378601	-2.1137270810	0.2351324665
C	-3.6574097050	-1.8558505804	0.5740374963
C	-3.1764095008	0.5364878589	0.5955749710
C	-4.0573977400	-0.5199982850	0.7786133946
C	1.3644787662	2.2331227878	-0.3882068655
C	-1.3587241163	2.7362997315	-0.1299547356
C	0.8877360504	3.5331338262	-0.4361404997
C	-0.4842558104	3.7931995843	-0.3156834110
H	-0.2919678166	-3.4328458005	-1.1237276257
H	2.0105812301	-4.0383756360	-0.5612057242
H	3.6208511553	-2.3502655244	0.2261256306
O	3.1434298271	0.2618982773	0.4988847095
H	-2.0107160758	-3.1375787187	0.1354565882
H	-4.3698320723	-2.6654144424	0.6931400754
H	-3.5421865708	1.5440431280	0.7497103148
H	-5.0806799905	-0.3079313287	1.0759080864
H	2.4219324884	2.0485061966	-0.5063543905
H	-2.4179594437	2.9491825693	-0.0456510416
H	1.5851493599	4.3525103710	-0.5858425715
H	-0.8607814496	4.8100461512	-0.3671826164
C	4.3512168382	-0.1565285175	1.1231142253
H	4.8106328938	0.7524243539	1.5144468302
H	5.0390172966	-0.6243793992	0.4074569689
H	4.1519663245	-0.8487045884	1.9483319030
H	-0.9512372993	-1.1749216854	1.2564985515
Cl	-0.2503531575	-1.4005052269	2.8372038229

Ground state coordinates for: S7

C	0.2762338217	0.7069121980	1.0044506027
C	1.4903330847	-0.2151099674	1.2092894783

H	1.2570612513	-0.7750878371	2.1400801635
C	0.3565237708	2.0797290518	1.2682113827
C	-0.7637475687	2.8932015023	1.1027015647
C	-1.9589262393	2.3485105290	0.6444975831
C	-2.0444039038	0.9800737436	0.3601647930
C	-0.9297942641	0.1173551080	0.5594532575
C	-0.9485570700	-1.3358479578	0.2459769013
C	0.2843088522	-1.9714836005	-0.0868786910
C	1.5293343514	-1.2361970195	0.0929074853
C	2.8046772247	0.4848845379	1.4265141619
C	3.9045901195	0.2192680895	0.6684198752
C	2.6803072769	-1.4472911196	-0.6420097866
C	3.8641745237	-0.7356378670	-0.3870862793
C	-2.1205626135	-2.1123317006	0.2180143087
C	0.2818475397	-3.3139189871	-0.5071855640
C	-2.0966142598	-3.4487942539	-0.1743173830
C	-0.8958132134	-4.0489712332	-0.5606860314
H	1.2868860663	2.5111170689	1.6185237232
H	-0.7041560361	3.9554984926	1.3203819464
H	-2.8169343173	2.9925516839	0.5019938240
O	-3.1850344038	0.4218643553	-0.1365645166
H	2.8719887162	1.1869331423	2.2523498945
H	4.8358190869	0.7414227211	0.8728868109
H	2.6630245426	-2.1670305665	-1.4563660334
H	4.7450054698	-0.9098858632	-0.9959444659
H	-3.0620220440	-1.6628387131	0.4978644639
H	1.2283317331	-3.7916316882	-0.7409682434
H	-3.0198716306	-4.0210970188	-0.1785295559
H	-0.8746531865	-5.0898524731	-0.8705860784
C	-4.2764951419	1.2610000046	-0.4842302452
H	-5.0270502094	0.6024421396	-0.9238752464
H	-3.9834127731	2.0190013595	-1.2207348498
H	-4.7050002183	1.7570781499	0.3957188151
H	0.9700993146	2.6303041985	-0.9375113683
Cl	1.3527598604	3.1265072403	-2.0749388131

Ground state coordinates for: S8

C	-0.0545406467	-1.2731578186	-0.6558909586
C	-1.4919515494	-1.0749546521	-0.1791255331
H	-0.1019693943	-1.0139625898	-1.7443345703
C	0.4333316387	-2.6697081944	-0.7444103268
C	1.7270795274	-2.9757696820	-0.4810816279
C	2.6164064387	-1.9669797781	-0.0292857989
C	2.2464049269	-0.6332429233	0.1190480895
C	0.9087934606	-0.2213701793	-0.1755604336
C	0.4240501154	1.1289180214	-0.1239191271
C	-0.9966163788	1.3609696771	-0.0643148553
C	-1.9297103987	0.2389768459	0.0862278038
C	-2.3790295579	-2.1459502313	-0.0475087091
C	-3.6913520210	-1.9314868837	0.3677959111
C	-3.2580453632	0.4321205409	0.5167883996
C	-4.1315012663	-0.6368437656	0.6513544478
C	1.2967788029	2.2529187091	-0.1961767756
C	-1.4585396590	2.6839233205	-0.1147888771
C	0.8031276830	3.5411498784	-0.2373846815
C	-0.5812363024	3.7576017512	-0.1979854947
H	-0.2525208328	-3.4277087510	-1.1013819494
H	2.0962672181	-3.9891258726	-0.5949552692
H	3.6330926887	-2.2577524322	0.2061640267
O	3.0943168985	0.3050395047	0.5860680500
H	-2.0570795334	-3.1628217344	-0.2330259429
H	-4.3593614003	-2.7774292374	0.4921118647
H	-3.6053760196	1.4262103078	0.7707349627
H	-5.1481952484	-0.4658004242	0.9887810186
H	2.3605756088	2.0908260131	-0.2624692513
H	-2.5229859610	2.8812108266	-0.1094247181
H	1.4860726258	4.3798615875	-0.3177367203
H	-0.9750182510	4.7682640378	-0.2410708271
C	4.4061898946	-0.0681939862	1.0313359145
H	4.8515773626	0.8497386060	1.4116550623

H 5.0108665334 -0.4520218889 0.2032566640  
H 4.3505722841 -0.8083818563 1.8363060890

Ground state coordinates for: S9

C -0.0373311687 -1.3770295749 -0.0905557940  
C -1.4803905758 -1.1090425909 -0.0297995057  
C 0.4213862960 -2.7046148382 -0.2411112956  
C 1.7651086632 -3.0058995076 -0.2112334113  
C 2.7012697951 -1.9924583669 0.0023398378  
C 2.2837218102 -0.6733915719 0.1398682774  
C 0.8983554814 -0.3083143088 0.0407102019  
C 0.4056191066 1.0814240885 0.0504843230  
C -0.9995043415 1.3315382106 0.0774945166  
C -1.9529246647 0.2207449104 0.0970202401  
C -2.4279332727 -2.1591027662 -0.0468428487  
C -3.7856148188 -1.9225993323 0.0622181003  
C -3.3447488124 0.4354170722 0.2250399204  
C -4.2499018927 -0.6089552173 0.2061531823  
C 1.2636369404 2.2080062216 -0.0248255876  
C -1.4600854630 2.6661218137 0.0561203785  
C 0.7810111044 3.5050870163 -0.0435557232  
C -0.5953227181 3.7429495495 0.0051307219  
H -0.2837012248 -3.5110519738 -0.3872358931  
H 2.1003315824 -4.0312916558 -0.3347098195  
H 3.7521367982 -2.2429182164 0.0601305806  
O 3.1893185821 0.3195333067 0.3966918631  
H -2.0983097368 -3.1866642964 -0.1272679415  
H -4.4829528250 -2.7549703780 0.0492543136  
H -3.7269413860 1.4401212124 0.3535291174  
H -5.3122251490 -0.4085039511 0.3093728899  
H 2.3269606775 2.0557158750 -0.0825569493  
H -2.5242196030 2.8645162050 0.0570709900  
H 1.4806919101 4.3337342425 -0.1054271937  
H -0.9862239750 4.7560935326 -0.0123919528  
C 4.5575798291 -0.0098803439 0.5747293651  
H 5.0593707640 0.9306734308 0.8070703984  
H 4.9962462191 -0.4367983062 -0.3358472921  
H 4.6993454716 -0.7105940005 1.4065412428

Mallory Coordinates

R1 : ethene, R2=R31: phenyl

Ground state coordinates: M1

C 0.6750525969 -1.8254143262 0.0041783451  
C -0.6739752140 -1.8265488482 -0.0008379784  
C 1.6441486249 -0.7153522693 -0.0645015855  
C -1.6441425150 -0.7170095150 0.0653584538  
H 1.1436154106 -2.8083481366 0.0489688598  
H -1.1411067958 -2.8102654555 -0.0432307626  
C 1.4165719938 0.4598702419 -0.8040331381  
C 2.8904654291 -0.8661213860 0.5696344327  
C 2.3894164116 1.4535259096 -0.8798515574  
C 3.6126961245 1.2987532448 -0.2228446696  
C 3.8602622042 0.1322280550 0.5019344536  
H 2.1954766509 2.3499346455 -1.4622970641  
H 4.3690600778 2.0757224182 -0.2851991632  
H 4.8113601269 -0.0040545704 1.0088009522  
C -2.8861582701 -0.8645070069 -0.5777161919  
C -1.4209884272 0.4544380600 0.8120751451  
C -2.3941369071 1.4479334780 0.8866996910  
C -3.6131846865 1.2965127437 0.2211339831  
C -3.8561947382 0.1337346461 -0.5111872449  
H -3.0847081168 -1.7729915657 -1.1408738366  
H -4.8039973240 0.0002594061 -1.0249400214  
H -2.2038130662 2.3414251927 1.4747908011  
H -4.3699067861 2.0732025681 0.2826140740  
H -0.4847110565 0.5759573425 1.3457686121

H 0.4772261700 0.5843807969 -1.3315355361  
H 3.0925089475 -1.7774808076 1.1268802527

Ground state coordinates: M2

C 0.6692720848 -0.1046814573 2.1728134293  
C -0.6692720848 0.1046814573 2.1728134293  
C 1.4185777570 -0.2052172192 0.9257664410  
C -1.4185777570 0.2052172192 0.9257664410  
H 1.2166365948 -0.1538255446 3.1096275049  
H -1.2166365948 0.1538255446 3.1096275049  
C 0.6828524507 -0.5793378787 -0.2980928795  
C 2.7393161182 0.2064755722 0.8407918867  
C 1.4359105103 -0.5612901001 -1.5370049932  
C 2.7417097410 -0.1230848178 -1.5819269784  
C 3.4007301746 0.2580042805 -0.3977310991  
H 0.9509217741 -0.9183870284 -2.4401844285  
H 3.2802341460 -0.1144792847 -2.5238716920  
H 4.4329306920 0.5904844709 -0.4392181659  
C -2.7393161182 -0.2064755722 0.8407918867  
C -0.6828524507 0.5793378787 -0.2980928795  
C -1.4359105103 0.5612901001 -1.5370049932  
C -2.7417097410 0.1230848178 -1.5819269784  
C -3.4007301746 -0.2580042805 -0.3977310991  
H -3.2614685840 -0.5145773113 1.7413539342  
H -4.4329306920 -0.5904844709 -0.4392181659  
H -0.9509217741 0.9183870284 -2.4401844285  
H -3.2802341460 0.1144792847 -2.5238716920  
H -0.0787143187 1.4823456430 -0.1954032588  
H 0.0787143187 -1.4823456430 -0.1954032588  
H 3.2614685840 0.5145773113 1.7413539342

Ground state coordinates: M3

C 0.7160401142 -2.0765394304 -0.0077209050  
C -0.7160373854 -2.0765502062 0.0077814877  
C 1.4355459789 -0.9193772216 -0.1020460707  
C -1.4355495939 -0.9193851851 0.1020544627  
H 1.2423735549 -3.0273753433 0.0325087465  
H -1.2423614026 -3.0273925555 -0.0324396374  
C 0.7025407620 0.4035080969 -0.3178070115  
C 2.8761011259 -0.9056318362 -0.1145276196  
C 1.5394631308 1.5931188804 0.0978539679  
C 2.8806072997 1.5186862939 0.1774737626  
C 3.5741424701 0.2553475255 -0.0113553661  
H 1.0357838272 2.5389103415 0.2744228222  
H 3.4652993759 2.4020297107 0.4204420481  
H 4.6599696464 0.2430890564 0.0034438430  
C -2.8761037545 -0.9056316712 0.1144757774  
C -0.7025439334 0.4034938433 0.3178121742  
C -1.5394637732 1.5931216422 -0.0978051729  
C -2.8806054020 1.5186923533 -0.1774764545  
C -3.5741431188 0.2553474902 0.0112829533  
H -3.3963473847 -1.8600887833 0.1519236677  
H -4.6599696060 0.2430886978 -0.0035728534  
H -1.0357860112 2.5389293534 -0.2743014032  
H -3.4652880196 2.4020510933 -0.4204106595  
H -0.5515237208 0.4888046945 1.4180857533  
H 0.5515480680 0.4888417412 -1.4180810021  
H 3.3963381496 -1.8600914567 -0.1519972378

Ground state coordinates: M4

C 0.6978541166 0.0082356158 2.1071569500  
C -0.6978541166 -0.0082356158 2.1071569500  
C 1.4317714995 -0.0707198823 0.9174979245  
C -1.4317714995 0.0707198823 0.9174979245  
H 1.2335320512 0.0666088212 3.0501499184  
H -1.2335320512 -0.0666088212 3.0501499184  
C 0.6968562672 -0.3498583563 -0.3796150077

C	2.8390345664	0.0424214359	0.9095496191
C	1.5295029361	-0.1463866519	-1.6101320108
C	2.8742625770	0.0106385593	-1.5443966699
C	3.5427318730	0.0762696114	-0.2763758972
H	1.0444053361	-0.2268634413	-2.5768003195
H	3.4613796112	0.0882739732	-2.4534624048
H	4.6222953370	0.1876429825	-0.2556592927
C	-2.8390345664	-0.0424214359	0.9095496191
C	-0.6968562672	0.3498583563	-0.3796150077
C	-1.5295029361	0.1463866519	-1.6101320108
C	-2.8742625770	-0.0106385593	-1.5443966699
C	-3.5427318730	-0.0762696114	-0.2763758972
H	-3.3609393855	-0.1579700423	1.8548975236
H	-4.6222953370	-0.1876429825	-0.2556592927
H	-1.0444053361	0.2268634413	-2.5768003195
H	-3.4613796112	-0.0882739732	-2.4534624048
H	-0.4837686465	1.4409338064	-0.3612338043
H	0.4837686465	-1.4409338064	-0.3612338043
H	3.3609393855	0.1579700423	1.8548975236

Ground state coordinates: M5=M6

C	1.0701864298	-1.8026937293	1.2121515090
C	-0.2877822171	-2.0725977960	1.1123576525
C	1.7042856326	-0.8470771529	0.4086162009
C	-1.1343925075	-1.3071887690	0.2728601864
H	1.6641263016	-2.3288314760	1.9556338811
H	-0.7359257462	-2.8395443505	1.7369937425
C	0.9318354155	-0.2357027500	-0.7498944419
C	3.0565385401	-0.4916525051	0.6006143211
C	1.5583476719	1.0309451737	-1.2696347845
C	2.8446567738	1.3487514199	-0.9936858241
C	3.6311002488	0.5522251484	-0.0911585233
H	0.9823572915	1.6572560204	-1.9419983504
H	3.2897783117	2.2365384942	-1.4332864113
H	4.6654230104	0.8238887125	0.0945922866
C	-2.5264897385	-1.5509358998	0.2183914021
C	-0.5883606860	-0.1645900571	-0.4621794411
C	-1.4568737680	0.4358923473	-1.4541146163
C	-2.7997380135	0.1576805972	-1.4939139304
C	-3.3400029870	-0.8293338843	-0.6313985042
H	-2.9445862031	-2.3381057782	0.8394961391
H	-4.4058644953	-1.0371710534	-0.6599489645
H	-1.0533145048	1.2041542894	-2.1045415778
H	-3.4492041131	0.6827500626	-2.1867090030
H	-0.6322814621	0.6918919222	0.3914069129
H	1.0272949606	-0.9747490919	-1.5785350548
H	3.6276605989	-1.0223231804	1.3581555433
Cl	-0.4989635581	1.9041279693	1.5657803238

Ground state coordinates: M7

C	1.1501105316	-1.9865243644	1.1130288743
C	-0.1870210689	-2.2613320653	0.9874407139
C	1.7780603463	-0.9692811797	0.3526380970
C	-1.0530966636	-1.4473318665	0.1608406721
H	1.7441906175	-2.5229642111	1.8496687517
H	-0.6455003161	-3.0363388615	1.5952607231
C	1.0283273348	-0.4100906746	-0.8485381463
C	3.0764440265	-0.5219390562	0.6304159063
C	1.6147758363	0.8853615279	-1.3523533334
C	2.8546465399	1.2966012653	-0.9837925758
C	3.6306460962	0.5683235707	-0.0243063265
H	1.0623019495	1.4488504959	-2.0961725930
H	3.2682055020	2.2059143184	-1.4118992933
H	4.6280646637	0.9108714321	0.2315530129
C	-2.4529222890	-1.5873507556	0.2276051999
C	-0.4944845431	-0.4536094152	-0.6878185327
C	-1.3572407575	0.3634024946	-1.4252358701
C	-2.7483979944	0.2132907696	-1.3441044865

C	-3.2958002650	-0.7687086417	-0.5169021127
H	-2.8711611513	-2.3452085832	0.8850998306
H	-4.3727491519	-0.8907003326	-0.4501748427
H	-0.9572390488	1.1208583040	-2.0909810439
H	-3.3935384810	0.8620705404	-1.9287513629
H	-1.2897124273	1.7266609400	0.5916132150
H	1.2188870945	-1.1549639533	-1.6592380619
H	3.6340177337	-1.0192780944	1.4211943258
Cl	-1.3700029273	2.6570210795	1.4899599331

Ground state coordinates: M8

C	0.7040955156	-2.1029789810	-0.0018609503
C	-0.6916331874	-2.1037912494	-0.0163648083
C	1.4372411043	-0.9131499972	-0.0852748872
C	-1.4260920669	-0.9143104831	0.0601897567
H	1.2403804550	-3.0455128308	0.0584804305
H	-1.2268771360	-3.0472392809	-0.0712711180
C	0.7012189807	0.3827456298	-0.3671182133
C	2.8446631751	-0.9041122290	0.0258686541
C	1.5334806698	1.6143041640	-0.1683606309
C	2.8784896753	1.5497547173	-0.0130371307
C	3.5477482355	0.2822959538	0.0553030445
H	1.0477294155	2.5804717746	-0.2509505404
H	3.4652138062	2.4593666728	0.0611462065
H	4.6274853318	0.2624891736	0.1652156386
C	-2.8335229024	-0.9074582911	-0.0509896609
C	-0.6915018508	0.3840027115	0.3345532699
C	-1.5251119311	1.6134736087	0.1287103746
C	-2.8700583645	1.5465436179	-0.0262335218
C	-3.5379171363	0.2779732795	-0.0872718563
H	-3.3550697144	-1.8534238618	-0.1630771331
H	-4.6176213648	0.2563502443	-0.1970648432
H	-1.0404378035	2.5806276406	0.2057185428
H	-3.4577860415	2.4550638080	-0.1056660392
H	-0.4768700212	0.3688804678	1.4253834476
H	3.3672535721	-1.8488285193	0.1434047669

Ground state coordinates: M9

C	0.6796942699	-2.0940979775	-0.0001421111
C	-0.6797064490	-2.0940946035	0.0001429160
C	1.4229560432	-0.8664222849	-0.0001957672
C	-1.4229585548	-0.8664140445	0.0001517477
H	1.2319664606	-3.0301067027	-0.0002232487
H	-1.2319841897	-3.0300972999	0.0003700421
C	0.7286977914	0.3804425750	0.0000157533
C	2.8371085962	-0.8789187866	-0.0002698944
C	1.4992359208	1.5667230164	0.0003846006
C	2.8815641062	1.5295280904	0.0002988094
C	3.5605444747	0.2969458840	-0.0000924411
H	1.0056152231	2.5320699554	0.0009386461
H	3.4449896076	2.4580075417	0.0005361102
H	4.6462265807	0.2728188569	-0.0001566994
C	-2.8371148519	-0.8789156676	0.0002739576
C	-0.7286978903	0.3804451723	-0.0000752975
C	-1.4992318920	1.5667344666	-0.0003678063
C	-2.8815531685	1.5295320416	-0.0002814474
C	-3.5605400067	0.2969476383	0.0000914066
H	-3.3485076559	-1.8381150254	0.0004996796
H	-4.6462223500	0.2728306279	0.0002175553
H	-1.0056051556	2.5320784471	-0.0008017081
H	-3.4449835162	2.4580107819	-0.0005839340
H	3.3485146607	-1.8381103032	-0.0004030001

R1 : pyrrole, R2=R3 : phenyl

Ground state coordinates: M1



C	1.6368297981	1.2796250622	0.4905897033
C	-1.6078031778	1.3064285610	-0.3826311652
H	0.7012811572	1.6360074070	0.8768744015
H	-0.6481762259	1.6828035813	-0.6707186973
C	1.8068819488	-0.0490376583	0.0421113617
C	3.1177224912	-0.4230422297	-0.3645375578
C	4.1832556815	0.4730446854	-0.3420987644
C	3.9828950990	1.7797988942	0.0779225276
C	2.7138935163	2.1846824039	0.4931489476
C	-1.8122757006	-0.0463542917	-0.0284095143
C	-3.1540945598	-0.4317828782	0.2522876988
C	-4.2121413091	0.4714614772	0.1980154256
C	-2.6781866485	2.2179623620	-0.4144487261
C	-3.9766191632	1.7989557920	-0.1259173354
C	0.7145057268	-1.1036300827	0.0163031327
C	-0.7216742511	-1.1047104112	0.0194858430
C	1.0736831549	-2.4549252304	0.0192426991
C	-1.0714966226	-2.4608983294	0.0283864987
N	0.0017150991	-3.2475757886	0.0274301813
H	3.3543625679	-1.4126704836	-0.7173213832
H	5.1674039202	0.1439297397	-0.6542757495
H	4.8169447996	2.4707608580	0.0896995469
H	2.5734323329	3.2028533047	0.8318071223
H	-3.4292296367	-1.4353856256	0.5231712646
H	-5.2190904991	0.1313402894	0.4097882618
H	-2.5080971956	3.2536319278	-0.6782429038
H	-4.8053077162	2.4952532400	-0.1625429130
H	2.0653194836	-2.8772421544	0.0357358007
H	-2.0580854890	-2.8945992773	0.0158187694
H	0.0049809040	-4.2891210441	0.0314905605

Ground state coordinates: M3

C	0.7111297072	-1.0523792367	-0.2882737874
C	-0.7111354223	-1.0523793331	0.2882607277
H	0.5943585576	-1.1738300182	-1.3976835152
H	-0.5943644872	-1.1738434598	1.3976692840
C	1.4737505063	0.2530510267	-0.0937782415
C	2.8864713900	0.2074293993	-0.1449748995
C	3.5729952316	-0.9816534984	-0.0485956416
C	2.8635520347	-2.2035572807	0.2235922305
C	1.5112941964	-2.2351934543	0.2057913730
C	-1.4737493763	0.2530583128	0.0937801215
C	-2.8864697842	0.2074418282	0.1449990654
C	-3.5729985870	-0.9816383993	0.0486211305
C	-1.5113073773	-2.2351835782	-0.2058142390
C	-2.8635653447	-2.2035427655	-0.2235936576
C	0.7335760445	1.4403230373	-0.0247828649
C	-0.7335688203	1.4403264086	0.0247797601
C	1.1355659758	2.7922508561	-0.0326791067
C	-1.1355499696	2.7922574299	0.0326812978
N	0.0000097385	3.5420421959	-0.0000134003
H	3.4427991643	1.1405245276	-0.1976144211
H	4.6585211161	-0.9867410480	-0.0691638124
H	3.4296088259	-3.0871783981	0.5077839093
H	0.9786393972	-3.1390084902	0.4852189452
H	-3.4427938286	1.1405383329	0.1976575386
H	-4.6585242210	-0.9867214052	0.0692082125
H	-0.9786562748	-3.1389960926	-0.4852583693
H	-3.4296306880	-3.0871576859	-0.5077870606
H	2.1098741734	3.2513968824	-0.0695385633
H	-2.1098552054	3.2514089465	0.0695444620
H	0.0000128726	4.5516480213	-0.0000224162

Ground state coordinates: M4

C	0.7111297072	-1.0523792367	-0.2882737874
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C	-0.7111354223	-1.0523793331	0.2882607277
H	0.5943585576	-1.1738300182	-1.3976835152
H	-0.5943644872	-1.1738434598	1.3976692840
C	1.4737505063	0.2530510267	-0.0937782415
C	2.8864713900	0.2074293993	-0.1449748995
C	3.5729952316	-0.9816534984	-0.0485956416
C	2.8635520347	-2.2035572807	0.2235922305
C	1.5112941964	-2.2351934543	0.2057913730
C	-1.4737493763	0.2530583128	0.0937801215
C	-2.8864697842	0.2074418282	0.1449990654
C	-3.5729985870	-0.9816383993	0.0486211305
C	-1.5113073773	-2.2351835782	-0.2058142390
C	-2.8635653447	-2.2035427655	-0.2235936576
C	0.7335760445	1.4403230373	-0.0247828649
C	-0.7335688203	1.4403264086	0.0247797601
C	1.1355659758	2.7922508561	-0.0326791067
C	-1.1355499696	2.7922574299	0.0326812978
N	0.0000097385	3.5420421959	-0.0000134003
H	3.4427991643	1.1405245276	-0.1976144211
H	4.6585211161	-0.9867410480	-0.0691638124
H	3.4296088259	-3.0871783981	0.5077839093
H	0.9786393972	-3.1390084902	0.4852189452
H	-3.4427938286	1.1405383329	0.1976575386
H	-4.6585242210	-0.9867214052	0.0692082125
H	-0.9786562748	-3.1389960926	-0.4852583693
H	-3.4296306880	-3.0871576859	-0.5077870606
H	2.1098741734	3.2513968824	-0.0695385633
H	-2.1098552054	3.2514089465	0.0695444620
H	0.0000128726	4.5516480213	-0.0000224162

Ground state coordinates: M5=M6

C	0.6796743114	-0.8832892930	0.3325994075
C	-0.7647398334	-0.7180781077	0.9535880218
H	-0.5403126826	-0.4913466907	2.0174924478
C	1.4805647820	0.3397245940	0.3184343398
C	2.8805301641	0.2464807471	0.3016177814
C	3.5115845781	-0.9828182612	0.4195668180
C	2.7690665526	-2.1722134528	0.5749039568
C	1.3962257325	-2.1163213055	0.5844887504
C	-1.4858593036	0.4980532837	0.3960382919
C	-2.8389616840	0.4555489682	0.1141817724
C	-3.5863805210	-0.7225806136	0.2384104728
C	-1.6136958503	-1.9579480504	0.9410115619
C	-2.9405467301	-1.9265118614	0.6352799928
C	0.7803198205	1.5898378703	0.2206527709
C	-0.6630120738	1.6707935540	0.2232660244
C	1.2689739454	2.8782029392	0.0224091906
C	-0.9857388276	3.0017506559	0.0278654339
N	0.1950436514	3.7074346061	-0.0876739668
H	3.4771140750	1.1493039353	0.2168843409
H	4.5970693875	-1.0279708750	0.4055213194
H	3.2822183381	-3.1218536726	0.6858917161
H	0.8257358608	-3.0348407442	0.6639260685
H	-3.3241323716	1.3533830543	-0.2604841069
H	-4.6416019077	-0.7280722215	-0.0122604574
H	-1.1651881995	-2.8885427841	1.2721846548
H	-3.5207679117	-2.8438607974	0.6898846690
H	2.2769776782	3.2536640766	-0.0662464247
H	-1.9391206398	3.5037128470	-0.0259436135
H	0.2533076742	4.7026257731	-0.2383911370
H	0.4353989586	-1.0132563997	-0.7805255642
Cl	-0.0417667174	-1.1746339850	-2.4576531570

Ground state coordinates: M7

C	-0.6894029951	0.2707696330	-0.9145872920
C	0.2059404977	-0.9618199876	-1.1662552202
H	0.6936920566	-0.7199080384	-2.1380466555
C	-0.0885332016	1.4700941405	-0.4533682022

C	-0.8770296159	2.6233191522	-0.3152630514
C	-2.2340694100	2.6128312220	-0.6279260290
C	-2.8312467079	1.4322580189	-1.0682585117
C	-2.0590037353	0.2724447511	-1.2050746616
C	1.3484941997	-1.0698335691	-0.1625819395
C	1.7107422399	-2.2887879536	0.3791081826
C	1.0148789244	-3.4715342470	0.0839086595
C	-0.5210243502	-2.2662583332	-1.3671417646
C	-0.1089316342	-3.4289074997	-0.7885800839
C	1.3222568731	1.4346891629	-0.0782967620
C	2.0070547280	0.1828644732	0.1197476612
C	2.1986942442	2.4427943116	0.2768199607
C	3.2752908715	0.4827083741	0.5944218918
N	3.3719827770	1.8503276960	0.6794951803
H	-0.4211190224	3.5343845517	0.0623172680
H	-2.8244392029	3.5170993149	-0.5126338775
H	-3.8915741792	1.4040230620	-1.3008355972
H	-2.5386991451	-0.6362188652	-1.5519411704
H	2.5405200306	-2.3221011036	1.0814582842
H	1.3130838360	-4.4087024764	0.5418094923
H	-1.3550877334	-2.2802135477	-2.0614862371
H	-0.6495797429	-4.3488095520	-0.9973489336
H	2.0889627921	3.5167742172	0.2814347511
H	4.1102178919	-0.1549630124	0.8423096014
H	4.2010741559	2.3505989090	0.9572474598
H	-2.3523259592	-0.2568553172	1.1158385415
Cl	-2.7390159286	-0.6219524653	2.2990219874

Ground state coordinates: M8

C	0.6568168352	-1.0578569833	0.2065158504
C	-0.8187198609	-0.8776032952	0.6243142333
H	-0.7434105614	-0.6634067485	1.7148406203
C	1.4686024943	0.0945366569	0.0478981585
C	2.8345315522	-0.0623440774	-0.2355347686
C	3.4069820722	-1.3260207880	-0.3575107679
C	2.6094428219	-2.4610035674	-0.2160868964
C	1.2441945928	-2.3203503760	0.0605973255
C	-1.4510640801	0.3690987714	0.0157700976
C	-2.7404220661	0.3459523347	-0.4817402160
C	-3.5076592019	-0.8291521309	-0.5084792318
C	-1.6891563152	-2.1000804565	0.4890523261
C	-2.9503029335	-2.0458430529	-0.0236721771
C	0.8284485189	1.4047695341	0.1236513140
C	-0.6040686584	1.5370802657	0.0487038211
C	1.3585968485	2.6812237869	0.1354886131
C	-0.8866698611	2.8944533448	0.0123513037
N	0.3096593714	3.5672263026	0.0684090745
H	3.4498003824	0.8210843897	-0.3820047990
H	4.4660407873	-1.4229537770	-0.5778110611
H	3.0378307261	-3.4529775057	-0.3240885368
H	0.6391519991	-3.2135843188	0.1708163126
H	-3.1571042990	1.2616838266	-0.8949761211
H	-4.5096137087	-0.8171592345	-0.9242082721
H	-1.3140947630	-3.0364511715	0.8896731482
H	-3.5485167436	-2.9528272573	-0.0640450241
H	2.3788551187	3.0311916111	0.1813347051
H	-1.8269458853	3.4238736402	-0.0156251750
H	0.4030747947	4.5697826272	0.0993167680

Ground state coordinates: M9

C	0.7430838534	-1.0301359447	0.0028219003
C	-0.7365097759	-1.0303210267	0.0076944854
C	1.4644003325	0.1977468963	-0.0020629424
C	2.8719448245	0.1781263398	-0.0072935685
C	3.5757847834	-1.0150878879	-0.0085648900
C	2.8754099440	-2.2285033976	-0.0074734829
C	1.4883115635	-2.2283259358	-0.0013694777
C	-1.4638070663	0.1963977984	-0.0109744753

C	-2.8721261602	0.1728904191	-0.0252307411
C	-3.5755125855	-1.0211009358	-0.0165578590
C	-1.4838553623	-2.2311387490	0.0287852321
C	-2.8730935319	-2.2331451693	0.0152122618
C	0.7161410267	1.4383922585	0.0005485309
C	-0.7186341722	1.4379260938	-0.0070392765
C	1.1267295205	2.7626270060	0.0111875203
C	-1.1328584254	2.7615546752	0.0015773153
N	-0.0040725963	3.5394428783	0.0121357773
H	3.4108345116	1.1212012957	-0.0085173969
H	4.6618299093	-1.0081710330	-0.0116951645
H	3.4140981055	-3.1714791139	-0.0112753799
H	0.9777635355	-3.1846628114	-0.0028461764
H	-3.4124800028	1.1147216764	-0.0388734168
H	-4.6612880855	-1.0165481220	-0.0293045900
H	-0.9723217734	-3.1865802780	0.0510990775
H	-3.4101009494	-3.1768197906	0.0284251045
H	2.1083671125	3.2105957270	0.0193828969
H	-2.1156041344	3.2070897851	0.0063967829
H	-0.0050426680	4.5471378741	0.0246946255

R1: thiophene, R2=R3 : phenyl

Ground state coordinates: M1

C	1.6594179219	1.5404136367	0.4568952588
C	-1.6245044217	1.5692808981	-0.3438711541
H	0.7421581739	1.9327499380	0.8379833187
H	-0.6795248839	1.9757763987	-0.6183757253
C	1.8039844719	0.2019949973	0.0329749639
C	3.1067341123	-0.2101321677	-0.3361410968
C	4.2013871665	0.6529978658	-0.3250569194
C	4.0243683917	1.9747030787	0.0648615538
C	2.7610822476	2.4129169228	0.4626818133
C	-1.8075749188	0.2097473441	-0.0179121361
C	-3.1380621815	-0.2111812511	0.2222189102
C	-4.2245447369	0.6614855544	0.1746976151
C	-2.7165924093	2.4519386029	-0.3826036175
C	-4.0101060521	2.0027679342	-0.1174699611
C	0.7211041546	-0.8628701910	0.0080845930
C	-0.7305807890	-0.8609769904	0.0272644896
C	1.2244994251	-2.1738631794	-0.0125704444
C	-1.2371786718	-2.1710718366	0.0485761791
S	-0.0075473125	-3.2859882895	0.0204265902
H	3.2522754630	-1.1900056112	-0.6254146270
H	5.1350422639	0.3131822438	-0.6040280382
H	4.8228143503	2.6285308198	0.0602212777
H	2.6338114679	3.3912814988	0.7653999281
H	-3.3107273415	-1.2047338549	0.4414287908
H	-5.1794884287	0.3141767958	0.3549322992
H	-2.5596766419	3.4461935922	-0.6103171672
H	-4.8032167236	2.6627532572	-0.1381874459
H	2.2276591987	-2.4140612008	-0.0440995450
H	-2.2409721612	-2.4089385570	0.0778512062

Ground state coordinates: M3

C	1.3142660379	-0.7093475050	0.2880333458
C	1.3142259835	0.7094516082	-0.2879290913
H	1.4310561575	-0.5929948137	1.3988073605
H	1.4311648925	0.5931324018	-1.3986918379
C	0.0107251224	-1.4687855072	0.0891201474
C	0.0604229845	-2.8788968199	0.1394675294
C	1.2517784430	-3.5658330966	0.0482338092
C	2.4735029332	-2.8586532131	-0.2177792495
C	2.5013257397	-1.5058889438	-0.1993138917

C	0.0105946039	1.4687686552	-0.0891687134
C	0.0601672638	2.8788800776	-0.1397483312
C	1.2514531741	3.5659300193	-0.0484696887
C	2.5011450065	1.5061308075	0.1995509119
C	2.4732009020	2.8588944032	0.2178437211
C	-1.1929776843	-0.7346724430	0.0215511406
C	-1.1930409883	0.7345617549	-0.0215478793
C	-2.5020010275	-1.2460191031	0.0266724222
C	-2.5021098814	1.2458019307	-0.0267798539
S	-3.6573620669	-0.0001571473	0.0001219916
H	-0.8679693720	-3.4414903707	0.1898292056
H	1.2549297756	-4.6511721052	0.0699632326
H	3.3593890107	-3.4232343036	-0.4968826580
H	3.4054505964	-0.9715007061	-0.4732293701
H	-0.8682710158	3.4413796546	-0.1903278852
H	1.2545195549	4.6512657787	-0.0703850921
H	3.4052649154	0.9718453449	0.4736835195
H	3.3589866488	3.4235933020	0.4970283321
H	-2.8213034337	-2.2761343786	0.0602157094
H	-2.8214963389	2.2758888030	-0.0603803537

Ground state coordinates: M4

C	1.3142660379	-0.7093475050	0.2880333458
C	1.3142259835	0.7094516082	-0.2879290913
H	1.4310561575	-0.5929948137	1.3988073605
H	1.4311648925	0.5931324018	-1.3986918379
C	0.0107251224	-1.4687855072	0.0891201474
C	0.0604229845	-2.8788968199	0.1394675294
C	1.2517784430	-3.5658330966	0.0482338092
C	2.4735029332	-2.8586532131	-0.2177792495
C	2.5013257397	-1.5058889438	-0.1993138917
C	0.0105946039	1.4687686552	-0.0891687134
C	0.0601672638	2.8788800776	-0.1397483312
C	1.2514531741	3.5659300193	-0.0484696887
C	2.5011450065	1.5061308075	0.1995509119
C	2.4732009020	2.8588944032	0.2178437211
C	-1.1929776843	-0.7346724430	0.0215511406
C	-1.1930409883	0.7345617549	-0.0215478793
C	-2.5020010275	-1.2460191031	0.0266724222
C	-2.5021098814	1.2458019307	-0.0267798539
S	-3.6573620669	-0.0001571473	0.0001219916
H	-0.8679693720	-3.4414903707	0.1898292056
H	1.2549297756	-4.6511721052	0.0699632326
H	3.3593890107	-3.4232343036	-0.4968826580
H	3.4054505964	-0.9715007061	-0.4732293701
H	-0.8682710158	3.4413796546	-0.1903278852
H	1.2545195550	4.6512657787	-0.0703850921
H	3.4052649154	0.9718453449	0.4736835195
H	3.3589866488	3.4235933020	0.4970283321
H	-2.8213034337	-2.2761343786	0.0602157094
H	-2.8214963389	2.2758888030	-0.0603803537

Ground state coordinates: M5=M6

C	1.1037808765	0.1986729954	-0.6903006077
C	0.0932073025	1.3805887131	-0.8870950404
H	-0.1961351992	1.2617983721	-1.9536181867
C	0.5465536487	-1.1332426144	-0.6537289254
C	1.3983155525	-2.2278427086	-0.8562482169
C	2.7341334467	-2.0480418147	-1.1970013012
C	3.2605517173	-0.7592507490	-1.3681660635
C	2.4447991019	0.3384205649	-1.1693750063
C	-1.1779666139	1.1960779593	-0.0786742481
C	-1.8011486110	2.2824977092	0.5113928624
C	-1.2517082071	3.5689874013	0.4734951714
C	0.6787949278	2.7614318256	-0.7586549954
C	0.0092026162	3.7789910539	-0.1524408771
C	-0.8626492711	-1.2961888935	-0.3168749507
C	-1.7044530732	-0.1522195020	-0.0180436428

C	-1.5398469692	-2.4890455978	-0.1966703682
C	-2.9841183226	-0.5391835537	0.3183241880
S	-3.1815209849	-2.2579401949	0.2735499050
H	1.0100903711	-3.2363292292	-0.7581906047
H	3.3690767479	-2.9166618570	-1.3447828763
H	4.2979734589	-0.6240556379	-1.6568122377
H	2.8635763770	1.3329527230	-1.2654628169
H	-2.7231236214	2.1219145069	1.0637484490
H	-1.7605295310	4.3918294515	0.9638597026
H	1.6267659488	2.9638228025	-1.2448336835
H	0.4520309044	4.7711840495	-0.1325079966
H	-1.1674888071	-3.4919616044	-0.3470075938
H	-3.8281489159	0.0886934813	0.5641672899
H	1.3804599965	0.3394210279	0.5401468046
Cl	1.5978420082	0.6276425609	2.0646915167

Ground state coordinates: M7

C	-0.7656583892	0.4057696367	-0.9562725131
C	-0.3162415591	-1.0494002537	-1.1946854235
H	0.2127464369	-1.0021680895	-2.1724157068
C	0.1841851277	1.3496352151	-0.4986220916
C	-0.2012823936	2.6908736286	-0.3433863268
C	-1.4941549680	3.1108678767	-0.6410125298
C	-2.4343589959	2.1813419425	-1.0865398284
C	-2.0675594658	0.8397552908	-1.2365975803
C	0.7307704607	-1.4883068273	-0.1808244597
C	0.6678614686	-2.7319825871	0.4196206799
C	-0.3800654240	-3.6290639408	0.1653426126
C	-1.4279415116	-2.0526214484	-1.3604411826
C	-1.4244007436	-3.2593757655	-0.7292256746
C	1.5351967067	0.8866224738	-0.1494917089
C	1.7867245206	-0.5241669918	0.0619825920
C	2.6427311742	1.6549587843	0.1066635384
C	3.0765600144	-0.7624478671	0.4839161776
S	3.9940672965	0.6982098244	0.6135328558
H	0.5187386992	3.4085467518	0.0378205778
H	-1.7701754528	4.1530373424	-0.5122836740
H	-3.4501640470	2.4912892345	-1.3134848270
H	-2.8089938656	0.1304703164	-1.5882521421
H	1.4371487197	-3.0055682425	1.1375340930
H	-0.4092616495	-4.5895018918	0.6686980863
H	-2.2175933792	-1.8206361111	-2.0682176598
H	-2.2363884663	-3.9589063610	-0.9105172193
H	2.7466893470	2.7286789228	0.0380695470
H	3.5453227047	-1.7150079867	0.6863931929
H	-2.8250655876	0.4896737462	1.0681096987
Cl	-3.3718986080	0.3402341281	2.2323213325

Ground state coordinates: M8

C	1.2010758398	-0.8331792700	-0.2333111539
C	1.2515274464	0.6490015694	-0.6539297257
H	1.0067350249	0.6207194931	-1.7389639047
C	-0.0585567488	-1.4434550314	-0.0249820468
C	-0.1146757389	-2.8100248655	0.2927346634
C	1.0420993422	-3.5766991795	0.3955782020
C	2.2856666877	-2.9762876239	0.1967288422
C	2.3577688709	-1.6134993747	-0.1107129055
C	0.1388284172	1.4572616476	-0.0017118301
C	0.3835336906	2.7069819880	0.5363750310
C	1.6673730442	3.2718326343	0.5528083363
C	2.6004221794	1.3101655948	-0.5392070947
C	2.7654031248	2.5449868033	0.0109815224
C	-1.2707006234	-0.6145758389	-0.0970251763
C	-1.1679860212	0.8287049797	-0.0284750338
C	-2.5744565220	-1.0405088416	-0.1343546203
C	-2.4049891810	1.4350761639	-0.0034641148
S	-3.6916168108	0.2812623813	-0.0771932195
H	-1.0791634610	-3.2706243714	0.4835763007

H	0.9746526061	-4.6316217396	0.6434929935
H	3.1982848074	-3.5585968217	0.2832574113
H	3.3319546433	-1.1628359598	-0.2667743657
H	-0.4404555794	3.2506793597	0.9918716479
H	1.8280061302	4.2466064343	1.0007765324
H	3.4520922067	0.8024491920	-0.9810192040
H	3.7572661702	2.9887931938	0.0385905044
H	-2.9499103883	-2.0529898910	-0.1824899786
H	-2.6275960337	2.4925348773	0.0145762023

Ground state coordinates: M9

C	1.3015411738	-0.7359194216	-0.0010336169
C	1.2942456652	0.7413548982	-0.0015212543
C	0.0792114184	-1.4607374696	0.0012770124
C	0.1077470946	-2.8676644469	0.0027869912
C	1.3047723384	-3.5655672393	0.0005259800
C	2.5135618261	-2.8591791601	-0.0037133806
C	2.5047381221	-1.4724152779	-0.0042695019
C	0.0677978483	1.4597399837	-0.0032593005
C	0.0863318687	2.8679673304	-0.0037412232
C	1.2756524943	3.5785555322	-0.0005628702
C	2.4929500514	1.4901493751	0.0026777240
C	2.4912310666	2.8809997556	0.0052340449
C	-1.1820465047	-0.7261126762	0.0014850881
C	-1.1882192049	0.7168590317	-0.0025078912
C	-2.4565454849	-1.2498001614	0.0040190121
C	-2.4667387322	1.2319219833	-0.0030839450
S	-3.6563714149	-0.0136137988	0.0009628804
H	-0.8280719017	-3.4174682214	0.0043410373
H	1.3026336154	-4.6515209469	0.0004451421
H	3.4598440219	-3.3918379913	-0.0074825700
H	3.4581089443	-0.9572275612	-0.0092883942
H	-0.8544875884	3.4089426826	-0.0084877173
H	1.2643773182	4.6640960888	-0.0006800673
H	3.4497762878	0.9816070728	0.0230246443
H	3.4336489481	3.4205820469	0.0172646518
H	-2.7612685730	-2.2858824521	0.0074244685
H	-2.7800046822	2.2656178387	-0.0078444947

R1: benzene, R2=R3 : phenyl

Ground state coordinates: M1

C	1.4888823682	0.7373076990	1.1982220806
C	-1.1889043364	1.1121832907	-1.0851730234
H	0.7616984110	0.5251237946	1.9759998157
H	-0.3989489523	0.8970237791	-1.7975717203
C	2.3656341417	1.8145188669	1.3390937271
C	3.2952558021	2.0719694176	0.3360109130
C	3.3472479490	1.2657335661	-0.8033894299
C	2.4636425975	0.1896601541	-0.9381078187
C	1.5181676660	-0.0928167892	0.0737480547
C	0.6067586565	-1.2744021994	-0.0240997084
C	-0.8021761048	-1.1529992572	-0.0399975884
C	-1.5053667363	0.1602678055	-0.1022990788
C	-1.8884000398	2.3147830203	-1.1636583007
C	-2.9173156969	2.5928259070	-0.2614427851
C	-2.5460828627	0.4500023710	0.7944861078
C	-3.2440364804	1.6553410214	0.7185877174
C	1.1759477205	-2.5575918129	-0.0198296083
C	-1.5814646770	-2.3230343319	-0.0238728013
C	0.3892409882	-3.7055885534	-0.0129257555
C	-1.0006710578	-3.5874531962	-0.0084491468
H	2.3219665850	2.4400783295	2.2250095850
H	3.9875225865	2.9038841434	0.4291646332
H	4.0729290825	1.4842888200	-1.5774873516
H	-1.6318665229	3.0358100842	-1.9348182778

H	-3.4601324918	3.5316270443	-0.3234849948
H	-2.7979082393	-0.2724426841	1.5659704553
H	-4.0407380776	1.8620120643	1.4277390298
H	2.2578174967	-2.6449410358	-0.0081774824
H	-2.6627527835	-2.2260903957	-0.0516788783
H	0.8590004792	-4.6849400209	-0.0054106396
H	-1.6291713449	-4.4733722816	-0.0041097536
H	2.5024243848	-0.4023035174	-1.7825657526

Ground state coordinates: M3

C	0.7062446835	-1.2585940797	-0.2957809354
C	-0.7064642885	-1.2584727322	0.2957774961
H	0.5856493316	-1.3658026674	-1.4020705772
H	-0.5858861226	-1.3657048007	1.4020668579
C	1.5041839571	-2.4561434314	0.1709847174
C	2.8500004129	-2.4271604122	0.2126121795
C	3.5559217127	-1.1961007361	-0.0554979724
C	2.8795619662	-0.0133251457	-0.1574806566
C	1.4498576554	0.0530271054	-0.0905190769
C	0.7336180504	1.2495749337	-0.0035060351
C	-0.7334009303	1.2497023061	0.0035072963
C	-1.4498492926	0.0532788108	0.0905189827
C	-1.5046113838	-2.4558828090	-0.1709886546
C	-2.8504229282	-2.4266667292	-0.2126111873
C	-2.8795648271	-0.0128259787	0.1574830441
C	-3.5561295978	-1.1954844875	0.0555019836
C	1.3999612253	2.5303818493	0.0450064119
C	-1.3995201738	2.5306258600	-0.0450060047
C	0.7155018654	3.7065088922	0.0326550266
C	-0.7148554874	3.7066335122	-0.0326569438
H	0.9682278652	-3.3664064404	0.4202155097
H	3.4157657272	-3.3124876542	0.4900488632
H	4.6411242730	-1.2029113472	-0.0944145955
H	-0.9688128043	-3.3662384007	-0.4202206161
H	-3.4163430053	-3.3118956119	-0.4900458406
H	-3.4556853103	0.9005322840	0.2529665608
H	-4.6413332899	-1.2021063458	0.0944209710
H	2.4815981475	2.5590044080	0.0946033167
H	-2.4811519986	2.5594385116	-0.0946024760
H	1.2522724048	4.6499826921	0.0654514990
H	-1.2514609175	4.6502011410	-0.0654550803
H	3.4558399838	0.8999338637	-0.2529624204

Ground state coordinates: M4

C	1.2014261950	-0.5986709990	0.3287514615
C	1.2014511024	0.5986215870	-0.3288542677
H	1.1146831136	-0.4004937525	1.4274674509
H	1.1146395433	0.4004514064	-1.4275648152
C	2.4741850265	-1.4193989355	0.2697357124
C	2.4813072734	-2.7631657353	0.1176804569
C	1.2561134777	-3.4726992932	-0.0809488893
C	0.0435401804	-2.8145500974	-0.1212098568
C	-0.0547102315	-1.4189363881	0.0252522759
C	-1.2996479763	-0.7210048558	-0.0296818469
C	-1.2996215406	0.7210821994	0.0296241873
C	-0.0546402579	1.4189578777	-0.0252593291
C	2.4742454415	1.4192879423	-0.2698842577
C	2.4814399625	2.7630393816	-0.1176936945
C	0.0436917715	2.8145376427	0.1214023741
C	1.2563047418	3.4726228829	0.0811448752
C	-2.5493625269	-1.3977001684	-0.0796323264
C	-2.5493058884	1.3978285793	0.0795762894
C	-3.7386733145	-0.7049903415	-0.0428409041
C	-3.7386447886	0.7051602705	0.0428047380
H	3.4077013107	-0.9052569621	0.4639226243
H	3.4160566156	-3.3133278889	0.1459195923



H	1.2817578328	-4.5497066141	-0.2131606527
H	3.4077248849	0.9051193164	-0.4641783703
H	3.4162137074	3.3131597350	-0.1459628994
H	-0.8478431513	3.3986927624	0.3123518052
H	1.2820292390	4.5496078738	0.2135159495
H	-2.5803004284	-2.4792270038	-0.1155987364
H	-2.5801837980	2.4793585303	0.1155147732
H	-4.6795511744	-1.2444230871	-0.0704961436
H	-4.6794998159	1.2446324847	0.0704764031
H	-0.8480197668	-3.3987160967	-0.3120089701

Ground state coordinates: M5=M6

C	-0.9312477470	0.7439291850	-0.5011210610
C	-0.8209342331	-0.6806568372	-1.1352248973
H	-0.4022586726	-0.4890849253	-2.1456055656
C	-2.0517210801	1.5809441140	-0.9019918462
C	-1.9871388038	2.9480771220	-0.8477615825
C	-0.7647409494	3.5588413869	-0.4955055040
C	0.3762933268	2.8109962534	-0.2466577562
C	0.3639745815	1.4069015785	-0.3213324976
C	1.5561302331	0.5984304700	-0.1075966193
C	1.4600361710	-0.8323690726	-0.0727520450
C	0.2074555061	-1.4931092699	-0.3748695070
C	-2.1293114552	-1.3928302953	-1.3359017532
C	-2.3150128182	-2.6863291294	-0.9666696625
C	-0.0633589312	-2.8116581648	-0.0248475208
C	-1.2851428551	-3.4203678290	-0.3081905349
C	2.8132723534	1.2007159337	0.1321373374
C	2.6263248418	-1.5706588313	0.2366967717
C	3.9383329587	0.4497597082	0.4202187115
C	3.8379134682	-0.9496501392	0.4810421465
H	-2.9960606406	1.0939857199	-1.1160918715
H	-2.8595447901	3.5551881322	-1.0655561741
H	-0.7087270698	4.6418534148	-0.4286749352
H	-2.9191239470	-0.8650469683	-1.8606254097
H	-3.2666123334	-3.1713079398	-1.1657086203
H	0.6748840186	-3.3745134992	0.5367390682
H	-1.4668710896	-4.4417273491	0.0083502613
H	2.9127515807	2.2788396673	0.0934101859
H	2.5794119906	-2.6534273339	0.2471302875
H	4.8896033522	0.9409409736	0.5985484373
H	4.7161315014	-1.5492063421	0.7020826902
H	1.2899747415	3.3398626252	-0.0060986915
H	-1.2253899797	0.5263267661	0.5362456639
Cl	-1.7138954052	0.0327120216	2.2105516457

Ground state coordinates: M7

C	-0.6469606618	0.3462821993	-0.9816637580
C	-0.0917610630	-1.0684369021	-1.2100607976
H	0.5029557623	-0.9802365707	-2.1454505358
C	-1.9665125892	0.6952029240	-1.2902319972
C	-2.4284327902	2.0032720331	-1.1101475935
C	-1.5669039696	2.9742491397	-0.5992151653
C	-0.2558245914	2.6333682412	-0.2777716483
C	0.2323750573	1.3292863264	-0.4732087506
C	1.6160601533	0.9556150525	-0.1049935583
C	1.9171385871	-0.4110917944	0.1515203680
C	0.8961680673	-1.4186834811	-0.1124715816
C	-1.1264875042	-2.1356563968	-1.4477700955
C	-1.1415290067	-3.3049773395	-0.7504826265
C	0.8163656565	-2.6282872761	0.5531167382
C	-0.1794874254	-3.5742932351	0.2640552761
C	2.6248506126	1.9151583993	0.0722176498
C	3.1995517107	-0.7496761562	0.6251781737
C	3.8907974086	1.5591996059	0.5276573769
C	4.1750753470	0.2206651965	0.8182738487
H	-2.6449969109	-0.0541293482	-1.6840185257
H	-3.4548815886	2.2545385918	-1.3613157392

H	-1.9183135263	3.9888047454	-0.4373034407
H	-1.8459628028	-1.9712661386	-2.2442903799
H	-1.8998403723	-4.0516814768	-0.9714487090
H	1.5272069074	-2.8396054056	1.3474616902
H	-0.2235561804	-4.5037237148	0.8217615346
H	2.4220933893	2.9556817880	-0.1599507237
H	3.4381908792	-1.7939009996	0.8019173576
H	4.6556523332	2.3204574574	0.6494690708
H	5.1626341937	-0.0653935141	1.1684838199
H	0.3903268233	3.3871578564	0.1595933251
H	-3.0331922687	0.4104192012	0.9646623163
Cl	-3.6979538019	0.2879822534	2.0686128108

Ground state coordinates: M8

C	1.3081948009	-0.5956212141	-0.1830897680
C	1.0417658184	0.8760154225	-0.4994772575
H	0.8131740492	0.8766651541	-1.5945731539
C	2.6145422871	-1.0756824759	-0.1364753943
C	2.8518132559	-2.4202206181	0.1357433056
C	1.7955471170	-3.2896246260	0.3710327451
C	0.4775807340	-2.8245339767	0.3286219460
C	0.1967556831	-1.4547916820	0.0105302208
C	-1.1652168098	-0.9050601878	-0.0680564916
C	-1.3700517791	0.5169059128	0.0470187175
C	-0.2498633154	1.4006278026	0.0484266120
C	2.2002480550	1.8123251845	-0.4518602561
C	2.0652288345	3.0992397123	-0.0473658803
C	-0.3170415762	2.7491413891	0.4521995824
C	0.7983878208	3.5610721623	0.4192438578
C	-2.3147595499	-1.7033052274	-0.2283458684
C	-2.6903128377	1.0423047161	0.0946490575
C	-3.5906171762	-1.1548995748	-0.2120721632
C	-3.7900218263	0.2220865080	-0.0268872698
H	3.4618247535	-0.4184272203	-0.2758573357
H	3.8713112141	-2.7877666248	0.1906393261
H	2.0009077149	-4.3268983708	0.5987119492
H	-0.5712997172	-3.6313066690	0.5980074250
H	3.1528146873	1.4615689947	-0.8299366050
H	2.9105982056	3.7783090997	-0.0629190322
H	-1.2411632504	3.1499530963	0.8492088989
H	0.7109857633	4.5863891169	0.7674357070
H	-2.2063435484	-2.7665415824	-0.3648977382
H	-2.8381987062	2.1131075902	0.1624429836
H	-4.4463338047	-1.8090392747	-0.3479963976
H	-4.7913545781	0.6381113255	-0.0132801999

Ground state coordinates: M9

C	0.6944957728	-1.2680251696	0.0048812888
C	-0.7715919345	-1.2188455999	0.0037188580
C	1.3928559864	-2.4964381540	0.0159560008
C	2.7751267106	-2.5502658095	0.0106515815
C	3.5139416682	-1.3600865930	-0.0076841956
C	2.8540967278	-0.1443083292	-0.0151921072
C	1.4435567730	-0.0601728831	-0.0058563433
C	0.7515878365	1.2333572750	-0.0035848327
C	-0.6687305163	1.2809115920	0.0020350030
C	-1.4429676709	0.0347334101	0.0007923141
C	-1.5528417941	-2.4003986730	-0.0006042008
C	-2.9395062277	-2.3629459087	-0.0053910824
C	-2.8565429219	0.0418398346	-0.0049997376
C	-3.5982221668	-1.1264859728	-0.0057057821
C	1.4654761917	2.4529138729	-0.0037714016
C	-1.3020983325	2.5440201109	0.0078437817
C	0.8210624851	3.6769252992	0.0011244992
C	-0.5791414779	3.7233282778	0.0072969155
H	0.8461966567	-3.4314997481	0.0305966044
H	3.2799880146	-3.5115835756	0.0206959639
H	4.5995282537	-1.3873303621	-0.0141999410

H	-1.0685947838	-3.3693691456	-0.0185219262
H	-3.5056625213	-3.2894508313	-0.0124270369
H	-3.3903536388	0.9839785075	-0.0062067688
H	-4.6828846962	-1.0815043444	-0.0075575852
H	2.5483782620	2.4458981769	-0.0059410984
H	-2.3831256089	2.6080623986	0.0153730022
H	1.4014379967	4.5948119152	0.0022874964
H	-1.0977752945	4.6774062185	0.0130522174
H	3.4495247032	0.7602413134	-0.0262142844

R1 : benzene, R2=R3 : 3-pyridine

Ground state coordinates: M1

C	1.2789869495	1.0405852716	1.0791220992
C	-1.2762722725	1.0403514960	-1.0756807063
H	0.4444171501	0.9163972039	1.7612141543
H	-0.4422919094	0.9152061970	-1.7583702038
N	2.0929341071	2.1674700332	1.1759795361
C	3.1732649255	2.3346635763	0.3069304423
C	3.4349515587	1.3624462102	-0.6587029957
C	2.6226610124	0.2322986149	-0.7523742327
C	1.5303769763	0.0539586699	0.1117588494
C	0.7065453321	-1.1879646405	0.0279160369
C	-0.7098748931	-1.1887018557	-0.0263399515
C	-1.5321453093	0.0536670525	-0.1094350358
N	-2.0866757636	2.1695275853	-1.1740206001
C	-3.1691107127	2.3387380133	-0.3083037355
C	-2.6277960929	0.2333129496	0.7504421945
C	-3.4371155150	1.3656243235	0.6547624054
C	1.3807466704	-2.4206770199	0.0408486438
C	-1.3822322708	-2.4225090150	-0.0397775637
C	0.6970628058	-3.6333444459	0.0161652245
C	-0.6963348741	-3.6341320274	-0.0176585925
H	3.8046893800	3.2151192076	0.3825761993
H	4.2701044962	1.4834100545	-1.3428613114
H	-3.7981319315	3.2208219792	-0.3849002994
H	-2.8335690369	-0.5166195165	1.5089755621
H	-4.2747330332	1.4876040884	1.3357087936
H	2.4649185941	-2.4163559852	0.1030079600
H	-2.4665292012	-2.4198322062	-0.1005454841
H	1.2492553940	-4.5683857711	0.0336000536
H	-1.2474144808	-4.5698227559	-0.0368994688
H	2.8231904325	-0.5164288654	-1.5132570003

Ground state coordinates: M2

C	1.1744935859	-0.6387051008	0.6219383274
C	1.1743558258	0.6388072030	-0.6218667223
H	1.0810636843	0.0510391135	1.4566107928
H	1.0809530396	-0.0510199361	-1.4564718394
N	2.4005502760	-1.3906844534	0.6441434790
C	2.5033855975	-2.6465516403	0.0718681611
C	1.3617657862	-3.2856139501	-0.4269274751
C	0.1167453451	-2.6503908445	-0.3136166954
C	-0.0181053683	-1.3950395144	0.2674292604
C	-1.3156280308	-0.6840356837	0.1970981022
C	-1.3157231658	0.6839418891	-0.1970448272
C	-0.0182795660	1.3950706292	-0.2673996327
N	2.4003884270	1.3908185489	-0.6440826389
C	2.5031371297	2.6467335198	-0.0718959938
C	0.1164775607	2.6504874587	0.3135342105
C	1.3614674702	3.2857762237	0.4268122953
C	-2.5359116210	-1.3257223779	0.4183625387
C	-2.5360727012	1.3254897100	-0.4183383843
C	-3.7505681460	-0.6612777755	0.2157275208
C	-3.7506542071	0.6609056801	-0.2157206162
H	3.4652894179	-3.1516329397	0.0440298527

H	1.4310892611	-4.2702427970	-0.8782030117
H	3.4650134423	3.1518673596	-0.0440495086
H	-0.7706678838	3.1453108033	0.6994943315
H	1.4307385848	4.2704406233	0.8780199914
H	-2.5352502805	-2.3554340059	0.7639026083
H	-2.5355060588	2.3551991060	-0.7638857717
H	-4.6870398741	-1.1824850024	0.3914166314
H	-4.6871911817	1.1819880623	-0.3914281201
H	-0.7703760409	-3.1452216133	-0.6996222533

Ground state coordinates: M3

C	0.7064974144	-1.2734660435	-0.2953942306
C	-0.7065351948	-1.2734469843	0.2953907362
H	0.5865154725	-1.3806833559	-1.4017497219
H	-0.5865549126	-1.3806703289	1.4017459454
N	1.5042677457	-2.4709576215	0.1718082180
C	2.8500591093	-2.4418771612	0.2141724293
C	3.5560379434	-1.2107663757	-0.0535512730
C	2.8796484928	-0.0280397584	-0.1559042494
C	1.4499029384	0.0382089769	-0.0897253620
C	0.7335291740	1.2347049434	-0.0031044731
C	-0.7334934317	1.2347260989	0.0031057495
C	-1.4499026936	0.0382507330	0.0897252493
N	-1.5043399447	-2.4709148436	-0.1718122435
C	-2.8501306134	-2.4417962049	-0.2141715245
C	-2.8796498829	-0.0279575729	0.1559066167
C	-3.5560730934	-1.2106650634	0.0535552313
C	1.3997529550	2.5155601009	0.0457727076
C	-1.3996787584	2.5156014204	-0.0457722489
C	0.7152153057	3.6916375836	0.0330465829
C	-0.7151060835	3.6916586415	-0.0330484154
H	3.4157365574	-3.3271634392	0.4919188249
H	4.6412621359	-1.2174984143	-0.0918738046
H	-3.4158346314	-3.3270660580	-0.4919159149
H	-3.4558886799	0.8853589740	0.2510746957
H	-4.6412974465	-1.2173654942	0.0918801271
H	2.4813604885	2.5442609732	0.0959617375
H	-2.4812853532	2.5443357587	-0.0959608444
H	1.2518994985	4.6351502448	0.0661368692
H	-1.2517617941	4.6351874160	-0.0661403389
H	3.4559125704	0.8852609736	-0.2510705509

Ground state coordinates: M4

C	1.2224914909	-0.6750862928	0.3844134512
C	1.2225004651	0.6750610810	-0.3844457210
H	1.1350144892	-0.4093718195	1.4613294529
H	1.1349928701	0.4093485167	-1.4613586979
N	2.4935938149	-1.4685241276	0.2897587403
C	2.4926162689	-2.8076360693	0.0995477380
C	1.2566668291	-3.5029210881	-0.1027853234
C	0.0459716545	-2.8395966554	-0.1281364148
C	-0.0407668264	-1.4445215813	0.0477094838
C	-1.2731727098	-0.7238551663	-0.0169869432
C	-1.2731553926	0.7238876228	0.0169827760
C	-0.0407309522	1.4445242071	-0.0477037194
N	2.4936239545	1.4684671985	-0.2898100890
C	2.4926844522	2.8075731465	-0.0995558747
C	0.0460468250	2.8395892349	0.1281939903
C	1.2567592403	3.5028834274	0.1028391619
C	-2.5263076744	-1.3972399762	-0.0525248435
C	-2.5262725684	1.3973044138	0.0525132199
C	-3.7158842477	-0.7058270790	-0.0280831106
C	-3.7158667224	0.7059214694	0.0280645143
H	3.4229738599	-3.3657301806	0.0955382152
H	1.2755372210	-4.5764534225	-0.2620798321
H	3.4230561310	3.3656439968	-0.0955568643
H	-0.8461265263	3.4149031525	0.3414369208
H	1.2756629560	4.5764086129	0.2621772112

H	-2.5572727627	-2.4792406521	-0.0608791949
H	-2.5572076468	2.4793061149	0.0608590315
H	-4.6562232598	-1.2466939875	-0.0421008708
H	-4.6561921136	1.2468123518	0.0420732457
H	-0.8462203973	-3.4148983472	-0.3413334848

Ground state coordinates: M5=M6

C	0.9646833808	-0.7803267836	-0.4927554067
C	0.9059368568	0.6584373065	-1.0886961538
H	0.5428215613	0.4837674716	-2.1240161614
N	2.0999009907	-1.6130093336	-0.7907360135
C	2.0398675218	-2.9816806945	-0.6610796815
C	0.8139305555	-3.5834129691	-0.3266475109
C	-0.3399035027	-2.8237995503	-0.1781970736
C	-0.3248739731	-1.4283865043	-0.3366179175
C	-1.5352756831	-0.6106557368	-0.2231735032
C	-1.4391828240	0.8166445910	-0.1809831514
C	-0.1606245684	1.4733859978	-0.3869972551
N	2.2279689879	1.3639879641	-1.2081857754
C	2.3977027601	2.6557954725	-0.8215360755
C	0.0948027210	2.7866550858	-0.0141314188
C	1.3358445373	3.3921125372	-0.2206233714
C	-2.8079191685	-1.2067384876	-0.0929302104
C	-2.6207401689	1.5614281679	0.0336809303
C	-3.9518434651	-0.4500124754	0.1039981303
C	-3.8527587282	0.9465819843	0.1790197001
H	2.9262541604	-3.5894221213	-0.8106907591
H	0.7603329610	-4.6603925949	-0.1959693150
H	3.3616329790	3.1367060974	-0.9635945037
H	-0.6742487188	3.3497274130	0.5046435402
H	1.5034384303	4.4111658892	0.1107748423
H	-2.9084791684	-2.2841312948	-0.1524409530
H	-2.5674255744	2.6441601652	0.0467718274
H	-4.9166505561	-0.9384926012	0.1977772854
H	-4.7430924984	1.5500631947	0.3294402565
H	-1.2643082586	-3.3356074185	0.0591267048
H	1.2391012154	-0.5396895996	0.7341062290
Cl	1.6075091829	-0.0612278037	2.6177966673

Ground state coordinates: M7

C	-0.7069856155	0.5191163911	-0.9604975083
C	-0.3135805006	-0.9338435320	-1.2679630311
H	0.2779673707	-0.8613250063	-2.2069847766
N	-1.9879948305	1.0239218201	-1.2110106967
C	-2.2958994508	2.3654841316	-0.9600038526
C	-1.3171833012	3.2109187188	-0.4390612583
C	-0.0430672288	2.7139014349	-0.1742863992
C	0.2904260435	1.3743470659	-0.4371441839
C	1.6296380127	0.8290086042	-0.1206219884
C	1.7742246093	-0.5724240712	0.0805001048
C	0.6413230837	-1.4454305323	-0.2060917924
N	-1.4599786823	-1.8686512209	-1.5448653087
C	-1.5933133660	-3.0662238355	-0.9109905103
C	0.4364981180	-2.6719428124	0.3994336933
C	-0.6574271713	-3.4897365164	0.0749497388
C	2.7460598143	1.6584993279	0.0667378005
C	3.0169605574	-1.0737045666	0.5137840117
C	3.9705624638	1.1417400179	0.4797536478
C	4.1020655212	-0.2303465290	0.7181047403
H	-3.2959433812	2.7376909044	-1.1619405768
H	-1.5484690985	4.2494649170	-0.2223152124
H	-2.4284972428	-3.7156498385	-1.1601327030
H	1.1277329892	-3.0007922757	1.1708366177
H	-0.7975961697	-4.4364965782	0.5856195175
H	2.6610567089	2.7237385716	-0.1228343514
H	3.1365205164	-2.1442583919	0.6489045279
H	4.8209812363	1.8044769785	0.6097036498
H	5.0558439854	-0.6417868363	1.0354647787

H	0.6946660771	3.3712294291	0.2734958288
H	-2.5829261305	0.5184417863	1.0795478106
Cl	-3.1216077535	0.1960113156	2.2130675088

Ground state coordinates: M8

C	1.4118793992	0.3884206479	-0.1662247149
C	0.2942015539	1.3857006124	-0.4451609155
H	0.1547316840	1.3119402302	-1.5558809760
N	2.7517181946	0.7822630461	-0.1281731620
C	3.7610507992	-0.1487525358	0.1021506644
C	3.4382267382	-1.4944700692	0.2914331462
C	2.1125928337	-1.8970925221	0.2433165753
C	1.0737195065	-0.9745636855	0.0006428744
C	-0.3302873802	-1.4015957208	-0.0539811203
C	-1.3891399426	-0.4349486050	-0.0073891394
C	-1.0730185527	0.9619052823	0.0003021899
N	0.6033126008	2.8373153635	-0.3244535263
C	-0.3443334750	3.7459531256	0.0177736883
C	-2.0070396028	1.9628475116	0.3322534707
C	-1.6551991432	3.2982603960	0.3511684659
C	-0.6867875061	-2.7599078517	-0.1152116048
C	-2.7403103580	-0.8766977689	0.0181708231
C	-2.0145596827	-3.1627149798	-0.0982248650
C	-3.0523214139	-2.2183905384	-0.0244993790
H	4.7937470301	0.1802432231	0.1523982618
H	4.2181375188	-2.2233141159	0.4842840047
H	1.8803612293	-2.9406699561	0.4153894678
H	-0.1121668161	4.8045814381	0.0531764724
H	-3.0078165439	1.6867926412	0.6386252010
H	-2.4016444442	4.0320522506	0.6417037159
H	0.0809920497	-3.5189039019	-0.1921251903
H	-3.5450138663	-0.1518122313	0.0250237505
H	-2.2509071228	-4.2208706768	-0.1501042990
H	-4.0876789267	-2.5408075616	-0.0232245454

Ground state coordinates: M9

C	0.7332237740	-1.2600024454	0.0011547749
C	-0.7335905887	-1.2601127333	0.0010182255
N	1.4726920546	-2.4641974715	0.0029181747
C	2.8555320717	-2.4737899265	0.0017969197
C	3.5558968323	-1.2607958600	-0.0012932486
C	2.8563161567	-0.0677299012	-0.0026159443
C	1.4440090685	-0.0292440749	-0.0010941540
C	0.7108103594	1.2414605031	-0.0010329480
C	-0.7103343772	1.2413493999	0.0005412595
C	-1.4440460460	-0.0289209801	0.0000032518
N	-1.4733132698	-2.4641801012	0.0009266651
C	-2.8562237822	-2.4729073875	-0.0006029045
C	-2.8564542182	-0.0667241119	-0.0019355159
C	-3.5562613974	-1.2596231131	-0.0022795247
C	1.3841358838	2.4837274005	-0.0016528930
C	-1.3832934795	2.4838750348	0.0026773862
C	0.7007843308	3.6861158341	-0.0002298385
C	-0.6998201575	3.6861724713	0.0022808025
H	3.3909078309	-3.4185358759	0.0032354236
H	4.6417649127	-1.2525759205	-0.0025061941
H	-3.3928870400	-3.4169241929	-0.0010262669
H	-3.4220260207	0.8568647242	-0.0036897215
H	-4.6421448020	-1.2509442513	-0.0040319050
H	2.4667789768	2.5114326180	-0.0029514367
H	-2.4659103236	2.5120943387	0.0052144191
H	1.2513009123	4.6221256792	-0.0007457207
H	-1.2498296635	4.6224536895	0.0041057440
H	3.4222871406	0.8555515416	-0.0049321123

R1 : benzene, R2=R3 : 2-thiophene

Ground state coordinates: M1

C	1.2796640953	-1.0564874891	1.2677588150
C	-1.2796640953	1.0564874891	1.2677588150
H	0.4140440763	-1.7036838104	1.3393163673
H	-0.4140440763	1.7036838104	1.3393163673
C	1.4988395270	-0.2328136010	0.1904132827
S	2.9960813655	0.6596137125	0.4128059344
C	3.2902015921	-0.0972184499	1.9441505169
C	2.2962997257	-0.9810793717	2.2632353565
C	0.7066370787	-0.0779671264	-1.0463970721
C	-0.7066370787	0.0779671264	-1.0463970721
C	-1.4988395270	0.2328136010	0.1904132827
S	-2.9960813655	-0.6596137125	0.4128059344
C	-3.2902015921	0.0972184499	1.9441505169
C	-2.2962997257	0.9810793717	2.2632353565
C	1.3771501903	-0.1250354408	-2.2813373188
C	0.6946721315	-0.0557225536	-3.4922303317
C	-0.6946721315	0.0557225536	-3.4922303317
C	-1.3771501903	0.1250354408	-2.2813373188
H	4.1733499746	0.1574739210	2.5132915113
H	2.2889700140	-1.5655847609	3.1761390236
H	-4.1733499746	-0.1574739210	2.5132915113
H	-2.2889700140	1.5655847609	3.1761390236
H	2.4550886420	-0.2533482660	-2.2803399327
H	1.2452229740	-0.1032986993	-4.4268343050
H	-1.2452229740	0.1032986993	-4.4268343050
H	-2.4550886420	0.2533482660	-2.2803399327

Ground state coordinates: M2

C	0.6228427711	-0.5922894176	1.2914971855
C	-0.6228427711	0.5922894176	1.2914971855
H	-0.0054511136	-1.4842762284	1.3324509831
H	0.0054511136	1.4842762284	1.3324509831
C	1.3556324864	-0.3580404785	0.0789039336
S	2.8267843458	0.5266276942	0.4076669322
C	2.6668646491	0.2673429972	2.1251132707
C	1.5220038160	-0.3862030713	2.4379382598
C	0.6842645874	-0.2282674081	-1.2174898799
C	-0.6842645874	0.2282674081	-1.2174898799
C	-1.3556324864	0.3580404785	0.0789039336
S	-2.8267843458	-0.5266276942	0.4076669322
C	-2.6668646491	-0.2673429972	2.1251132707
C	-1.5220038160	0.3862030713	2.4379382598
C	1.3068855935	-0.4766100126	-2.4357163537
C	0.6497386720	-0.2380038474	-3.6569528053
C	-0.6497386720	0.2380038474	-3.6569528053
C	-1.3068855935	0.4766100126	-2.4357163537
H	3.4595628044	0.5798285474	2.7919027159
H	1.2482362740	-0.6536848676	3.4526557160
H	-3.4595628044	-0.5798285474	2.7919027159
H	-1.2482362740	0.6536848676	3.4526557160
H	2.3173465371	-0.8750063751	-2.4361760043
H	1.1682144161	-0.4285106062	-4.5918221064
H	-1.1682144161	0.4285106062	-4.5918221064
H	-2.3173465371	0.8750063751	-2.4361760043

Ground state coordinates: M3

C	0.6564654044	-0.3892379264	1.3692535600
C	-0.6564654044	0.3892379264	1.3692535600
H	0.3952580487	-1.4698337718	1.3705674857
H	-0.3952580487	1.4698337718	1.3705674857
C	1.3999445523	-0.0911539385	0.0731886305
S	3.1504594480	-0.0042163406	0.3418094360
C	2.8979684241	0.0319250766	2.1024503036
C	1.6297460518	-0.1274799321	2.4914702070
C	0.7421696965	0.0388002097	-1.1156735731

C	-0.7421696965	-0.0388002097	-1.1156735731
C	-1.3999445523	0.0911539385	0.0731886305
S	-3.1504594480	0.0042163406	0.3418094360
C	-2.8979684241	-0.0319250766	2.1024503036
C	-1.6297460518	0.1274799321	2.4914702070
C	1.4050954395	0.1905743131	-2.3944297730
C	0.7136515355	0.1152113099	-3.5595170895
C	-0.7136515355	-0.1152113099	-3.5595170895
C	-1.4050954395	-0.1905743131	-2.3944297730
H	3.7657341408	0.1615750888	2.7377321790
H	1.3301451470	-0.1531995629	3.5338963366
H	-3.7657341408	-0.1615750888	2.7377321790
H	-1.3301451470	0.1531995629	3.5338963366
H	2.4813793083	0.3399648722	-2.4030483739
H	1.2320818803	0.2132445014	-4.5085521935
H	-1.2320818803	-0.2132445014	-4.5085521935
H	-2.4813793083	-0.3399648722	-2.4030483739

Ground state coordinates: M4

C	0.6584995341	-0.3998726593	1.3710500067
C	-0.6584995341	0.3998726593	1.3710500067
H	0.3858371092	-1.4732959118	1.3392004199
H	-0.3858371092	1.4732959118	1.3392004199
C	1.4003790163	-0.1002682225	0.0835751994
S	3.0965605661	0.0786329077	0.3474725251
C	2.8904096340	-0.0081676025	2.1137054124
C	1.6268657978	-0.2039318099	2.5023012313
C	0.7299610169	0.0087893976	-1.1416437781
C	-0.7299610169	-0.0087893976	-1.1416437781
C	-1.4003790163	0.1002682225	0.0835751994
S	-3.0965605661	-0.0786329077	0.3474725251
C	-2.8904096340	0.0081676025	2.1137054124
C	-1.6268657978	0.2039318099	2.5023012313
C	1.4083311003	0.0779224162	-2.3934442047
C	0.7090420818	0.0481717578	-3.5758769697
C	-0.7090420818	-0.0481717578	-3.5758769697
C	-1.4083311003	-0.0779224162	-2.3934442047
H	3.7741034597	0.0892922586	2.7315177831
H	1.3344789917	-0.3077925406	3.5409336178
H	-3.7741034597	-0.0892922586	2.7315177831
H	-1.3344789917	0.3077925406	3.5409336178
H	2.4930350703	0.1182547113	-2.4092620024
H	1.2421687565	0.0839548904	-4.5199516028
H	-1.2421687565	-0.0839548904	-4.5199516028
H	-2.4930350703	-0.1182547113	-2.4092620024

Ground state coordinates: M5=M6

C	1.1398750413	0.5564016377	-0.5460735764
C	-0.1192799352	1.2861766524	-1.0177692087
H	1.1811965017	0.8831356686	0.6794463311
H	-0.1725951399	1.1258793305	-2.1172610630
C	1.0135050971	-0.8641328213	-0.4516339877
S	2.5653761114	-1.6337832053	-0.5649063563
C	3.3548330384	-0.1149121703	-0.9519915836
C	2.4929333778	0.9253863087	-0.9566617808
C	-0.2255171406	-1.5319998080	-0.2031802956
C	-1.4231924993	-0.7213330701	-0.1128431876
C	-1.3466060149	0.6493449054	-0.4042766098
S	-2.5939591236	1.8364990337	-0.0859574501
C	-1.4566035935	3.1651071547	-0.4009527705
C	-0.2444944608	2.7712451232	-0.7989163349
C	-0.3153242329	-2.9218112837	0.0215987099
C	-1.5164961828	-3.5175304728	0.3590986697
C	-2.6779413223	-2.7250743521	0.4988680912
C	-2.6332847780	-1.3664781656	0.2765493040
H	4.4234366252	-0.1046222091	-1.1165925164
H	2.7977511539	1.9507397933	-1.1290912171
H	-1.8021755094	4.1789247249	-0.2455135068



H	0.5567807361	3.4617988576	-1.0349458539
H	0.5813603866	-3.5304455387	-0.0564030447
H	-1.5643589430	-4.5876408459	0.5311017333
H	-3.6168612049	-3.1929342617	0.7789847649
H	-3.5369125037	-0.7727971098	0.3760503627
Cl	1.2046866623	1.4740427767	2.1548204218

Ground state coordinates: M7

C	1.0811314267	0.4937773810	-0.9135530833
C	-0.1960038698	1.2682909731	-1.2007727491
H	1.3420362553	0.8793429145	1.4803817295
H	-0.3659137639	1.1746009287	-2.2987691140
C	0.9924204296	-0.8375512664	-0.5400883807
S	2.5868577716	-1.5510908799	-0.4256053208
C	3.3415289249	-0.0616386578	-0.8996126530
C	2.4251448379	0.9282675344	-1.1271522184
C	-0.2525479592	-1.5321625253	-0.2576819868
C	-1.4542241409	-0.7379259218	-0.1900865968
C	-1.3784339376	0.6398697308	-0.4983736592
S	-2.5785982843	1.8499488001	-0.0637796540
C	-1.4186615425	3.1560823483	-0.3877220382
C	-0.2536639639	2.7488636849	-0.9018430821
C	-0.3197999645	-2.9025782992	0.0218417692
C	-1.5194630271	-3.5074460263	0.3882292522
C	-2.6865679168	-2.7337290335	0.4962126981
C	-2.6548898656	-1.3780309731	0.2182724888
H	4.4188827785	-0.0037012826	-0.9676956733
H	2.6984148085	1.9322624238	-1.4309925953
H	-1.7179952775	4.1724996268	-0.1640034291
H	0.5470670589	3.4276620906	-1.1741116399
H	0.5843753786	-3.5027995312	-0.0383043506
H	-1.5473524679	-4.5719154476	0.5984076655
H	-3.6213825680	-3.2005326017	0.7922309915
H	-3.5662369985	-0.7910230750	0.2898148133
Cl	1.5800080243	1.3198437373	2.6763048608

Ground state coordinates: M8

C	0.7944362087	-1.3533556040	0.1392111712
C	-0.6744021293	-1.4020772893	0.4302287437
H	-0.7138251494	-1.3747070379	1.5478466411
C	1.3985404069	-0.1043888548	0.0369290968
S	3.1230195578	-0.2728884538	-0.1795313982
C	3.0001499650	-1.9932261696	-0.1086231795
C	1.7107443547	-2.4313193807	0.0711728370
C	0.6798194769	1.1405913181	0.0734085835
C	-0.7661175887	1.1195158760	0.1034113342
C	-1.4105827534	-0.1340213163	0.1196063643
S	-3.0600403225	-0.4453344169	-0.2207770865
C	-2.8176256130	-2.2040443436	-0.1928389068
C	-1.5594690407	-2.5625974475	0.0893845978
C	1.3213610342	2.3940053458	0.0267741725
C	0.5881922166	3.5681730385	-0.0014708280
C	-0.8251468232	3.5500295546	0.0104306591
C	-1.4884080446	2.3465315678	0.0560890503
H	3.8919732660	-2.5955781580	-0.2199564480
H	1.4442446818	-3.4793103356	0.1344348571
H	-3.6711618000	-2.8384008862	-0.3954097259
H	-1.2287520978	-3.5914051898	0.1669171468
H	2.4054458540	2.4404549115	0.0107610876
H	1.1091122003	4.5200028101	-0.0360107209
H	-1.3797597312	4.4816436575	-0.0095253884
H	-2.5738950089	2.3259683903	0.0835961294

Ground state coordinates: M9

C	0.7203905805	-1.3709539284	0.0103922910
C	-0.7160951612	-1.3717007892	0.0165494034
C	1.3900792664	-0.1430413507	0.0022375811

S	3.1253258776	-0.3825472435	-0.0096710313
C	2.9266781636	-2.1127345636	-0.0016725844
C	1.6187045976	-2.4903143117	0.0087234541
C	0.7164197566	1.1228348799	0.0030471996
C	-0.7167673873	1.1236076829	0.0108602330
C	-1.3900630188	-0.1428479044	0.0152850430
S	-3.1264889070	-0.3843345350	-0.0113410941
C	-2.9254503258	-2.1146838062	-0.0132108866
C	-1.61711613321	-2.4922860929	0.0025731592
C	1.3974371857	2.3629918308	-0.0044850161
C	0.7037725608	3.5568962734	-0.0060571829
C	-0.7056782265	3.5570367392	0.0017506850
C	-1.3989837883	2.3629110203	0.0111491183
H	3.8020796437	-2.7475504915	-0.0052104337
H	1.2981212711	-3.5254395737	0.0141076320
H	-3.8000047300	-2.7506735172	-0.0207203053
H	-1.2973565998	-3.5275733994	0.0037119100
H	2.4837940378	2.3693714550	-0.0081397265
H	1.2453963631	4.4979061275	-0.0119011336
H	-1.2476999574	4.4978149049	0.0022839502
H	-2.4854187846	2.3699588738	0.0192071273

R1: benzene, R2=R3 : 2-pyrrole

Ground state coordinates: M1

C	1.3404771575	1.3375456643	0.9781887196
C	-1.3404597289	1.3375619721	-0.9781853748
H	0.5150466832	1.4091092399	1.6759199965
H	-0.5150290732	1.4091083965	-1.6759171704
C	1.5100701147	0.2602024216	0.1428993602
N	2.9513518126	0.4825870411	-0.8373448558
C	3.2901417206	2.0139292863	-0.0994277773
C	2.3507985416	2.3330238904	0.8422090335
C	0.7100256950	-0.9766069529	0.0356324091
C	-0.7100344642	-0.9765954107	-0.0356319529
C	-1.5100655829	0.2602152148	-0.1428980377
N	-2.9513467168	0.4826105953	0.8373445661
C	-3.2901225768	2.0139583501	0.0994262187
C	-2.3507785887	2.3330437460	-0.8422129053
C	1.3821522817	-2.2115477799	0.0425798777
C	0.6967434818	-3.4224370140	0.0141389495
C	-0.6967787826	-3.4224353497	-0.0141404274
C	-1.3821743472	-2.2115345837	-0.0425803014
H	4.1565115218	2.5830670751	-0.4063976580
H	2.3783855270	3.2459259719	1.4261079722
H	-4.1564907688	2.5831005612	0.4064019721
H	-2.3783630931	3.2459416645	-1.4261084634
H	2.4658205261	-2.2105589229	0.1062926240
H	1.2491513700	-4.3570476614	0.0287556201
H	-1.2491892069	-4.3570347023	-0.0287603213
H	-2.4658425891	-2.2105334407	-0.1062930550
H	-3.3940189117	-0.0536863174	1.5342480730
H	3.3940128151	-0.0537160462	-1.5342343101

Ground state coordinates: M3

C	-0.3860297166	-0.6531401640	1.4990821555
C	0.3860297166	0.6531401640	1.4990821555
H	-1.4685697690	-0.3976154686	1.5323499571
H	1.4685697690	0.3976154686	1.5323499571
C	-0.1155308041	-1.3875640322	0.1882556569
N	-0.0596850059	-2.7486924202	0.4877280267
C	0.0568752064	-2.8984876636	1.8804800368
C	-0.0827985130	-1.7280011648	2.5245688227
C	0.0176460918	-0.7436452246	-1.0099724362

C	-0.0176460918	0.7436452246	-1.0099724362
C	0.1155308041	1.3875640322	0.1882556569
N	0.0596850059	2.7486924202	0.4877280267
C	-0.0568752064	2.8984876636	1.8804800368
C	0.0827985130	1.7280011648	2.5245688227
C	0.1298836179	-1.4103697022	-2.2882426633
C	0.0795378102	-0.7186118916	-3.4567595917
C	-0.0795378102	0.7186118916	-3.4567595917
C	-0.1298836179	1.4103697022	-2.2882426633
H	0.1993792098	-3.8900640011	2.2916153057
H	-0.1213007507	-1.5973043894	3.5971384094
H	-0.1993792098	3.8900640011	2.2916153057
H	0.1213007507	1.5973043894	3.5971384094
H	0.2155227438	-2.4946666983	-2.3104410968
H	0.1446777578	-1.2433746943	-4.4053739039
H	-0.1446777578	1.2433746943	-4.4053739039
H	-0.2155227438	2.4946666983	-2.3104410968
H	-0.3684679113	3.4090291082	-0.1438567446
H	0.3684679113	-3.4090291082	-0.1438567446

Ground state coordinates: M4

C	-0.3940180750	-0.6569391385	1.4984487365
C	0.3940180750	0.6569391385	1.4984487365
H	-1.4712711769	-0.4001747881	1.4952719216
H	1.4712711769	0.4001747881	1.4952719216
C	-0.0960627631	-1.3815365924	0.1980202910
N	0.0654793006	-2.6875151710	0.5024106562
C	0.0520494314	-2.8881375471	1.9003293174
C	-0.1536107834	-1.7246002171	2.5369104023
C	0.0065455044	-0.7281457654	-1.0402574745
C	-0.0065455044	0.7281457654	-1.0402574745
C	0.0960627631	1.3815365924	0.1980202910
N	-0.0654793006	2.6875151710	0.5024106562
C	-0.0520494314	2.8881375471	1.9003293174
C	0.1536107834	1.7246002171	2.5369104023
C	0.0628790581	-1.4083063917	-2.2900206339
C	0.0388740483	-0.7098537884	-3.4730412773
C	-0.0388740483	0.7098537884	-3.4730412773
C	-0.0628790581	1.4083063917	-2.2900206339
H	0.1887887042	-3.8858510850	2.2929625937
H	-0.2493166437	-1.5912841111	3.6046932107
H	-0.1887887042	3.8858510850	2.2929625937
H	0.2493166437	1.5912841111	3.6046932107
H	0.0852141309	-2.4938733238	-2.3137461786
H	0.0661033034	-1.2434042387	-4.4170539691
H	-0.0661033034	1.2434042387	-4.4170539691
H	-0.0852141309	2.4938733238	-2.3137461786
H	-0.3039415453	3.4111046504	-0.1613383407
H	0.3039415453	-3.4111046504	-0.1613383407

Ground state coordinates: M5=M6

C	-1.0535592427	0.3322808012	-0.9356018178
C	-0.6475624332	-1.0997195824	-1.2541146344
H	-0.3031063035	-1.1130311642	-2.3103160919
C	0.0280588342	1.2286934673	-0.6640157603
N	-0.4216580299	2.4856650122	-0.9133385947
C	-1.7139240423	2.4466257552	-1.4349202165
C	-2.1028259363	1.1453772342	-1.5357405169
C	1.3110356652	0.8313487474	-0.1550797370
C	1.5104062316	-0.5860429726	0.0659232025
C	0.5116047936	-1.4781298057	-0.3536754035
N	0.3396498342	-2.7963773363	0.0209797170
C	-0.9550376743	-3.2120059964	-0.3496562976
C	-1.5895765447	-2.2683070894	-1.0622654590
C	2.3212209385	1.7371365235	0.2069125522
C	3.4963327664	1.3038950142	0.8053630957
C	3.6776172612	-0.0708741274	1.0687893946
C	2.7123921735	-0.9920520902	0.7155753434

H	-2.2382535078	3.3628425909	-1.6623310760
H	-3.0648100879	0.7938908654	-1.8796292637
H	-1.2909968102	-4.2007112641	-0.0669860013
H	-2.5639409918	-2.3631566804	-1.5196368468
H	2.1807273859	2.8009474825	0.0288326495
H	4.2660000805	2.0185914512	1.0774329088
H	4.5938450001	-0.4099049628	1.5436078303
H	2.8897191057	-2.0491402545	0.8934142921
H	0.7774161150	-3.1586882398	0.8571207941
H	0.0659066784	3.3337307653	-0.6671648470
H	-1.5363735083	0.2259417149	0.3206157688
Cl	-2.1288502061	0.0104369197	1.7575284438

Ground state coordinates: M7

C	-0.8872472880	-0.0273870849	-1.0612063411
C	-0.2896386566	-1.4057156688	-1.1205994445
H	0.0020771216	-1.5931309758	-2.1795574943
C	-0.0851305012	1.0508389236	-0.7081846436
N	-0.8568711284	2.1911126033	-0.8246478070
C	-2.1240572023	1.8576465452	-1.2305274847
C	-2.1755035516	0.4808851061	-1.3943012839
C	1.2877075815	0.9656411418	-0.2482337091
C	1.7873509985	-0.3606829885	0.0317995704
C	0.9546698012	-1.4609486623	-0.2591800762
N	1.0256761987	-2.7342687394	0.2936606027
C	-0.2212546906	-3.3665038001	0.1225294984
C	-1.0427912985	-2.6394852224	-0.6532496379
C	2.0981372690	2.0722574282	0.0171884166
C	3.3685629542	1.9245737465	0.5778746612
C	3.8445349723	0.6417949809	0.8919135808
C	3.0718440892	-0.4785324846	0.6277441357
H	-2.8824923501	2.6123837366	-1.3766443876
H	-3.0243506043	-0.0779990946	-1.7653706018
H	-0.3853081629	-4.3381145324	0.5706197773
H	-2.0180525787	-2.9436387159	-1.0068847731
H	1.7346573643	3.0725632870	-0.2091857598
H	3.9811517943	2.7994266262	0.7718150590
H	4.8313551932	0.5227172614	1.3302874106
H	3.4710406621	-1.4675001010	0.8386403117
H	1.5661727151	-2.8927984619	1.1335996128
H	-0.5707267991	3.1140514700	-0.5396740897
H	-3.1045116920	0.5035116214	0.6984204257
Cl	-3.6650444128	0.5273134746	1.8758494993

Ground state coordinates: M8

C	1.4995246369	-0.7147349835	-0.1931344476
C	1.5259719804	0.7390512032	-0.5755788498
H	1.6476151813	0.7865877994	-1.6821728629
C	0.2782283534	-1.3608087811	-0.0461513728
N	0.5470117781	-2.6915320061	0.2113375493
C	1.9030263338	-2.8966244642	0.2407501944
C	2.5275789612	-1.6843854866	-0.0148494764
C	-1.0240317123	-0.7244846276	-0.0981525157
C	-1.0295482700	0.7199655299	-0.1250615010
C	0.2092001851	1.3890479878	-0.2054408022
N	0.4802242715	2.6981060461	0.1752547265
C	1.8664529299	2.8234514974	0.3908960040
C	2.5284054483	1.7168115090	0.0134395998
C	-2.2383747838	-1.4122410118	-0.0334074791
C	-3.4557333176	-0.7317958056	0.0386381901
C	-3.4671387615	0.6718649251	0.0554727926
C	-2.2809174746	1.3851673215	-0.0223337789
H	2.3177567117	-3.8751627016	0.4322343154
H	3.5942043553	-1.5345944107	-0.1171393661
H	2.2569190688	3.7544901733	0.7813103586
H	3.6022811088	1.5939095461	-0.0066305128
H	-2.2415446635	-2.5003457658	-0.0318941969
H	-4.3865622347	-1.2883055615	0.0846791446

H	-4.4118732412	1.2050140092	0.1137209820
H	-2.3089676512	2.4716069684	-0.0496510995
H	-0.1737697601	3.2018518862	0.7594535338
H	-0.1425782776	-3.3827791044	0.4594244304

Ground state coordinates: M9

C	1.5139682108	-0.7140051443	0.0023389617
C	1.5068417062	0.7158718340	0.0005829068
C	0.2738616108	-1.3779203544	0.0012355502
N	0.5404538693	-2.7322054873	0.0007425291
C	1.9027921170	-2.9333681525	-0.0021473145
C	2.5354039049	-1.7116801849	0.0008714978
C	-0.9988963074	-0.7203092386	0.0007211807
C	-1.0041512910	0.7152790429	0.0004159618
C	0.2671670216	1.3767317506	0.0020113819
N	0.5285639094	2.7355322033	0.0056938709
C	1.8840226922	2.9472493774	-0.0015744011
C	2.5264879391	1.7226452648	-0.0090345738
C	-2.2368890867	-1.4012328312	0.0003123823
C	-3.4358690029	-0.7112883131	-0.0000601652
C	-3.4401787043	0.6962019095	0.0002156726
C	-2.2441855862	1.3915042958	0.0005262484
H	2.3129852314	-3.9326703942	-0.0065653339
H	3.6041410936	-1.5527566182	-0.0000394972
H	2.2902663622	3.9481147939	0.0020588256
H	3.5959236078	1.5712747276	0.0373913352
H	-2.2520006345	-2.4885085347	-0.0007157325
H	-4.3748163741	-1.2568800475	-0.0003056215
H	-4.3819645222	1.2366901249	-0.0001501772
H	-2.2645985552	2.4788457123	0.0022379485
H	-0.1656796448	3.4629774616	-0.0436348420
H	-0.1496323601	-3.4644497742	-0.0138234426

R1 : benzene, R2=R3 : 3-pyridine

Ground state coordinates: M1

C	1.2789869495	1.0405852716	1.0791220992
C	-1.2762722725	1.0403514960	-1.0756807063
H	0.4444171501	0.9163972039	1.7612141543
H	-0.4422919094	0.9152061970	-1.7583702038
N	2.0929341071	2.1674700332	1.1759795361
C	3.1732649255	2.3346635763	0.3069304423
C	3.4349515587	1.3624462102	-0.6587029957
C	2.6226610124	0.2322986149	-0.7523742327
C	1.5303769763	0.0539586699	0.1117588494
C	0.7065453321	-1.1879646405	0.0279160369
C	-0.7098748931	-1.1887018557	-0.0263399515
C	-1.5321453093	0.0536670525	-0.1094350358
N	-2.0866757636	2.1695275853	-1.1740206001
C	-3.1691107127	2.3387380133	-0.3083037355
C	-2.6277960929	0.2333129496	0.7504421945
C	-3.4371155150	1.3656243235	0.6547624054
C	1.3807466704	-2.4206770199	0.0408486438
C	-1.3822322708	-2.4225090150	-0.0397775637
C	0.6970628058	-3.6333444459	0.0161652245
C	-0.6963348741	-3.6341320274	-0.0176585925
H	3.8046893800	3.2151192076	0.3825761993
H	4.2701044962	1.4834100545	-1.3428613114
H	-3.7981319315	3.2208219792	-0.3849002994
H	-2.8335690369	-0.5166195165	1.5089755621
H	-4.2747330332	1.4876040884	1.3357087936
H	2.4649185941	-2.4163559852	0.1030079600
H	-2.4665292012	-2.4198322062	-0.1005454841
H	1.2492553940	-4.5683857711	0.0336000536
H	-1.2474144808	-4.5698227559	-0.0368994688
H	2.8231904325	-0.5164288654	-1.5132570003

## Ground state coordinates: M2

C	1.1744935859	-0.6387051008	0.6219383274
C	1.1743558258	0.6388072030	-0.6218667223
H	1.0810636843	0.0510391135	1.4566107928
H	1.0809530396	-0.0510199361	-1.4564718394
N	2.4005502760	-1.3906844534	0.6441434790
C	2.5033855975	-2.6465516403	0.0718681611
C	1.3617657862	-3.2856139501	-0.4269274751
C	0.1167453451	-2.6503908445	-0.3136166954
C	-0.0181053683	-1.3950395144	0.2674292604
C	-1.3156280308	-0.6840356837	0.1970981022
C	-1.3157231658	0.6839418891	-0.1970448272
C	-0.0182795660	1.3950706292	-0.2673996327
N	2.4003884270	1.3908185489	-0.6440826389
C	2.5031371297	2.6467335198	-0.0718959938
C	0.1164775607	2.6504874587	0.3135342105
C	1.3614674702	3.2857762237	0.4268122953
C	-2.5359116210	-1.3257223779	0.4183625387
C	-2.5360727012	1.3254897100	-0.4183383843
C	-3.7505681460	-0.6612777755	0.2157275208
C	-3.7506542071	0.6609056801	-0.2157206162
H	3.4652894179	-3.1516329397	0.0440298527
H	1.4310892611	-4.2702427970	-0.8782030117
H	3.4650134423	3.1518673596	-0.0440495086
H	-0.7706678838	3.1453108033	0.6994943315
H	1.4307385848	4.2704406233	0.8780199914
H	-2.5352502805	-2.3554340059	0.7639026083
H	-2.5355060588	2.3551991060	-0.7638857717
H	-4.6870398741	-1.1824850024	0.3914166314
H	-4.6871911817	1.1819880623	-0.3914281201
H	-0.7703760409	-3.1452216133	-0.6996222533

## Ground state coordinates: M3

C	0.7064974144	-1.2734660435	-0.2953942306
C	-0.7065351948	-1.2734469843	0.2953907362
H	0.5865154725	-1.3806833559	-1.4017497219
H	-0.5865549126	-1.3806703289	1.4017459454
N	1.5042677457	-2.4709576215	0.1718082180
C	2.8500591093	-2.4418771612	0.2141724293
C	3.5560379434	-1.2107663757	-0.0535512730
C	2.8796484928	-0.0280397584	-0.1559042494
C	1.4499029384	0.0382089769	-0.0897253620
C	0.7335291740	1.2347049434	-0.0031044731
C	-0.7334934317	1.2347260989	0.0031057495
C	-1.4499026936	0.0382507330	0.0897252493
N	-1.5043399447	-2.4709148436	-0.1718122435
C	-2.8501306134	-2.4417962049	-0.2141715245
C	-2.8796498829	-0.0279575729	0.1559066167
C	-3.5560730934	-1.2106650634	0.0535552313
C	1.3997529550	2.5155601009	0.0457727076
C	-1.3996787584	2.5156014204	-0.0457722489
C	0.7152153057	3.6916375836	0.0330465829
C	-0.7151060835	3.6916586415	-0.0330484154
H	3.4157365574	-3.3271634392	0.4919188249
H	4.6412621359	-1.2174984143	-0.0918738046
H	-3.4158346314	-3.3270660580	-0.4919159149
H	-3.4558886799	0.8853589740	0.2510746957
H	-4.6412974465	-1.2173654942	0.0918801271
H	2.4813604885	2.5442609732	0.0959617375
H	-2.4812853532	2.5443357587	-0.0959608444
H	1.2518994985	4.6351502448	0.0661368692
H	-1.2517617941	4.6351874160	-0.0661403389
H	3.4559125704	0.8852609736	-0.2510705509

## Ground state coordinates: M4

C	1.2224914909	-0.6750862928	0.3844134512
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C	1.2225004651	0.6750610810	-0.3844457210
H	1.1350144892	-0.4093718195	1.4613294529
H	1.1349928701	0.4093485167	-1.4613586979
N	2.4935938149	-1.4685241276	0.2897587403
C	2.4926162689	-2.8076360693	0.0995477380
C	1.2566668291	-3.5029210881	-0.1027853234
C	0.0459716545	-2.8395966554	-0.1281364148
C	-0.0407668264	-1.4445215813	0.0477094838
C	-1.2731727098	-0.7238551663	-0.0169869432
C	-1.2731553926	0.7238876228	0.0169827760
C	-0.0407309522	1.4445242071	-0.0477037194
N	2.4936239545	1.4684671985	-0.2898100890
C	2.4926844522	2.8075731465	-0.0995558747
C	0.0460468250	2.8395892349	0.1281939903
C	1.2567592403	3.5028834274	0.1028391619
C	-2.5263076744	-1.3972399762	-0.0525248435
C	-2.5262725684	1.3973044138	0.0525132199
C	-3.7158842477	-0.7058270790	-0.0280831106
C	-3.7158667224	0.7059214694	0.0280645143
H	3.4229738599	-3.3657301806	0.0955382152
H	1.2755372210	-4.5764534225	-0.2620798321
H	3.4230561310	3.3656439968	-0.0955568643
H	-0.8461265263	3.4149031525	0.3414369208
H	1.2756629560	4.5764086129	0.2621772112
H	-2.5572727627	-2.4792406521	-0.0608791949
H	-2.5572076468	2.4793061149	0.0608590315
H	-4.6562232598	-1.2466939875	-0.0421008708
H	-4.6561921136	1.2468123518	0.0420732457
H	-0.8462203973	-3.4148983472	-0.3413334848

Ground state coordinates: M5=M6

C	0.9646833808	-0.7803267836	-0.4927554067
C	0.9059368568	0.6584373065	-1.0886961538
H	0.5428215613	0.4837674716	-2.1240161614
N	2.0999009907	-1.6130093336	-0.7907360135
C	2.0398675218	-2.9816806945	-0.6610796815
C	0.8139305555	-3.5834129691	-0.3266475109
C	-0.3399035027	-2.8237995503	-0.1781970736
C	-0.3248739731	-1.4283865043	-0.3366179175
C	-1.5352756831	-0.6106557368	-0.2231735032
C	-1.4391828240	0.8166445910	-0.1809831514
C	-0.1606245684	1.4733859978	-0.3869972551
N	2.2279689879	1.3639879641	-1.2081857754
C	2.3977027601	2.6557954725	-0.8215360755
C	0.0948027210	2.7866550858	-0.0141314188
C	1.3358445373	3.3921125372	-0.2206233714
C	-2.8079191685	-1.2067384876	-0.0929302104
C	-2.6207401689	1.5614281679	0.0336809303
C	-3.9518434651	-0.4500124754	0.1039981303
C	-3.8527587282	0.9465819843	0.1790197001
H	2.9262541604	-3.5894221213	-0.8106907591
H	0.7603329610	-4.6603925949	-0.1959693150
H	3.3616329790	3.1367060974	-0.9635945037
H	-0.6742487188	3.3497274130	0.5046435402
H	1.5034384303	4.4111658892	0.1107748423
H	-2.9084791684	-2.2841312948	-0.1524409530
H	-2.5674255744	2.6441601652	0.0467718274
H	-4.9166505561	-0.9384926012	0.1977772854
H	-4.7430924984	1.5500631947	0.3294402565
H	-1.2643082586	-3.3356074185	0.0591267048
H	1.2391012154	-0.5396895996	0.7341062290
Cl	1.6075091829	-0.0612278037	2.6177966673

Ground state coordinates: M7

C	-0.7069856155	0.5191163911	-0.9604975083
C	-0.3135805006	-0.9338435320	-1.2679630311
H	0.2779673707	-0.8613250063	-2.2069847766
N	-1.9879948305	1.0239218201	-1.2110106967

C	-2.2958994508	2.3654841316	-0.9600038526
C	-1.3171833012	3.2109187188	-0.4390612583
C	-0.0430672288	2.7139014349	-0.1742863992
C	0.2904260435	1.3743470659	-0.4371441839
C	1.6296380127	0.8290086042	-0.1206219884
C	1.7742246093	-0.5724240712	0.0805001048
C	0.6413230837	-1.4454305323	-0.2060917924
N	-1.4599786823	-1.8686512209	-1.5448653087
C	-1.5933133660	-3.0662238355	-0.9109905103
C	0.4364981180	-2.6719428124	0.3994336933
C	-0.6574271713	-3.4897365164	0.0749497388
C	2.7460598143	1.6584993279	0.0667378005
C	3.0169605574	-1.0737045666	0.5137840117
C	3.9705624638	1.1417400179	0.4797536478
C	4.1020655212	-0.2303465290	0.7181047403
H	-3.2959433812	2.7376909044	-1.1619405768
H	-1.5484690985	4.2494649170	-0.2223152124
H	-2.4284972428	-3.7156498385	-1.1601327030
H	1.1277329892	-3.0007922757	1.1708366177
H	-0.7975961697	-4.4364965782	0.5856195175
H	2.6610567089	2.7237385716	-0.1228343514
H	3.1365205164	-2.1442583919	0.6489045279
H	4.8209812363	1.8044769785	0.6097036498
H	5.0558439854	-0.6417868363	1.0354647787
H	0.6946660771	3.3712294291	0.2734958288
H	-2.5829261305	0.5184417863	1.0795478106
Cl	-3.1216077535	0.1960113156	2.2130675088

Ground state coordinates: M8

C	1.4118793992	0.3884206479	-0.1662247149
C	0.2942015539	1.3857006124	-0.4451609155
H	0.1547316840	1.3119402302	-1.5558809760
N	2.7517181946	0.7822630461	-0.1281731620
C	3.7610507992	-0.1487525358	0.1021506644
C	3.4382267382	-1.4944700692	0.2914331462
C	2.1125928337	-1.8970925221	0.2433165753
C	1.0737195065	-0.9745636855	0.0006428744
C	-0.3302873802	-1.4015957208	-0.0539811203
C	-1.3891399426	-0.4349486050	-0.0073891394
C	-1.0730185527	0.9619052823	0.0003021899
N	0.6033126008	2.8373153635	-0.3244535263
C	-0.3443334750	3.7459531256	0.0177736883
C	-2.0070396028	1.9628475116	0.3322534707
C	-1.6551991432	3.2982603960	0.3511684659
C	-0.6867875061	-2.7599078517	-0.1152116048
C	-2.7403103580	-0.8766977689	0.0181708231
C	-2.0145596827	-3.1627149798	-0.0982248650
C	-3.0523214139	-2.2183905384	-0.0244993790
H	4.7937470301	0.1802432231	0.1523982618
H	4.2181375188	-2.2233141159	0.4842840047
H	1.8803612293	-2.9406699561	0.4153894678
H	-0.1121668161	4.8045814381	0.0531764724
H	-3.0078165439	1.6867926412	0.6386252010
H	-2.4016444442	4.0320522506	0.6417037159
H	0.0809920497	-3.5189039019	-0.1921251903
H	-3.5450138663	-0.1518122313	0.0250237505
H	-2.2509071228	-4.2208706768	-0.1501042990
H	-4.0876789267	-2.5408075616	-0.0232245454

Ground state coordinates: M9

C	0.7332237740	-1.2600024454	0.0011547749
C	-0.7335905887	-1.2601127333	0.0010182255
N	1.4726920546	-2.4641974715	0.0029181747
C	2.8555320717	-2.4737899265	0.0017969197
C	3.5558968323	-1.2607958600	-0.0012932486
C	2.8563161567	-0.0677299012	-0.0026159443
C	1.4440090685	-0.0292440749	-0.0010941540
C	0.7108103594	1.2414605031	-0.0010329480



C	-0.7103343772	1.2413493999	0.0005412595
C	-1.4440460460	-0.0289209801	0.0000032518
N	-1.4733132698	-2.4641801012	0.0009266651
C	-2.8562237822	-2.4729073875	-0.0006029045
C	-2.8564542182	-0.0667241119	-0.0019355159
C	-3.5562613974	-1.2596231131	-0.0022795247
C	1.3841358838	2.4837274005	-0.0016528930
C	-1.3832934795	2.4838750348	0.0026773862
C	0.7007843308	3.6861158341	-0.0002298385
C	-0.6998201575	3.6861724713	0.0022808025
H	3.3909078309	-3.4185358759	0.0032354236
H	4.6417649127	-1.2525759205	-0.0025061941
H	-3.3928870400	-3.4169241929	-0.0010262669
H	-3.4220260207	0.8568647242	-0.0036897215
H	-4.6421448020	-1.2509442513	-0.0040319050
H	2.4667789768	2.5114326180	-0.0029514367
H	-2.4659103236	2.5120943387	0.0052144191
H	1.2513009123	4.6221256792	-0.0007457207
H	-1.2498296635	4.6224536895	0.0041057440
H	3.4222871406	0.8555515416	-0.0049321123

R1: benzene R2=R3 : 3-thiophene

Ground state coordinates: M1

C	1.3828514938	0.9019605344	-0.9809488365
C	-1.3828514938	-0.9019605344	-0.9809488365
H	0.6349755234	1.6745551268	-1.0842100853
H	-0.6349755234	-1.6745551268	-1.0842100853
C	1.5359009278	0.0127345428	0.0550723966
C	2.6546140237	-0.8637931309	-0.1682057109
C	3.3030690408	-0.6280885518	-1.3463306650
S	2.5709463940	0.6802634429	-2.2193242075
C	0.7086327234	-0.0167119097	1.2893732695
C	-0.7086327234	0.0167119097	1.2893732695
C	-1.5359009278	-0.0127345428	0.0550723966
C	-2.6546140237	0.8637931309	-0.1682057109
C	-3.3030690408	0.6280885518	-1.3463306650
S	-2.5709463940	-0.6802634429	-2.2193242075
C	1.3811332557	-0.0501024765	2.5226811387
C	0.6963223360	-0.0295320799	3.7346745613
C	-0.6963223360	0.0295320799	3.7346745613
C	-1.3811332557	0.0501024765	2.5226811387
H	4.1571884458	-1.1471504155	-1.7576940606
H	-4.1571884458	1.1471504155	-1.7576940606
H	2.4671243503	-0.0616568626	2.5209692510
H	1.2482479924	-0.0490588671	4.6697452651
H	-1.2482479924	0.0490588671	4.6697452651
H	-2.4671243503	0.0616568626	2.5209692510
H	2.9398991207	-1.6494479116	0.5224829798
H	-2.9398991207	1.6494479116	0.5224829798

Ground state coordinates: M2

C	-0.5626925218	-0.7036888839	1.0550459839
C	0.5626925218	0.7036888839	1.0550459839
H	-1.5052225304	-0.1679383472	1.1302219128
H	1.5052225304	0.1679383472	1.1302219128
C	-0.1817192664	-1.4030607941	-0.1478448732
C	0.5096962134	-2.6028954265	0.1190851633
C	0.5465566883	-2.9554425592	1.4503841572
S	-0.3326456756	-1.8259584539	2.4356468589
C	-0.1452782339	-0.6999322715	-1.4454653163
C	0.1452782339	0.6999322715	-1.4454653163
C	0.1817192664	1.4030607941	-0.1478448732
C	-0.5096962134	2.6028954265	0.1190851633
C	-0.5465566883	2.9554425592	1.4503841572
S	0.3326456756	1.8259584539	2.4356468589

C	-0.3158679837	-1.3545810074	-2.6613424792
C	-0.1606129693	-0.6738486349	-3.8816250729
C	0.1606129693	0.6738486349	-3.8816250729
C	0.3158679837	1.3545810074	-2.6613424792
H	1.0710678266	-3.7855113321	1.9020925357
H	-1.0710678266	3.7855113321	1.9020925357
H	-0.5849615581	-2.4068901937	-2.6619562818
H	-0.2905205605	-1.2103573676	-4.8167926479
H	0.2905205605	1.2103573676	-4.8167926479
H	0.5849615581	2.4068901937	-2.6619562818
H	1.0183355196	-3.1709045849	-0.6526356484
H	-1.0183355196	3.1709045849	-0.6526356484

Ground state coordinates: M3

C	-0.3791703824	-0.6504009993	1.0666982515
C	0.3791703824	0.6504009993	1.0666982515
H	-1.4618786533	-0.4364982718	1.1112056669
H	1.4618786533	0.4364982718	1.1112056669
C	-0.0754759734	-1.4237885383	-0.2111658094
C	-0.0052801074	-2.8327234499	0.0413492642
C	0.0226267350	-3.1667220057	1.3564791854
S	-0.0067028532	-1.8058776367	2.4712668892
C	0.0236127239	-0.7356172361	-1.4095845233
C	-0.0236127239	0.7356172361	-1.4095845233
C	0.0754759734	1.4237885383	-0.2111658094
C	0.0052801074	2.8327234499	0.0413492642
C	-0.0226267350	3.1667220057	1.3564791854
S	0.0067028532	1.8058776367	2.4712668892
C	0.1224143364	-1.4055019704	-2.6835903512
C	0.0731607884	-0.7151132315	-3.8552650230
C	-0.0731607884	0.7151132315	-3.8552650230
C	-0.1224143364	1.4055019704	-2.6835903512
H	0.0714842765	-4.1699395601	1.7611191561
H	-0.0714842765	4.1699395601	1.7611191561
H	0.2119857768	-2.4869484362	-2.6982824150
H	0.1323234845	-1.2435344356	-4.8020921350
H	-0.1323234845	1.2435344356	-4.8020921350
H	-0.2119857768	2.4869484362	-2.6982824150
H	0.0490942401	-3.5803095120	-0.7417464665
H	-0.0490942401	3.5803095120	-0.7417464665

Ground state coordinates: M4

C	-0.3913157366	-0.6504321398	1.0603556708
C	0.3913157366	0.6504321398	1.0603556708
H	-1.4704638004	-0.4283511608	1.0772902911
H	1.4704638004	0.4283511608	1.0772902911
C	-0.0766325422	-1.4236920658	-0.2061042107
C	0.0887461901	-2.7979150459	0.0448773107
C	0.0951125847	-3.1219388623	1.3838997372
S	-0.0956863772	-1.7993916686	2.4783648677
C	-0.0005323122	-0.7253760854	-1.4380594410
C	0.0005323122	0.7253760854	-1.4380594410
C	0.0766325422	1.4236920658	-0.2061042107
C	-0.0887461901	2.7979150459	0.0448773107
C	-0.0951125847	3.1219388623	1.3838997372
S	0.0956863772	1.7993916686	2.4783648677
C	0.0330669414	-1.4056536471	-2.6854255727
C	0.0209523572	-0.7076389192	-3.8726774586
C	-0.0209523572	0.7076389192	-3.8726774586
C	-0.0330669414	1.4056536471	-2.6854255727
H	0.2211598153	-4.1198086234	1.7883082299
H	-0.2211598153	4.1198086234	1.7883082299
H	0.0354188290	-2.4896644295	-2.7036528710
H	0.0332737987	-1.2446059708	-4.8152426684
H	-0.0332737987	1.2446059708	-4.8152426684
H	-0.0354188290	2.4896644295	-2.7036528710
H	0.2506709813	-3.5455513913	-0.7217370800
H	-0.2506709813	3.5455513913	-0.7217370800

## Ground state coordinates: M5=M6

C	0.9474270616	-0.5734615284	-0.2681218691
C	0.8540173357	0.8462434811	-0.7843185882
H	1.0521834599	-0.4532747159	1.0079573232
H	0.8239153962	0.8287310525	-1.8858845694
C	-0.2555243710	-1.3516883814	-0.4005173759
C	0.0210763247	-2.7371423067	-0.5362023151
C	1.3584645056	-3.0046724587	-0.6824350028
S	2.3565836944	-1.6022552327	-0.6756183024
C	-1.5459797506	-0.7143593568	-0.2985733224
C	-1.6083098275	0.7181452916	-0.1731657705
C	-0.4118255181	1.4925513983	-0.2550158174
C	-0.2045289858	2.8288364345	0.1316121744
C	1.1087559909	3.2322152113	0.1189718492
S	2.2483443581	2.0051336495	-0.3734892176
C	-2.7411798815	-1.4624145769	-0.2599330938
C	-3.9675852900	-0.8475489503	-0.0810514973
C	-4.0295752144	0.5506159500	0.0765476699
C	-2.8787679642	1.3131459534	0.0352289516
H	1.8133895826	-3.9847079390	-0.7525404555
H	1.4816329061	4.2016141541	0.4230290068
H	-2.6976467389	-2.5420280423	-0.3578823765
H	-4.8755969577	-1.4409046318	-0.0518639095
H	-4.9902398219	1.0349198628	0.2240177683
H	-2.9484235034	2.3907497405	0.1386201571
H	-0.7279863524	-3.5185797984	-0.5202913380
H	-0.9944760599	3.4811508862	0.4857473195
Cl	1.1891896878	-0.2122324171	2.5873309249

## Ground state coordinates: M7

C	0.8916627631	-0.5392730647	-0.7620659276
C	0.7911109537	0.9264155296	-1.0463996925
H	0.9778154990	-0.6034262198	1.7221073334
H	0.7100111694	1.0717619012	-2.1376269506
C	-0.2344325276	-1.3064219345	-0.5116092722
C	0.0837977357	-2.7068608784	-0.4344898324
C	1.4040577151	-2.9671308876	-0.6532365363
S	2.3152884747	-1.5197784124	-0.9591276366
C	-1.5560424394	-0.6843255263	-0.3661077762
C	-1.6350413433	0.7410566951	-0.2683604624
C	-0.4271329587	1.5208602895	-0.3666971936
C	-0.1779529393	2.8001366547	0.1532909094
C	1.1418626710	3.1958784096	0.1223301556
S	2.2364859264	2.0077365339	-0.5601343580
C	-2.7298726849	-1.4423213025	-0.2690077663
C	-3.9660168231	-0.8352984007	-0.0606253206
C	-4.0453792124	0.5576913613	0.0616742258
C	-2.8974570992	1.3313272057	-0.0381723837
H	1.9102878966	-3.9218056965	-0.6187825476
H	1.5480861151	4.1151274988	0.5239109366
H	-2.6769779214	-2.5232610779	-0.3537401699
H	-4.8627706678	-1.4432504559	0.0101992461
H	-5.0066215080	1.0365769247	0.2246522375
H	-2.9723807384	2.4122165168	0.0328536808
H	-0.6361954849	-3.4823563610	-0.2032480560
H	-0.9419979341	3.4098090084	0.6234367335
Cl	1.1331394289	-0.6723015816	3.0071347475

## Ground state coordinates: M8

C	1.0679118891	-0.7320306701	-0.1238880582
C	1.0632210222	0.7145560817	-0.4550628451
H	1.1200956269	0.8080568372	-1.5585928170
C	-0.1243834731	-1.4253065612	0.0169066983
C	0.1041580044	-2.8322630303	0.2022773858
C	1.4264377455	-3.1559260195	0.1831503540
S	2.4450640968	-1.7662516104	-0.0663771229

C	-1.4029896136	-0.7302404770	-0.0288693526
C	-1.4381180563	0.7085961871	-0.0922386088
C	-0.2113033707	1.4286668607	-0.1060212426
C	0.0176980277	2.7829899107	0.1873263713
C	1.3591734289	3.0989138349	0.2941091319
S	2.4635623311	1.8180040620	0.0432825187
C	-2.6245689401	-1.4182272398	0.0321548731
C	-3.8328563047	-0.7321690774	0.0347449175
C	-3.8700705143	0.6744886100	-0.0164598553
C	-2.6885051949	1.3832976313	-0.0704365161
H	1.8818906731	-4.1272286401	0.3189431171
H	1.7485208354	4.0867039169	0.5192311234
H	-2.6306842602	-2.5011119695	0.0757426322
H	-4.7623619265	-1.2914330348	0.0782160864
H	-4.8216977985	1.1945940531	-0.0190979307
H	-2.7139193939	2.4662240358	-0.1284971058
H	-0.6751466239	-3.5674675357	0.3570923105
H	-0.7595478792	3.5115468639	0.3803167318

Ground state coordinates: M9

C	1.0630858930	-0.7088868337	-0.0038514313
C	1.0640901568	0.7056833066	-0.0071977664
C	-0.1444957452	-1.4200777181	0.0000415857
C	0.0826801400	-2.8397451901	0.0027907558
C	1.4023235949	-3.1713564908	0.0010171682
S	2.4471808715	-1.7746598252	-0.0045630000
C	-1.4045254920	-0.7142100009	0.0006235905
C	-1.4060948860	0.7166517897	-0.0050544003
C	-0.1434512516	1.4226354935	-0.0119994565
C	0.0892216354	2.8442738292	-0.0045684765
C	1.4104680800	3.1708390800	0.0050898593
S	2.4498140191	1.7693028898	0.0091089601
C	-2.6451331951	-1.3940022190	0.0064731060
C	-3.8408820907	-0.7023537645	0.0061967184
C	-3.8417786763	0.7054058288	0.0002791148
C	-2.6461210565	1.3976380088	-0.0047567973
H	1.8393157600	-4.1603176991	0.0007921736
H	1.8514910516	4.1579349449	0.0071344633
H	-2.6561952182	-2.4791472146	0.0105406286
H	-4.7811392929	-1.2456382219	0.0091456149
H	-4.7822880768	1.2481268533	-0.0005950604
H	-2.6568054465	2.4829222098	-0.0089058010
H	-0.7056466309	-3.5823974498	0.0056193297
H	-0.6969730351	3.5892568270	-0.0069681335

R1: benzene, R2=R3 : 3-pyrrole

Ground state coordinates: M1

C	1.3278190570	1.2881320501	0.9811618372
C	-1.3278417277	1.2881177680	-0.9811587058
H	0.5361141297	1.3913879735	1.7087762189
H	-0.5361278901	1.3913818447	-1.7087731517
C	1.5325348621	0.2521130088	0.1023846813
C	2.7005170406	0.4753990593	-0.7073251844
C	3.3340912035	1.6535324398	-0.4341681759
N	2.5268270875	2.5265183550	0.8292151197
C	0.7084084094	-0.9821913500	0.0246900114
C	-0.7083971239	-0.9821988318	-0.0246862890
C	-1.5325366367	0.2520968093	-0.1023912995
C	-2.7005211354	0.4753607588	0.7073285045
C	-3.3341177655	1.6534873783	0.4341612066
N	-2.5268628254	2.5264814630	-0.8292123301
C	1.3817204248	-2.2154977968	0.0306236583
C	0.6968829173	-3.4274914127	0.0111715036
C	-0.6968358649	-3.4274987690	-0.0111771419
C	-1.3816861256	-2.2155123849	-0.0306196312

H	4.2170608565	2.0648970337	-0.9024671848
H	-4.2170817234	2.0648427845	0.9024700661
H	2.4665327519	-2.2137720662	0.0824966005
H	1.2490169014	-4.3625584979	0.0239082676
H	-1.2489499465	-4.3625716837	-0.0239036836
H	-2.4664984707	-2.2138081155	-0.0824925739
H	3.0311890007	-0.2152893020	-1.4749818834
H	-3.0311858074	-0.2153208798	1.4749853941
H	-2.6874331580	3.3863405535	-1.2809914325
H	2.6873883111	3.3863792645	1.2809839849

Ground state coordinates: M3

C	1.4277238021	-0.6409588620	0.3901608344
C	1.4277246038	0.6409586264	-0.3901583953
H	1.4317993738	-0.3840852207	1.4706325287
H	1.4318024672	0.3840868876	-1.4706302579
C	0.1371218003	-1.4047474027	0.0920529298
C	0.5216933844	-2.7829267432	-0.0259732884
C	1.8820704670	-2.8560981662	-0.0534973309
N	2.5032730103	-1.6196215779	0.1464074057
C	-1.0676236525	-0.7387426156	-0.0047969247
C	-1.0676232909	0.7387425351	0.0047989273
C	0.1371219662	1.4047466179	-0.0920521575
C	0.5216934966	2.7829268235	0.0259665501
C	1.8820698980	2.8560994081	0.0534912854
N	2.5032757679	1.6196201508	-0.1464032266
C	-2.3410890661	-1.4121066580	-0.0774886953
C	-3.5120176933	-0.7185714720	-0.0496948386
C	-3.5120174391	0.7185716354	0.0496953923
C	-2.3410888829	1.4121067664	0.0774899953
H	2.4932369125	-3.7422771987	-0.1795641092
H	2.4932355883	3.7422799062	0.1795511998
H	-2.3512881898	-2.4972641543	-0.1295292102
H	-4.4602788502	-1.2466766357	-0.0906868435
H	-4.4602785199	1.2466770157	0.0906871206
H	-2.3512879770	2.4972641873	0.1295310410
H	-0.1432797754	-3.6307175916	-0.1214756604
H	-0.1432801861	3.6307181357	0.1214618447
H	3.2196022965	1.3557602671	0.5230475182
H	3.2196190517	-1.3557585673	-0.5230201289

Ground state coordinates: M4

C	-0.3994987757	-0.6446394803	1.4308391362
C	0.3994987757	0.6446394803	1.4308391362
H	-1.4754911806	-0.3957085723	1.4509751117
H	1.4754911806	0.3957085723	1.4509751117
C	-0.0829205344	-1.4077637710	0.1517462301
C	0.0940970828	-2.7551920327	0.5049068135
C	0.0427383792	-2.8490712039	1.8877083030
N	-0.1063600824	-1.6309670255	2.4729130881
C	0.0067066040	-0.7245263980	-1.0838145634
C	-0.0067066040	0.7245263980	-1.0838145634
C	0.0829205344	1.4077637710	0.1517462301
C	-0.0940970828	2.7551920327	0.5049068135
C	-0.0427383792	2.8490712039	1.8877083030
N	0.1063600824	1.6309670255	2.4729130881
C	0.0578598480	-1.4071169497	-2.3284841407
C	0.0356098284	-0.7079678441	-3.5145642985
C	-0.0356098284	0.7079678441	-3.5145642985
C	-0.0578598480	1.4071169497	-2.3284841407
H	0.1262110034	-3.7416575268	2.4955182080
H	-0.1262110034	3.7416575268	2.4955182080
H	0.0801263964	-2.4918082350	-2.3403208335
H	0.0606595865	-1.2428011509	-4.4581680322
H	-0.0606595865	1.2428011509	-4.4581680322
H	-0.0801263964	2.4918082350	-2.3403208335

H	0.3005764233	-3.5832380635	-0.1575164560
H	-0.3005764233	3.5832380635	-0.1575164560
H	0.4775773093	1.5402979829	3.4090949198
H	-0.4775773093	-1.5402979829	3.4090949198

Ground state coordinates: M5=M6

C	1.2295938586	0.0575881233	-0.5207103233
C	0.6478030098	1.4365841388	-0.7406061417
H	0.5091764864	1.5952905349	-1.8312267506
C	0.2879479411	-1.0270558959	-0.7407852063
C	1.0067655501	-2.1111295850	-1.2841040634
C	2.3066110809	-1.6748616377	-1.4995206934
N	2.4262656986	-0.3617468703	-1.1937592778
C	-1.1070169468	-0.8864760340	-0.4147812502
C	-1.5855921511	0.4095721656	-0.0070586568
C	-0.6989265982	1.5197957700	-0.0351780501
C	-0.7678900314	2.7894811578	0.5755573156
C	0.4590679492	3.4067563438	0.4440150410
N	1.3680553727	2.5876000194	-0.1887679568
C	-1.9923054733	-1.9822564412	-0.4211063126
C	-3.3119547743	-1.8386000514	-0.0263403011
C	-3.7803609250	-0.5768664176	0.3943027842
C	-2.9387868391	0.5185288164	0.4100154240
H	3.1641344334	-2.2451404615	-1.8327904149
H	0.7689418776	4.3740888499	0.8176755403
H	-1.6216516816	-2.9594440211	-0.7177982372
H	-3.9782188093	-2.6948666732	-0.0272188408
H	-4.8151787153	-0.4639912580	0.7047101207
H	-3.3192838253	1.4864185245	0.7215718922
H	0.6354344435	-3.0998301909	-1.5115797720
H	-1.5976193871	3.1818641427	1.1465295169
H	2.1422810613	2.9874066790	-0.6982791816
H	3.3239059251	0.0379684441	-0.9482220249
H	1.5921756128	-0.0216868688	0.7189212673
Cl	2.3890147472	-0.1073960392	2.1906235061

Ground state coordinates: M7

C	1.1026988481	-0.3118854839	-0.9356430445
C	0.8526765919	1.1465177275	-1.1301891579
H	0.6843804962	1.3373421630	-2.2135506430
C	0.0853462362	-1.2150220778	-0.6403173382
C	0.6551359741	-2.5266363693	-0.7430228009
C	1.9747632977	-2.3752243756	-1.0996515266
N	2.2335850822	-1.0275492707	-1.2454419785
C	-1.2711126637	-0.7634602504	-0.3295772366
C	-1.4888560457	0.6441542150	-0.1592941253
C	-0.3896213673	1.5487591372	-0.3515944530
C	-0.1358418967	2.8267363840	0.1869725565
C	1.1830402016	3.1567633199	-0.0377606230
N	1.8724762439	2.1068244212	-0.6553186064
C	-2.3360580567	-1.6492304642	-0.1344462153
C	-3.5993443882	-1.1893588532	0.2357490253
C	-3.8120611962	0.1819335300	0.4282752762
C	-2.7718648526	1.0821700944	0.2382334509
H	2.7564136391	-3.1082230550	-1.2325484940
H	1.7201383136	4.0419978729	0.2765410413
H	-2.1698085658	-2.7146557825	-0.2671837335
H	-4.4124695998	-1.8948126674	0.3783828767
H	-4.7936606260	0.5452655710	0.7189982425
H	-2.9478643265	2.1459494989	0.3717342880
H	0.1605904060	-3.4690140146	-0.5563967885
H	-0.8231401566	3.4144199146	0.7814010275
H	2.5802061545	2.3719891577	-1.3298174253
H	3.1469021678	-0.6285192162	-1.3945837917
H	1.3597554370	-0.6537203278	1.3995119259
Cl	1.9825131343	-0.7223673159	2.5415548731

Ground state coordinates: M8

C	1.4020327169	-0.7142725748	-0.1241794398
C	1.4640284635	0.7153671907	-0.5479538714
H	1.5629025476	0.7542427755	-1.6557047077
C	0.2002687822	-1.3987446694	0.0343724076
C	0.5341455640	-2.7795671710	0.2277777592
C	1.9044191758	-2.8832863057	0.1720614924
N	2.4255161904	-1.6291048404	-0.0728204670
C	-1.0876306716	-0.7082714734	-0.0363218844
C	-1.0799790423	0.7250322963	-0.0943684055
C	0.1792349012	1.4152228272	-0.1346434755
C	0.5399464322	2.7109239014	0.2881345788
C	1.9139893219	2.8026371860	0.3377311907
N	2.5174333131	1.5777373725	0.0302569527
C	-2.3110922545	-1.3846902394	0.0123583445
C	-3.5203690321	-0.6904075255	0.0196893282
C	-3.5190423485	0.7102331415	-0.0112851985
C	-2.3178446516	1.4052388615	-0.0625859465
H	2.5520844268	-3.7353542380	0.3150258371
H	2.5234613277	3.6374685247	0.6579161272
H	-2.3146980975	-2.4703857038	0.0529104567
H	-4.4584231595	-1.2363337162	0.0542862226
H	-4.4582338949	1.2560507874	-0.0033659665
H	-2.3240625801	2.4908873927	-0.1044742886
H	-0.1493633883	-3.5968074110	0.4078028510
H	-0.1395552324	3.4805854229	0.6301798144
H	3.3863289389	1.6248564635	-0.4883389297
H	3.4062684444	-1.3981306941	-0.0530140940

Ground state coordinates: M9

C	1.4275267064	-0.7105957735	-0.0021128797
C	1.4302760223	0.7043968305	-0.0030731020
C	0.2102141705	-1.4141908714	-0.0008391419
C	0.5451356901	-2.8072034273	0.0007228149
C	1.9141519169	-2.9045489965	-0.0010050512
N	2.4524955108	-1.6306497528	-0.0004372520
C	-1.0525982618	-0.7152074191	-0.0009465603
C	-1.0530524703	0.7170697517	-0.0063934942
C	0.2132950591	1.4135704051	-0.0132557354
C	0.5557198696	2.8101670554	-0.0040278200
C	1.9259146086	2.9005766388	0.0085969816
N	2.4564818876	1.6228735748	0.0165333012
C	-2.2917447247	-1.3928107291	0.0062476413
C	-3.4888652550	-0.6993363101	0.0061965733
C	-3.4882895216	0.7077311921	0.0003512307
C	-2.2896722417	1.3988552396	-0.0056751175
H	2.5561769555	-3.7729018232	-0.0020858369
H	2.5718886077	3.7657543708	0.0112953154
H	-2.2979044177	-2.4790914444	0.0109397991
H	-4.4298324337	-1.2419841212	0.0106710964
H	-4.4282520306	1.2520469255	0.0001780941
H	-2.2931826252	2.4853247758	-0.0086683440
H	-0.1398683434	-3.6426111448	0.0020119173
H	-0.1269693408	3.6476860658	0.0014729321
H	3.4400400942	1.4140225182	-0.0270468474
H	3.4369923362	-1.4246543945	-0.0201585074

R1 : benzene, R2 : Phenyl, R3 : 2-methoxyphenyl

Ground state coordinates: M1

C	0.6912166487	-0.9458091091	-1.6873652309
C	-1.4529039302	-0.9720445137	1.1281286623
H	-0.1587799536	-0.6600711598	-2.2994326786
H	-0.5083581968	-0.8417159807	1.6464581887
C	1.3903368870	-2.1205101198	-1.9705827214
C	2.4804085713	-2.4719682462	-1.1800864839

C	2.8679994983	-1.6621014575	-0.1101115207
C	2.1607659298	-0.4878105546	0.1686136716
C	1.0562209333	-0.1097538957	-0.6280315462
C	0.3258462500	1.1720815451	-0.3834295206
C	-1.0506898580	1.2175427157	-0.0622167656
C	-1.8661968394	-0.0028875912	0.1995417071
C	-2.2489368545	-2.0828033454	1.4006341114
C	-3.4733979499	-2.2500253111	0.7504900736
C	-3.1022368913	-0.1802530667	-0.4423218362
C	-3.8976369366	-1.2939477010	-0.1725669162
C	1.0206035195	2.3792065470	-0.5587544468
C	-1.6789181884	2.4708252382	0.0433379559
C	0.3847100534	3.6116041034	-0.4417594076
C	-0.9774243634	3.6577852619	-0.1446261936
H	1.0859891509	-2.7485168263	-2.8018840721
H	3.0384266482	-3.3807458145	-1.3867852437
H	3.7150267382	-1.9540387224	0.4989310691
O	2.4572538929	0.3476995642	1.2112921255
H	-1.9137849406	-2.8185076510	2.1264335313
H	-4.0915069977	-3.1174999803	0.9632758320
H	-3.4327306544	0.5563020606	-1.1695030571
H	-4.8470754927	-1.4150166166	-0.6866136745
H	2.0770620813	2.3384716268	-0.8046393938
H	-2.7323791893	2.5021772542	0.3052402030
H	0.9483193526	4.5286764509	-0.5872795876
H	-1.4886819282	4.6113728665	-0.0488037836
C	3.5576198592	0.0267149648	2.0454222166
H	3.6062712849	0.8180486478	2.7948920926
H	4.5005330670	0.0029191150	1.4837460337
H	3.4193198559	-0.9385245684	2.5497326826

Ground state coordinates: M3

C	-0.0984355381	-1.3797966904	-0.2336292380
C	-1.5192037997	-1.0371593333	0.1562178999
H	-0.2117744512	-1.3780535842	-1.3165654194
H	-1.4551742032	-1.1903488597	1.2331606208
C	0.2877811295	-2.6743311342	-0.0395931197
C	1.6950869984	-3.0812263012	-0.0179117613
C	2.6473845194	-2.1597533358	-0.0160011511
C	2.2989257492	-0.7114246608	-0.0058620845
C	0.9770739463	-0.3193267756	-0.0895339805
C	0.5061445283	1.1234096242	-0.0737184227
C	-0.8918121823	1.3983309997	0.0323714931
C	-1.9055294171	0.2811620665	0.1337269868
C	-2.6091067601	-2.0432602984	-0.1590268865
C	-3.9066411683	-1.7239125561	-0.1303445235
C	-3.3781635991	0.6031258586	0.2576614009
C	-4.3093231060	-0.3471290097	0.1470156178
C	1.3927155467	2.2330188142	-0.1801580911
C	-1.3197384818	2.7522247900	0.0314047405
C	0.9317919167	3.5439295382	-0.1730694419
C	-0.4189839696	3.8029128002	-0.0662139830
H	-0.4108428163	-3.4871046372	0.0890147375
H	1.9547127521	-4.1347870685	0.0219749726
H	3.6790619345	-2.4920349439	0.0204252215
O	3.3006922873	0.1961311803	0.1221766149
H	-2.3878812805	-3.0737415611	-0.3985465597
H	-4.6629032249	-2.4773280649	-0.3285993325
H	-3.7539705174	1.6005133585	0.4173298463
H	-5.3633558230	-0.0954576174	0.2159817259
H	2.4528113075	2.1584197245	-0.2911922716
H	-2.3487978822	3.0480206409	0.1002870794
H	1.6311283774	4.3665106062	-0.2584996626
H	-0.7739667514	4.8259497586	-0.0654591767
C	4.6502981371	-0.0695642218	0.2282508152
H	5.2004906402	0.8892549580	0.3192891136
H	5.0108893749	-0.5972681638	-0.6802024129



H 4.8524475687 -0.6789750345 1.1346709781

Ground state coordinates: M4

C -0.1292291870 -1.2618125092 -0.5917906294  
C -1.3593197239 -1.0418304381 0.3308700561  
H -0.4695071910 -0.9959830979 -1.6136541097  
H -0.9582044161 -1.0492286419 1.3700888973  
C 0.3315372670 -2.6809710855 -0.6840359985  
C 1.6305037884 -3.0127175036 -0.5030761955  
C 2.5926254627 -2.0271063228 -0.1404098577  
C 2.2597561170 -0.6799684477 0.0118315126  
C 0.9229880547 -0.2293081314 -0.2039452137  
C 0.4725583237 1.1275556662 -0.1272926802  
C -0.9563359212 1.4109636486 -0.0730704218  
C -1.8945592257 0.3559091497 0.1162399900  
C -2.3866508229 -2.1348532228 0.3299480781  
C -3.7113089087 -1.8686470733 0.3485491961  
C -3.2943223809 0.5497615180 0.1706600164  
C -4.1667458274 -0.5102438866 0.2812607377  
C 1.3602780680 2.2409605337 -0.1846461358  
C -1.3868899328 2.7675248083 -0.1346705999  
C 0.8933619891 3.5362753540 -0.2339695241  
C -0.4915055225 3.8070207348 -0.2114018984  
H -0.3921470666 -3.4294723681 -0.9858879828  
H 1.9617441384 -4.0386219267 -0.6278664009  
H 3.6129317777 -2.3464945510 0.0276670030  
O 3.1665546734 0.2353441648 0.4152287403  
H -2.0304569762 -3.1549175962 0.4187478115  
H -4.4384832889 -2.6710557020 0.4140872989  
H -3.7104448287 1.5445597447 0.0800911921  
H -5.2344534971 -0.3140616938 0.2995728483  
H 2.4214396167 2.0612593195 -0.2357059665  
H -2.4437261541 2.9979689567 -0.1036458565  
H 1.6013813500 4.3556408288 -0.3059161572  
H -0.8482784341 4.8307588965 -0.2509941863  
C 4.4957145159 -0.1701697362 0.7667154466  
H 4.9928645867 0.7374901406 1.1062175126  
H 5.0276739514 -0.5760671432 -0.0996746827  
H 4.4804922438 -0.9045868196 1.5784475838

Ground state coordinates: M5=M6

C -0.0812153131 -1.2626500430 -0.6880530683  
C -1.3630000068 -1.0587068864 0.1858187827  
H -0.4154339409 -0.9808966739 -1.7068707170  
C 0.3986072159 -2.6773988875 -0.7636764972  
C 1.6806871176 -3.0071579572 -0.4691751134  
C 2.6211494303 -2.0322790681 -0.0371207780  
C 2.2598222159 -0.6814811069 0.0616428054  
C 0.9629658017 -0.2462633617 -0.2646365404  
C 0.4955837739 1.1278923411 -0.2222392988  
C -0.9069789757 1.4004105569 -0.0654687178  
C -1.8427009407 0.3149530651 0.2085525893  
C -2.3524378601 -2.1137270810 0.2351324665  
C -3.6574097050 -1.8558505804 0.5740374963  
C -3.1764095008 0.5364878589 0.5955749710  
C -4.0573977400 -0.5199982850 0.7786133946  
C 1.3644787662 2.2331227878 -0.3882068655  
C -1.3587241163 2.7362997315 -0.1299547356  
C 0.8877360504 3.5331338262 -0.4361404997  
C -0.4842558104 3.7931995843 -0.3156834110  
H -0.2919678166 -3.4328458005 -1.1237276257  
H 2.0105812301 -4.0383756360 -0.5612057242  
H 3.6208511553 -2.3502655244 0.2261256306  
O 3.1434298271 0.2618982773 0.4988847095  
H -2.0107160758 -3.1375787187 0.1354565882  
H -4.3698320723 -2.6654144424 0.6931400754  
H -3.5421865708 1.5440431280 0.7497103148  
H -5.0806799905 -0.3079313287 1.0759080864

H	2.4219324884	2.0485061966	-0.5063543905
H	-2.4179594437	2.9491825693	-0.0456510416
H	1.5851493599	4.3525103710	-0.5858425715
H	-0.8607814496	4.8100461512	-0.3671826164
C	4.3512168382	-0.1565285175	1.1231142253
H	4.8106328938	0.7524243539	1.5144468302
H	5.0390172966	-0.6243793992	0.4074569689
H	4.1519663245	-0.8487045884	1.9483319030
H	-0.9512372993	-1.1749216854	1.2564985515
Cl	-0.2503531575	-1.4005052269	2.8372038229

Ground state coordinates: M7

C	0.2814735574	0.7224867001	1.0109672846
C	1.4952203292	-0.1982357785	1.2165294303
H	1.2575584454	-0.7575123962	2.1468522733
C	0.3615598183	2.0946613251	1.2761385175
C	-0.7611196579	2.9054884497	1.1232097625
C	-1.9567749309	2.3602920361	0.6703899376
C	-2.0400806714	0.9943613847	0.3765671637
C	-0.9239921042	0.1323442191	0.5651019531
C	-0.9385382195	-1.3177965266	0.2380910019
C	0.2960514406	-1.9503413421	-0.0945924211
C	1.5419360121	-1.2227240810	0.1033217941
C	2.8084291186	0.5009369914	1.4415534023
C	3.9158364257	0.2242060096	0.7005392157
C	2.7028997021	-1.4458233380	-0.6120266336
C	3.8857880207	-0.7403432954	-0.3454136309
C	-2.1103149121	-2.0935098591	0.1928200504
C	0.2926456847	-3.2858479031	-0.5367151067
C	-2.0864464728	-3.4226729892	-0.2206762608
C	-0.8848664336	-4.0174538179	-0.6105932732
H	1.2943395631	2.5274340982	1.6168298758
H	-0.7017812171	3.9671014097	1.3427688193
H	-2.8179820617	3.0013357583	0.5346859544
O	-3.1828440199	0.4381262103	-0.1204794615
H	2.8672627792	1.2115780077	2.2603658223
H	4.8457456105	0.7459224526	0.9108192448
H	2.6919419727	-2.1691710753	-1.4227763917
H	4.7738138488	-0.9237522209	-0.9405006681
H	-3.0519290652	-1.6491179175	0.4783559918
H	1.2386358906	-3.7627553557	-0.7731713310
H	-3.0102539007	-3.9933300076	-0.2387616790
H	-0.8629727090	-5.0525337520	-0.9385018729
C	-4.2767835606	1.2806744038	-0.4555488095
H	-5.0262868871	0.6265072038	-0.9025791899
H	-3.9853254240	2.0485984969	-1.1815939785
H	-4.7041871970	1.7638724208	0.4317587388
H	0.8544090571	2.4235817699	-1.0106883575
Cl	1.1871896809	2.7860597584	-2.2110592840

Ground state coordinates: M8

C	-0.1795078889	-1.3069034834	0.3995307949
C	-1.5856240288	-0.7713596990	0.7148070734
H	-1.5181515905	-0.4333410291	1.7711977261
C	0.0671403126	-2.6818356528	0.3096144564
C	1.3555876240	-3.1487407428	0.0578816232
C	2.3964739001	-2.2480971329	-0.1371299031
C	2.1558081003	-0.8708185177	-0.0723935243
C	0.8595154685	-0.3636174277	0.2230554563
C	0.5313064820	1.0859249763	0.2655352449
C	-0.8095659476	1.4856067887	-0.0130523523
C	-1.8464946022	0.4681112710	-0.1138915429
C	-2.6960834486	-1.7841945947	0.6419636358
C	-3.8146349593	-1.5845194756	-0.1073502908
C	-3.0045801911	0.5988735110	-0.8565306758
C	-3.9881348090	-0.4014392684	-0.8794754725
C	1.4799463396	2.0922006095	0.5198055559
C	-1.1179355287	2.8546797570	-0.1118688104

C	1.1458404143	3.4417756037	0.4447818212
C	-0.1520235726	3.8282613286	0.1040946037
H	-0.7423743862	-3.3880880638	0.4489003337
H	1.5481976950	-4.2157310485	-0.0001283303
H	3.3902006506	-2.6193019523	-0.3513182072
O	3.1441825383	0.0390543190	-0.3124310612
H	-2.6054043223	-2.6763606032	1.2542098099
H	-4.5960457218	-2.3398673481	-0.1162113157
H	-3.1452718094	1.4905365212	-1.4614785330
H	-4.8756609776	-0.2771045165	-1.4904454634
H	2.4922788524	1.8150418540	0.7728178091
H	-2.1440364660	3.1485753977	-0.3097311835
H	1.9031790859	4.1920889502	0.6520711531
H	-0.4151237356	4.8799688499	0.0393773201
C	4.4179212765	-0.4183919754	-0.7447903102
H	5.0013681241	0.4809891130	-0.9457063944
H	4.3414622396	-1.0141795194	-1.6619396879
H	4.9221924085	-1.0087564091	0.0303091527

Ground state coordinates: M9

C	-0.0589293812	-1.3634375986	-0.1100379066
C	-1.4959677951	-1.0656485616	-0.0409049560
C	0.3704622572	-2.7051407142	-0.2148428900
C	1.7081488020	-3.0325562631	-0.2060839817
C	2.6690636099	-2.0301162216	-0.0645856845
C	2.2811170513	-0.6983600353	0.0296982603
C	0.8998683798	-0.3092072724	-0.0383590913
C	0.4330322511	1.0899363401	-0.0493238484
C	-0.9667033215	1.3673333044	0.0008734488
C	-1.9412985987	0.2761077444	0.0539780707
C	-2.4646882180	-2.0964929370	-0.0262235045
C	-3.8166522501	-1.8305384050	0.0845390072
C	-3.3281655427	0.5213522682	0.1825049133
C	-4.2539541163	-0.5046717365	0.1962746463
C	1.3096274060	2.1996939693	-0.1567662819
C	-1.4019480573	2.7102733311	-0.0286219877
C	0.8513703733	3.5053607238	-0.1841792882
C	-0.5187896155	3.7699490636	-0.1114263865
H	-0.3528004291	-3.5033452940	-0.3057474628
H	2.0201189218	-4.0690321280	-0.2926567763
H	3.7160652380	-2.3002601597	-0.0274455012
O	3.2153585641	0.2846300442	0.2095062566
H	-2.1573231532	-3.1320994922	-0.0878647616
H	-4.5304075334	-2.6489187195	0.0948151897
H	-3.6911577735	1.5362732835	0.2827422394
H	-5.3115724503	-0.2801185576	0.2981605016
H	2.3685659672	2.0274401535	-0.2307830134
H	-2.4615494949	2.9301695381	-0.0050841750
H	1.5654459843	4.3194757343	-0.2697644996
H	-0.8913498247	4.7899003944	-0.1335081637
C	4.5848397511	-0.0632445808	0.3328317445
H	5.1143846680	0.8771627404	0.4929857076
H	4.9676453029	-0.5412443854	-0.5773720029
H	4.7584681512	-0.7259979735	1.1894069635

R1: Benzene, R2 : phenyl , R3: 3-methoxyphenyl

Ground state coordinates: M1e

C	1.5550211284	0.6287473135	0.7021118255
C	-1.1602997019	0.9757192006	-1.4348130067

O	0.6453062939	0.6519094996	1.7175677117
H	-0.3877950746	0.6121149536	-2.1039959013
C	2.5890536649	1.5615816398	0.5664743207
C	3.5056210287	1.4461350192	-0.4813255438
C	3.4009016006	0.4033882730	-1.3962036334
C	2.3641437139	-0.5220571945	-1.2577427131
C	1.4213109308	-0.4280970463	-0.2282384042
C	0.3617441994	-1.4725660013	-0.0939376090
C	-1.0257323500	-1.1924253541	-0.1369200361
C	-1.5815117894	0.1719028940	-0.3636810030
C	-1.7343417743	2.2275925153	-1.6560830772
C	-2.7404110358	2.7018354134	-0.8128012284
C	-2.5967112738	0.6607954705	0.4750080562
C	-3.1698281471	1.9122933562	0.2551423185
C	0.7786249170	-2.8016515915	0.0788377760
C	-1.9303456061	-2.2554440743	0.0172416645
C	-0.1340304725	-3.8444798388	0.2230951835
C	-1.4993811081	-3.5676101768	0.1974973175
H	2.6944180923	2.3725532131	1.2769468940
H	4.3031364240	2.1781435405	-0.5715249511
H	4.1120143224	0.3083679965	-2.2108380715
H	2.2673897631	-1.3366062065	-1.9701638990
H	-1.3987758371	2.8301647746	-2.4954942099
H	-3.1868209311	3.6765106613	-0.9878849551
H	-2.9242134470	0.0562979531	1.3157749052
H	-3.9505032657	2.2720337794	0.9198078392
H	1.8442498970	-3.0069345207	0.1229452336
H	-2.9939201051	-2.0423114454	-0.0358645051
H	0.2208871331	-4.8617709673	0.3602313536
H	-2.2267878140	-4.3668668113	0.3070729756
C	0.6747467406	1.7373180864	2.6295283317
H	-0.1566920911	1.5737954778	3.3163465397
H	0.5367515296	2.6979486121	2.1179868986
H	1.6127630611	1.7634155666	3.1989689243

Ground state coordinates: M2e

C	0.8919073305	0.8291155717	0.1754143734
C	-0.4663225413	1.0440414436	-0.7774483128
O	0.3405125698	0.8531018962	1.5005318569
H	-0.0314963159	0.7938334517	-1.7467554422
C	1.8988009918	1.8408315797	-0.1168459218
C	2.9944543936	1.5958612405	-0.9228439657
C	3.2677542670	0.3079465931	-1.3906852275
C	2.4163307537	-0.7411346283	-0.9990505743
C	1.3198228262	-0.5453071346	-0.1813299160
C	0.3522862417	-1.6473458951	0.0045275160
C	-1.0272749671	-1.3636994838	-0.1930927980
C	-1.4369227732	0.0532415048	-0.2737476690
C	-0.9622162062	2.4186493389	-0.7672692165
C	-2.1497672110	2.7871719241	-0.1772928687
C	-2.6114509563	0.4687809483	0.3405635101
C	-2.9916461529	1.8131861472	0.3856005201
C	0.7448706766	-2.9601214893	0.2617188863
C	-1.9393924574	-2.4200434848	-0.2200936242
C	-0.1867719031	-4.0070088706	0.2616331390
C	-1.5252908020	-3.7396820138	0.0031750815
H	1.7209256497	2.8538037069	0.2245351360
H	3.6631285854	2.4171554470	-1.1678935928
H	4.1292384882	0.1116162712	-2.0197051339
H	2.6139553524	-1.7477877435	-1.3573681195
H	-0.3368111426	3.1791038976	-1.2271308880
H	-2.4498657824	3.8317448759	-0.1724073014
H	-3.2507611834	-0.2787575680	0.8003077122
H	-3.9246264259	2.1000699713	0.8601914082
H	1.7911094400	-3.1667695833	0.4672731801
H	-2.9845055705	-2.2157746937	-0.4336056194
H	0.1440647424	-5.0232485792	0.4547596692
H	-2.2538139805	-4.5446832189	-0.0203679902
C	0.5527771221	1.9883086567	2.3158922687

H	0.0423269880	1.7674038042	3.2566338462
H	0.1162453153	2.9046711893	1.8957532923
H	1.6184072535	2.1634689083	2.5174961073

Ground state coordinates: M3e

C	1.1826181766	-0.3763992638	0.0575428498
C	0.7755126021	1.0078477524	-0.4588520333
O	1.0182943268	-0.1529231177	1.4028804596
H	0.7595304298	0.7955557536	-1.5288948616
C	2.6176247396	-0.7954295853	-0.2431260997
C	2.9382768778	-2.0282580360	-0.6487554698
C	1.8921376275	-3.0284204536	-0.8576027933
C	0.6124947957	-2.7019084467	-0.6699346468
C	0.2105139575	-1.3174394668	-0.2408324558
C	-1.2580833963	-0.9934067116	-0.0950184144
C	-1.6868134816	0.3576608826	-0.0735383295
C	-0.6628773141	1.4344410921	-0.2533556585
C	1.7056652436	2.0100459439	-0.4362532672
C	1.3276483285	3.4360295588	-0.5107821898
C	-0.9894378532	2.7539731364	-0.2771697521
C	0.0449563425	3.7887258732	-0.4452346865
C	-2.2276695713	-2.0166625025	0.0272917652
C	-3.0663024595	0.6380123758	0.0797079709
C	-3.5786632385	-1.7136578609	0.1769152989
C	-3.9963452613	-0.3907353027	0.2047893076
H	3.4484027000	-0.1184201110	-0.0967768541
H	3.9761347150	-2.2922636100	-0.8274182939
H	2.1604685112	-4.0289010145	-1.1828581636
H	-0.1154225092	-3.4744272730	-0.8727993467
H	2.7676296947	1.8272285669	-0.3951212178
H	2.0972912805	4.1967859066	-0.5958354287
H	-2.0004480711	3.1140186317	-0.1646610530
H	-0.2358339239	4.8366123496	-0.4823356810
H	-1.9676591653	-3.0619060024	0.0325645054
H	-3.4585831140	1.6406265747	0.1002462775
H	-4.3048332096	-2.5104841854	0.2761436042
H	-5.0476608055	-0.1596717091	0.3208799218
C	1.9950059481	-0.0058160713	2.3731748420
H	2.6470367460	0.8606736142	2.1350452590
H	2.6037603566	-0.9312245446	2.4533486319
H	1.5062593663	0.1775645098	3.3516315976

Ground state coordinates: M4e

C	1.1744870887	0.3384747147	-0.2202433322
C	0.1129629882	1.3610493374	-0.5392908003
O	1.2215432033	0.6836929911	1.6078511299
H	0.1184822426	1.3875307348	-1.6609632194
C	2.5267267053	0.6647679000	-0.6709021307
C	3.4632652866	-0.3028331730	-0.8534071371
C	3.1112296703	-1.6847710187	

R1 : ethene, R2=R31: phenyl

Ground state coordinates: M1

C	0.6750525969	-1.8254143262	0.0041783451
C	-0.6739752140	-1.8265488482	-0.0008379784
C	1.6441486249	-0.7153522693	-0.0645015855
C	-1.6441425150	-0.7170095150	0.0653584538
H	1.1436154106	-2.8083481366	0.0489688598
H	-1.1411067958	-2.8102654555	-0.0432307626
C	1.4165719938	0.4598702419	-0.8040331381
C	2.8904654291	-0.8661213860	0.5696344327
C	2.3894164116	1.4535259096	-0.8798515574
C	3.6126961245	1.2987532448	-0.2228446696
C	3.8602622042	0.1322280550	0.5019344536
H	2.1954766509	2.3499346455	-1.4622970641

H	4.3690600778	2.0757224182	-0.2851991632
H	4.8113601269	-0.0040545704	1.0088009522
C	-2.8861582701	-0.8645070069	-0.5777161919
C	-1.4209884272	0.4544380600	0.8120751451
C	-2.3941369071	1.4479334780	0.8866996910
C	-3.6131846865	1.2965127437	0.2211339831
C	-3.8561947382	0.1337346461	-0.5111872449
H	-3.0847081168	-1.7729915657	-1.1408738366
H	-4.8039973240	0.0002594061	-1.0249400214
H	-2.2038130662	2.3414251927	1.4747908011
H	-4.3699067861	2.0732025681	0.2826140740
H	-0.4847110565	0.5759573425	1.3457686121
H	0.4772261700	0.5843807969	-1.3315355361
H	3.0925089475	-1.7774808076	1.1268802527

Ground state coordinates: M2

C	0.6692720848	-0.1046814573	2.1728134293
C	-0.6692720848	0.1046814573	2.1728134293
C	1.4185777570	-0.2052172192	0.9257664410
C	-1.4185777570	0.2052172192	0.9257664410
H	1.2166365948	-0.1538255446	3.1096275049
H	-1.2166365948	0.1538255446	3.1096275049
C	0.6828524507	-0.5793378787	-0.2980928795
C	2.7393161182	0.2064755722	0.8407918867
C	1.4359105103	-0.5612901001	-1.5370049932
C	2.7417097410	-0.1230848178	-1.5819269784
C	3.4007301746	0.2580042805	-0.3977310991
H	0.9509217741	-0.9183870284	-2.4401844285
H	3.2802341460	-0.1144792847	-2.5238716920
H	4.4329306920	0.5904844709	-0.4392181659
C	-2.7393161182	-0.2064755722	0.8407918867
C	-0.6828524507	0.5793378787	-0.2980928795
C	-1.4359105103	0.5612901001	-1.5370049932
C	-2.7417097410	0.1230848178	-1.5819269784
C	-3.4007301746	-0.2580042805	-0.3977310991
H	-3.2614685840	-0.5145773113	1.7413539342
H	-4.4329306920	-0.5904844709	-0.4392181659
H	-0.9509217741	0.9183870284	-2.4401844285
H	-3.2802341460	0.1144792847	-2.5238716920
H	-0.0787143187	1.4823456430	-0.1954032588
H	0.0787143187	-1.4823456430	-0.1954032588
H	3.2614685840	0.5145773113	1.7413539342

Ground state coordinates: M3

C	0.7160401142	-2.0765394304	-0.0077209050
C	-0.7160373854	-2.0765502062	0.0077814877
C	1.4355459789	-0.9193772216	-0.1020460707
C	-1.4355495939	-0.9193851851	0.1020544627
H	1.2423735549	-3.0273753433	0.0325087465
H	-1.2423614026	-3.0273925555	-0.0324396374
C	0.7025407620	0.4035080969	-0.3178070115
C	2.8761011259	-0.9056318362	-0.1145276196
C	1.5394631308	1.5931188804	0.0978539679
C	2.8806072997	1.5186862939	0.1774737626
C	3.5741424701	0.2553475255	-0.0113553661
H	1.0357838272	2.5389103415	0.2744228222
H	3.4652993759	2.4020297107	0.4204420481
H	4.6599696464	0.2430890564	0.0034438430
C	-2.8761037545	-0.9056316712	0.1144757774
C	-0.7025439334	0.4034938433	0.3178121742
C	-1.5394637732	1.5931216422	-0.0978051729
C	-2.8806054020	1.5186923533	-0.1774764545
C	-3.5741431188	0.2553474902	0.0112829533
H	-3.3963473847	-1.8600887833	0.1519236677
H	-4.6599696060	0.2430886978	-0.0035728534
H	-1.0357860112	2.5389293534	-0.2743014032
H	-3.4652880196	2.4020510933	-0.4204106595
H	-0.5515237208	0.4888046945	1.4180857533

H 0.5515480680 0.4888417412 -1.4180810021  
H 3.3963381496 -1.8600914567 -0.1519972378

Ground state coordinates: M4

C 0.6978541166 0.0082356158 2.1071569500  
C -0.6978541166 -0.0082356158 2.1071569500  
C 1.4317714995 -0.0707198823 0.9174979245  
C -1.4317714995 0.0707198823 0.9174979245  
H 1.2335320512 0.0666088212 3.0501499184  
H -1.2335320512 -0.0666088212 3.0501499184  
C 0.6968562672 -0.3498583563 -0.3796150077  
C 2.8390345664 0.0424214359 0.9095496191  
C 1.5295029361 -0.1463866519 -1.6101320108  
C 2.8742625770 0.0106385593 -1.5443966699  
C 3.5427318730 0.0762696114 -0.2763758972  
H 1.0444053361 -0.2268634413 -2.5768003195  
H 3.4613796112 0.0882739732 -2.4534624048  
H 4.6222953370 0.1876429825 -0.2556592927  
C -2.8390345664 -0.0424214359 0.9095496191  
C -0.6968562672 0.3498583563 -0.3796150077  
C -1.5295029361 0.1463866519 -1.6101320108  
C -2.8742625770 -0.0106385593 -1.5443966699  
C -3.5427318730 -0.0762696114 -0.2763758972  
H -3.3609393855 -0.1579700423 1.8548975236  
H -4.6222953370 -0.1876429825 -0.2556592927  
H -1.0444053361 0.2268634413 -2.5768003195  
H -3.4613796112 -0.0882739732 -2.4534624048  
H -0.4837686465 1.4409338064 -0.3612338043  
H 0.4837686465 -1.4409338064 -0.3612338043  
H 3.3609393855 0.1579700423 1.8548975236

Ground state coordinates: M5=M6

C 1.0701864298 -1.8026937293 1.2121515090  
C -0.2877822171 -2.0725977960 1.1123576525  
C 1.7042856326 -0.8470771529 0.4086162009  
C -1.1343925075 -1.3071887690 0.2728601864  
H 1.6641263016 -2.3288314760 1.9556338811  
H -0.7359257462 -2.8395443505 1.7369937425  
C 0.9318354155 -0.2357027500 -0.7498944419  
C 3.0565385401 -0.4916525051 0.6006143211  
C 1.5583476719 1.0309451737 -1.2696347845  
C 2.8446567738 1.3487514199 -0.9936858241  
C 3.6311002488 0.5522251484 -0.0911585233  
H 0.9823572915 1.6572560204 -1.9419983504  
H 3.2897783117 2.2365384942 -1.4332864113  
H 4.6654230104 0.8238887125 0.0945922866  
C -2.5264897385 -1.5509358998 0.2183914021  
C -0.5883606860 -0.1645900571 -0.4621794411  
C -1.4568737680 0.4358923473 -1.4541146163  
C -2.7997380135 0.1576805972 -1.4939139304  
C -3.3400029870 -0.8293338843 -0.6313985042  
H -2.9445862031 -2.3381057782 0.8394961391  
H -4.4058644953 -1.0371710534 -0.6599489645  
H -1.0533145048 1.2041542894 -2.1045415778  
H -3.4492041131 0.6827500626 -2.1867090030  
H -0.6322814621 0.6918919222 0.3914069129  
H 1.0272949606 -0.9747490919 -1.5785350548  
H 3.6276605989 -1.0223231804 1.3581555433  
Cl -0.4989635581 1.9041279693 1.5657803238

Ground state coordinates: M7

C 1.1501105316 -1.9865243644 1.1130288743  
C -0.1870210689 -2.2613320653 0.9874407139  
C 1.7780603463 -0.9692811797 0.3526380970  
C -1.0530966636 -1.4473318665 0.1608406721  
H 1.7441906175 -2.5229642111 1.8496687517  
H -0.6455003161 -3.0363388615 1.5952607231

C	1.0283273348	-0.4100906746	-0.8485381463
C	3.0764440265	-0.5219390562	0.6304159063
C	1.6147758363	0.8853615279	-1.3523533334
C	2.8546465399	1.2966012653	-0.9837925758
C	3.6306460962	0.5683235707	-0.0243063265
H	1.0623019495	1.4488504959	-2.0961725930
H	3.2682055020	2.2059143184	-1.4118992933
H	4.6280646637	0.9108714321	0.2315530129
C	-2.4529222890	-1.5873507556	0.2276051999
C	-0.4944845431	-0.4536094152	-0.6878185327
C	-1.3572407575	0.3634024946	-1.4252358701
C	-2.7483979944	0.2132907696	-1.3441044865
C	-3.2958002650	-0.7687086417	-0.5169021127
H	-2.8711611513	-2.3452085832	0.8850998306
H	-4.3727491519	-0.8907003326	-0.4501748427
H	-0.9572390488	1.1208583040	-2.0909810439
H	-3.3935384810	0.8620705404	-1.9287513629
H	-1.2897124273	1.7266609400	0.5916132150
H	1.2188870945	-1.1549639533	-1.6592380619
H	3.6340177337	-1.0192780944	1.4211943258
Cl	-1.3700029273	2.6570210795	1.4899599331

Ground state coordinates: M8

C	0.7040955156	-2.1029789810	-0.0018609503
C	-0.6916331874	-2.1037912494	-0.0163648083
C	1.4372411043	-0.9131499972	-0.0852748872
C	-1.4260920669	-0.9143104831	0.0601897567
H	1.2403804550	-3.0455128308	0.0584804305
H	-1.2268771360	-3.0472392809	-0.0712711180
C	0.7012189807	0.3827456298	-0.3671182133
C	2.8446631751	-0.9041122290	0.0258686541
C	1.5334806698	1.6143041640	-0.1683606309
C	2.8784896753	1.5497547173	-0.0130371307
C	3.5477482355	0.2822959538	0.0553030445
H	1.0477294155	2.5804717746	-0.2509505404
H	3.4652138062	2.4593666728	0.0611462065
H	4.6274853318	0.2624891736	0.1652156386
C	-2.8335229024	-0.9074582911	-0.0509896609
C	-0.6915018508	0.3840027115	0.3345532699
C	-1.5251119311	1.6134736087	0.1287103746
C	-2.8700583645	1.5465436179	-0.0262335218
C	-3.5379171363	0.2779732795	-0.0872718563
H	-3.3550697144	-1.8534238618	-0.1630771331
H	-4.6176213648	0.2563502443	-0.1970648432
H	-1.0404378035	2.5806276406	0.2057185428
H	-3.4577860415	2.4550638080	-0.1056660392
H	-0.4768700212	0.3688804678	1.4253834476
H	3.3672535721	-1.8488285193	0.1434047669

Ground state coordinates: M9

C	0.6796942699	-2.0940979775	-0.0001421111
C	-0.6797064490	-2.0940946035	0.0001429160
C	1.4229560432	-0.8664222849	-0.0001957672
C	-1.4229585548	-0.8664140445	0.0001517477
H	1.2319664606	-3.0301067027	-0.0002232487
H	-1.2319841897	-3.0300972999	0.0003700421
C	0.7286977914	0.3804425750	0.0000157533
C	2.8371085962	-0.8789187866	-0.0002698944
C	1.4992359208	1.5667230164	0.0003846006
C	2.8815641062	1.5295280904	0.0002988094
C	3.5605444747	0.2969458840	-0.0000924411
H	1.0056152231	2.5320699554	0.0009386461
H	3.4449896076	2.4580075417	0.0005361102
H	4.6462265807	0.2728188569	-0.0001566994
C	-2.8371148519	-0.8789156676	0.0002739576
C	-0.7286978903	0.3804451723	-0.0000752975
C	-1.4992318920	1.5667344666	-0.0003678063
C	-2.8815531685	1.5295320416	-0.0002814474



C	-3.5605400067	0.2969476383	0.0000914066
H	-3.3485076559	-1.8381150254	0.0004996796
H	-4.6462223500	0.2728306279	0.0002175553
H	-1.0056051556	2.5320784471	-0.0008017081
H	-3.4449835162	2.4580107819	-0.0005839340
H	3.3485146607	-1.8381103032	-0.0004030001

R1 : pyrrole, R2=R3 : phenyl

Ground state coordinates: M1

C	1.6368297981	1.2796250622	0.4905897033
C	-1.6078031778	1.3064285610	-0.3826311652
H	0.7012811572	1.6360074070	0.8768744015
H	-0.6481762259	1.6828035813	-0.6707186973
C	1.8068819488	-0.0490376583	0.0421113617
C	3.1177224912	-0.4230422297	-0.3645375578
C	4.1832556815	0.4730446854	-0.3420987644
C	3.9828950990	1.7797988942	0.0779225276
C	2.7138935163	2.1846824039	0.4931489476
C	-1.8122757006	-0.0463542917	-0.0284095143
C	-3.1540945598	-0.4317828782	0.2522876988
C	-4.2121413091	0.4714614772	0.1980154256
C	-2.6781866485	2.2179623620	-0.4144487261
C	-3.9766191632	1.7989557920	-0.1259173354
C	0.7145057268	-1.1036300827	0.0163031327
C	-0.7216742511	-1.1047104112	0.0194858430
C	1.0736831549	-2.4549252304	0.0192426991
C	-1.0714966226	-2.4608983294	0.0283864987
N	0.0017150991	-3.2475757886	0.0274301813
H	3.3543625679	-1.4126704836	-0.7173213832
H	5.1674039202	0.1439297397	-0.6542757495
H	4.8169447996	2.4707608580	0.0896995469
H	2.5734323329	3.2028533047	0.8318071223
H	-3.4292296367	-1.4353856256	0.5231712646
H	-5.2190904991	0.1313402894	0.4097882618
H	-2.5080971956	3.2536319278	-0.6782429038
H	-4.8053077162	2.4952532400	-0.1625429130
H	2.0653194836	-2.8772421544	0.0357358007
H	-2.0580854890	-2.8945992773	0.0158187694
H	0.0049809040	-4.2891210441	0.0314905605

Ground state coordinates: M3

C	0.7111297072	-1.0523792367	-0.2882737874
C	-0.7111354223	-1.0523793331	0.2882607277
H	0.5943585576	-1.1738300182	-1.3976835152
H	-0.5943644872	-1.1738434598	1.3976692840
C	1.4737505063	0.2530510267	-0.0937782415
C	2.8864713900	0.2074293993	-0.1449748995
C	3.5729952316	-0.9816534984	-0.0485956416
C	2.8635520347	-2.2035572807	0.2235922305
C	1.5112941964	-2.2351934543	0.2057913730
C	-1.4737493763	0.2530583128	0.0937801215
C	-2.8864697842	0.2074418282	0.1449990654
C	-3.5729985870	-0.9816383993	0.0486211305
C	-1.5113073773	-2.2351835782	-0.2058142390
C	-2.8635653447	-2.2035427655	-0.2235936576
C	0.7335760445	1.4403230373	-0.0247828649
C	-0.7335688203	1.4403264086	0.0247797601
C	1.1355659758	2.7922508561	-0.0326791067
C	-1.1355499696	2.7922574299	0.0326812978
N	0.0000097385	3.5420421959	-0.0000134003
H	3.4427991643	1.1405245276	-0.1976144211
H	4.6585211161	-0.9867410480	-0.0691638124
H	3.4296088259	-3.0871783981	0.5077839093

H	0.9786393972	-3.1390084902	0.4852189452
H	-3.4427938286	1.1405383329	0.1976575386
H	-4.6585242210	-0.9867214052	0.0692082125
H	-0.9786562748	-3.1389960926	-0.4852583693
H	-3.4296306880	-3.0871576859	-0.5077870606
H	2.1098741734	3.2513968824	-0.0695385633
H	-2.1098552054	3.2514089465	0.0695444620
H	0.0000128726	4.5516480213	-0.0000224162

Ground state coordinates: M4

C	0.7111297072	-1.0523792367	-0.2882737874
C	-0.7111354223	-1.0523793331	0.2882607277
H	0.5943585576	-1.1738300182	-1.3976835152
H	-0.5943644872	-1.1738434598	1.3976692840
C	1.4737505063	0.2530510267	-0.0937782415
C	2.8864713900	0.2074293993	-0.1449748995
C	3.5729952316	-0.9816534984	-0.0485956416
C	2.8635520347	-2.2035572807	0.2235922305
C	1.5112941964	-2.2351934543	0.2057913730
C	-1.4737493763	0.2530583128	0.0937801215
C	-2.8864697842	0.2074418282	0.1449990654
C	-3.5729985870	-0.9816383993	0.0486211305
C	-1.5113073773	-2.2351835782	-0.2058142390
C	-2.8635653447	-2.2035427655	-0.2235936576
C	0.7335760445	1.4403230373	-0.0247828649
C	-0.7335688203	1.4403264086	0.0247797601
C	1.1355659758	2.7922508561	-0.0326791067
C	-1.1355499696	2.7922574299	0.0326812978
N	0.0000097385	3.5420421959	-0.0000134003
H	3.4427991643	1.1405245276	-0.1976144211
H	4.6585211161	-0.9867410480	-0.0691638124
H	3.4296088259	-3.0871783981	0.5077839093
H	0.9786393972	-3.1390084902	0.4852189452
H	-3.4427938286	1.1405383329	0.1976575386
H	-4.6585242210	-0.9867214052	0.0692082125
H	-0.9786562748	-3.1389960926	-0.4852583693
H	-3.4296306880	-3.0871576859	-0.5077870606
H	2.1098741734	3.2513968824	-0.0695385633
H	-2.1098552054	3.2514089465	0.0695444620
H	0.0000128726	4.5516480213	-0.0000224162

Ground state coordinates: M5=M6

C	0.6796743114	-0.8832892930	0.3325994075
C	-0.7647398334	-0.7180781077	0.9535880218
H	-0.5403126826	-0.4913466907	2.0174924478
C	1.4805647820	0.3397245940	0.3184343398
C	2.8805301641	0.2464807471	0.3016177814
C	3.5115845781	-0.9828182612	0.4195668180
C	2.7690665526	-2.1722134528	0.5749039568
C	1.3962257325	-2.1163213055	0.5844887504
C	-1.4858593036	0.4980532837	0.3960382919
C	-2.8389616840	0.4555489682	0.1141817724
C	-3.5863805210	-0.7225806136	0.2384104728
C	-1.6136958503	-1.9579480504	0.9410115619
C	-2.9405467301	-1.9265118614	0.6352799928
C	0.7803198205	1.5898378703	0.2206527709
C	-0.6630120738	1.6707935540	0.2232660244
C	1.2689739454	2.8782029392	0.0224091906
C	-0.9857388276	3.0017506559	0.0278654339
N	0.1950436514	3.7074346061	-0.0876739668
H	3.4771140750	1.1493039353	0.2168843409
H	4.5970693875	-1.0279708750	0.4055213194
H	3.2822183381	-3.1218536726	0.6858917161
H	0.8257358608	-3.0348407442	0.6639260685
H	-3.3241323716	1.3533830543	-0.2604841069
H	-4.6416019077	-0.7280722215	-0.0122604574
H	-1.1651881995	-2.8885427841	1.2721846548
H	-3.5207679117	-2.8438607974	0.6898846690

H	2.2769776782	3.2536640766	-0.0662464247
H	-1.9391206398	3.5037128470	-0.0259436135
H	0.2533076742	4.7026257731	-0.2383911370
H	0.4353989586	-1.0132563997	-0.7805255642
Cl	-0.0417667174	-1.1746339850	-2.4576531570

Ground state coordinates: M7

C	-0.6894029951	0.2707696330	-0.9145872920
C	0.2059404977	-0.9618199876	-1.1662552202
H	0.6936920566	-0.7199080384	-2.1380466555
C	-0.0885332016	1.4700941405	-0.4533682022
C	-0.8770296159	2.6233191522	-0.3152630514
C	-2.2340694100	2.6128312220	-0.6279260290
C	-2.8312467079	1.4322580189	-1.0682585117
C	-2.0590037353	0.2724447511	-1.2050746616
C	1.3484941997	-1.0698335691	-0.1625819395
C	1.7107422399	-2.2887879536	0.3791081826
C	1.0148789244	-3.4715342470	0.0839086595
C	-0.5210243502	-2.2662583332	-1.3671417646
C	-0.1089316342	-3.4289074997	-0.7885800839
C	1.3222568731	1.4346891629	-0.0782967620
C	2.0070547280	0.1828644732	0.1197476612
C	2.1986942442	2.4427943116	0.2768199607
C	3.2752908715	0.4827083741	0.5944218918
N	3.3719827770	1.8503276960	0.6794951803
H	-0.4211190224	3.5343845517	0.0623172680
H	-2.8244392029	3.5170993149	-0.5126338775
H	-3.8915741792	1.4040230620	-1.3008355972
H	-2.5386991451	-0.6362188652	-1.5519411704
H	2.5405200306	-2.3221011036	1.0814582842
H	1.3130838360	-4.4087024764	0.5418094923
H	-1.3550877334	-2.2802135477	-2.0614862371
H	-0.6495797429	-4.3488095520	-0.9973489336
H	2.0889627921	3.5167742172	0.2814347511
H	4.1102178919	-0.1549630124	0.8423096014
H	4.2010741559	2.3505989090	0.9572474598
H	-2.3523259592	-0.2568553172	1.1158385415
Cl	-2.7390159286	-0.6219524653	2.2990219874

Ground state coordinates: M8

C	0.6568168352	-1.0578569833	0.2065158504
C	-0.8187198609	-0.8776032952	0.6243142333
H	-0.7434105614	-0.6634067485	1.7148406203
C	1.4686024943	0.0945366569	0.0478981585
C	2.8345315522	-0.0623440774	-0.2355347686
C	3.4069820722	-1.3260207880	-0.3575107679
C	2.6094428219	-2.4610035674	-0.2160868964
C	1.2441945928	-2.3203503760	0.0605973255
C	-1.4510640801	0.3690987714	0.0157700976
C	-2.7404220661	0.3459523347	-0.4817402160
C	-3.5076592019	-0.8291521309	-0.5084792318
C	-1.6891563152	-2.1000804565	0.4890523261
C	-2.9503029335	-2.0458430529	-0.0236721771
C	0.8284485189	1.4047695341	0.1236513140
C	-0.6040686584	1.5370802657	0.0487038211
C	1.3585968485	2.6812237869	0.1354886131
C	-0.8866698611	2.8944533448	0.0123513037
N	0.3096593714	3.5672263026	0.0684090745
H	3.4498003824	0.8210843897	-0.3820047990
H	4.4660407873	-1.4229537770	-0.5778110611
H	3.0378307261	-3.4529775057	-0.3240885368
H	0.6391519991	-3.2135843188	0.1708163126
H	-3.1571042990	1.2616838266	-0.8949761211
H	-4.5096137087	-0.8171592345	-0.9242082721
H	-1.3140947630	-3.0364511715	0.8896731482
H	-3.5485167436	-2.9528272573	-0.0640450241
H	2.3788551187	3.0311916111	0.1813347051
H	-1.8269458853	3.4238736402	-0.0156251750

H 0.4030747947 4.5697826272 0.0993167680

Ground state coordinates: M9

C 0.7430838534 -1.0301359447 0.0028219003  
C -0.7365097759 -1.0303210267 0.0076944854  
C 1.4644003325 0.1977468963 -0.0020629424  
C 2.8719448245 0.1781263398 -0.0072935685  
C 3.5757847834 -1.0150878879 -0.0085648900  
C 2.8754099440 -2.2285033976 -0.0074734829  
C 1.4883115635 -2.2283259358 -0.0013694777  
C -1.4638070663 0.1963977984 -0.0109744753  
C -2.8721261602 0.1728904191 -0.0252307411  
C -3.5755125855 -1.0211009358 -0.0165578590  
C -1.4838553623 -2.2311387490 0.0287852321  
C -2.8730935319 -2.2331451693 0.0152122618  
C 0.7161410267 1.4383922585 0.0005485309  
C -0.7186341722 1.4379260938 -0.0070392765  
C 1.1267295205 2.7626270060 0.0111875203  
C -1.1328584254 2.7615546752 0.0015773153  
N -0.0040725963 3.5394428783 0.0121357773  
H 3.4108345116 1.1212012957 -0.0085173969  
H 4.6618299093 -1.0081710330 -0.0116951645  
H 3.4140981055 -3.1714791139 -0.0112753799  
H 0.9777635355 -3.1846628114 -0.0028461764  
H -3.4124800028 1.1147216764 -0.0388734168  
H -4.6612880855 -1.0165481220 -0.0293045900  
H -0.9723217734 -3.1865802780 0.0510990775  
H -3.4101009494 -3.1768197906 0.0284251045  
H 2.1083671125 3.2105957270 0.0193828969  
H -2.1156041344 3.2070897851 0.0063967829  
H -0.0050426680 4.5471378741 0.0246946255

R1: thiophene, R2=R3 : phenyl

Ground state coordinates: M1

C 1.6594179219 1.5404136367 0.4568952588  
C -1.6245044217 1.5692808981 -0.3438711541  
H 0.7421581739 1.9327499380 0.8379833187  
H -0.6795248839 1.9757763987 -0.6183757253  
C 1.8039844719 0.2019949973 0.0329749639  
C 3.1067341123 -0.2101321677 -0.3361410968  
C 4.2013871665 0.6529978658 -0.3250569194  
C 4.0243683917 1.9747030787 0.0648615538  
C 2.7610822476 2.4129169228 0.4626818133  
C -1.8075749188 0.2097473441 -0.0179121361  
C -3.1380621815 -0.2111812511 0.2222189102  
C -4.2245447369 0.6614855544 0.1746976151  
C -2.7165924093 2.4519386029 -0.3826036175  
C -4.0101060521 2.0027679342 -0.1174699611  
C 0.7211041546 -0.8628701910 0.0080845930  
C -0.7305807890 -0.8609769904 0.0272644896  
C 1.2244994251 -2.1738631794 -0.0125704444  
C -1.2371786718 -2.1710718366 0.0485761791  
S -0.0075473125 -3.2859882895 0.0204265902  
H 3.2522754630 -1.1900056112 -0.6254146270  
H 5.1350422639 0.3131822438 -0.6040280382  
H 4.8228143503 2.6285308198 0.0602212777  
H 2.6338114679 3.3912814988 0.7653999281  
H -3.3107273415 -1.2047338549 0.4414287908  
H -5.1794884287 0.3141767958 0.3549322992  
H -2.5596766419 3.4461935922 -0.6103171672  
H -4.8032167236 2.6627532572 -0.1381874459  
H 2.2276591987 -2.4140612008 -0.0440995450  
H -2.2409721612 -2.4089385570 0.0778512062

Ground state coordinates: M3

C	1.3142660379	-0.7093475050	0.2880333458
C	1.3142259835	0.7094516082	-0.2879290913
H	1.4310561575	-0.5929948137	1.3988073605
H	1.4311648925	0.5931324018	-1.3986918379
C	0.0107251224	-1.4687855072	0.0891201474
C	0.0604229845	-2.8788968199	0.1394675294
C	1.2517784430	-3.5658330966	0.0482338092
C	2.4735029332	-2.8586532131	-0.2177792495
C	2.5013257397	-1.5058889438	-0.1993138917
C	0.0105946039	1.4687686552	-0.0891687134
C	0.0601672638	2.8788800776	-0.1397483312
C	1.2514531741	3.5659300193	-0.0484696887
C	2.5011450065	1.5061308075	0.1995509119
C	2.4732009020	2.8588944032	0.2178437211
C	-1.1929776843	-0.7346724430	0.0215511406
C	-1.1930409883	0.7345617549	-0.0215478793
C	-2.5020010275	-1.2460191031	0.0266724222
C	-2.5021098814	1.2458019307	-0.0267798539
S	-3.6573620669	-0.0001571473	0.0001219916
H	-0.8679693720	-3.4414903707	0.1898292056
H	1.2549297756	-4.6511721052	0.0699632326
H	3.3593890107	-3.4232343036	-0.4968826580
H	3.4054505964	-0.9715007061	-0.4732293701
H	-0.8682710158	3.4413796546	-0.1903278852
H	1.2545195549	4.6512657787	-0.0703850921
H	3.4052649154	0.9718453449	0.4736835195
H	3.3589866488	3.4235933020	0.4970283321
H	-2.8213034337	-2.2761343786	0.0602157094
H	-2.8214963389	2.2758888030	-0.0603803537

Ground state coordinates: M4

C	1.3142660379	-0.7093475050	0.2880333458
C	1.3142259835	0.7094516082	-0.2879290913
H	1.4310561575	-0.5929948137	1.3988073605
H	1.4311648925	0.5931324018	-1.3986918379
C	0.0107251224	-1.4687855072	0.0891201474
C	0.0604229845	-2.8788968199	0.1394675294
C	1.2517784430	-3.5658330966	0.0482338092
C	2.4735029332	-2.8586532131	-0.2177792495
C	2.5013257397	-1.5058889438	-0.1993138917
C	0.0105946039	1.4687686552	-0.0891687134
C	0.0601672638	2.8788800776	-0.1397483312
C	1.2514531741	3.5659300193	-0.0484696887
C	2.5011450065	1.5061308075	0.1995509119
C	2.4732009020	2.8588944032	0.2178437211
C	-1.1929776843	-0.7346724430	0.0215511406
C	-1.1930409883	0.7345617549	-0.0215478793
C	-2.5020010275	-1.2460191031	0.0266724222
C	-2.5021098814	1.2458019307	-0.0267798539
S	-3.6573620669	-0.0001571473	0.0001219916
H	-0.8679693720	-3.4414903707	0.1898292056
H	1.2549297756	-4.6511721052	0.0699632326
H	3.3593890107	-3.4232343036	-0.4968826580
H	3.4054505964	-0.9715007061	-0.4732293701
H	-0.8682710158	3.4413796546	-0.1903278852
H	1.2545195550	4.6512657787	-0.0703850921
H	3.4052649154	0.9718453449	0.4736835195
H	3.3589866488	3.4235933020	0.4970283321
H	-2.8213034337	-2.2761343786	0.0602157094
H	-2.8214963389	2.2758888030	-0.0603803537

Ground state coordinates: M5=M6

C	1.1037808765	0.1986729954	-0.6903006077
C	0.0932073025	1.3805887131	-0.8870950404
H	-0.1961351992	1.2617983721	-1.9536181867

C	0.5465536487	-1.1332426144	-0.6537289254
C	1.3983155525	-2.2278427086	-0.8562482169
C	2.7341334467	-2.0480418147	-1.1970013012
C	3.2605517173	-0.7592507490	-1.3681660635
C	2.4447991019	0.3384205649	-1.1693750063
C	-1.1779666139	1.1960779593	-0.0786742481
C	-1.8011486110	2.2824977092	0.5113928624
C	-1.2517082071	3.5689874013	0.4734951714
C	0.6787949278	2.7614318256	-0.7586549954
C	0.0092026162	3.7789910539	-0.1524408771
C	-0.8626492711	-1.2961888935	-0.3168749507
C	-1.7044530732	-0.1522195020	-0.0180436428
C	-1.5398469692	-2.4890455978	-0.1966703682
C	-2.9841183226	-0.5391835537	0.3183241880
S	-3.1815209849	-2.2579401949	0.2735499050
H	1.0100903711	-3.2363292292	-0.7581906047
H	3.3690767479	-2.9166618570	-1.3447828763
H	4.2979734589	-0.6240556379	-1.6568122377
H	2.8635763770	1.3329527230	-1.2654628169
H	-2.7231236214	2.1219145069	1.0637484490
H	-1.7605295310	4.3918294515	0.9638597026
H	1.6267659488	2.9638228025	-1.2448336835
H	0.4520309044	4.7711840495	-0.1325079966
H	-1.1674888071	-3.4919616044	-0.3470075938
H	-3.8281489159	0.0886934813	0.5641672899
H	1.3804599965	0.3394210279	0.5401468046
Cl	1.5978420082	0.6276425609	2.0646915167

Ground state coordinates: M7

C	-0.7656583892	0.4057696367	-0.9562725131
C	-0.3162415591	-1.0494002537	-1.1946854235
H	0.2127464369	-1.0021680895	-2.1724157068
C	0.1841851277	1.3496352151	-0.4986220916
C	-0.2012823936	2.6908736286	-0.3433863268
C	-1.4941549680	3.1108678767	-0.6410125298
C	-2.4343589959	2.1813419425	-1.0865398284
C	-2.0675594658	0.8397552908	-1.2365975803
C	0.7307704607	-1.4883068273	-0.1808244597
C	0.6678614686	-2.7319825871	0.4196206799
C	-0.3800654240	-3.6290639408	0.1653426126
C	-1.4279415116	-2.0526214484	-1.3604411826
C	-1.4244007436	-3.2593757655	-0.7292256746
C	1.5351967067	0.8866224738	-0.1494917089
C	1.7867245206	-0.5241669918	0.0619825920
C	2.6427311742	1.6549587843	0.1066635384
C	3.0765600144	-0.7624478671	0.4839161776
S	3.9940672965	0.6982098244	0.6135328558
H	0.5187386992	3.4085467518	0.0378205778
H	-1.7701754528	4.1530373424	-0.5122836740
H	-3.4501640470	2.4912892345	-1.3134848270
H	-2.8089938656	0.1304703164	-1.5882521421
H	1.4371487197	-3.0055682425	1.1375340930
H	-0.4092616495	-4.5895018918	0.6686980863
H	-2.2175933792	-1.8206361111	-2.0682176598
H	-2.2363884663	-3.9589063610	-0.9105172193
H	2.7466893470	2.7286789228	0.0380695470
H	3.5453227047	-1.7150079867	0.6863931929
H	-2.8250655876	0.4896737462	1.0681096987
Cl	-3.3718986080	0.3402341281	2.2323213325

Ground state coordinates: M8

C	1.2010758398	-0.8331792700	-0.2333111539
C	1.2515274464	0.6490015694	-0.6539297257
H	1.0067350249	0.6207194931	-1.7389639047
C	-0.0585567488	-1.4434550314	-0.0249820468
C	-0.1146757389	-2.8100248655	0.2927346634
C	1.0420993422	-3.5766991795	0.3955782020
C	2.2856666877	-2.9762876239	0.1967288422

C	2.3577688709	-1.6134993747	-0.1107129055
C	0.1388284172	1.4572616476	-0.0017118301
C	0.3835336906	2.7069819880	0.5363750310
C	1.6673730442	3.2718326343	0.5528083363
C	2.6004221794	1.3101655948	-0.5392070947
C	2.7654031248	2.5449868033	0.0109815224
C	-1.2707006234	-0.6145758389	-0.0970251763
C	-1.1679860212	0.8287049797	-0.0284750338
C	-2.5744565220	-1.0405088416	-0.1343546203
C	-2.4049891810	1.4350761639	-0.0034641148
S	-3.6916168108	0.2812623813	-0.0771932195
H	-1.0791634610	-3.2706243714	0.4835763007
H	0.9746526061	-4.6316217396	0.6434929935
H	3.1982848074	-3.5585968217	0.2832574113
H	3.3319546433	-1.1628359598	-0.2667743657
H	-0.4404555794	3.2506793597	0.9918716479
H	1.8280061302	4.2466064343	1.0007765324
H	3.4520922067	0.8024491920	-0.9810192040
H	3.7572661702	2.9887931938	0.0385905044
H	-2.9499103883	-2.0529898910	-0.1824899786
H	-2.6275960337	2.4925348773	0.0145762023

Ground state coordinates: M9

C	1.3015411738	-0.7359194216	-0.0010336169
C	1.2942456652	0.7413548982	-0.0015212543
C	0.0792114184	-1.4607374696	0.0012770124
C	0.1077470946	-2.8676644469	0.0027869912
C	1.3047723384	-3.5655672393	0.0005259800
C	2.5135618261	-2.8591791601	-0.0037133806
C	2.5047381221	-1.4724152779	-0.0042695019
C	0.0677978483	1.4597399837	-0.0032593005
C	0.0863318687	2.8679673304	-0.0037412232
C	1.2756524943	3.5785555322	-0.0005628702
C	2.4929500514	1.4901493751	0.0026777240
C	2.4912310666	2.8809997556	0.0052340449
C	-1.1820465047	-0.7261126762	0.0014850881
C	-1.1882192049	0.7168590317	-0.0025078912
C	-2.4565454849	-1.2498001614	0.0040190121
C	-2.4667387322	1.2319219833	-0.0030839450
S	-3.6563714149	-0.0136137988	0.0009628804
H	-0.8280719017	-3.4174682214	0.0043410373
H	1.3026336154	-4.6515209469	0.0004451421
H	3.4598440219	-3.3918379913	-0.0074825700
H	3.4581089443	-0.9572275612	-0.0092883942
H	-0.8544875884	3.4089426826	-0.0084877173
H	1.2643773182	4.6640960888	-0.0006800673
H	3.4497762878	0.9816070728	0.0230246443
H	3.4336489481	3.4205820469	0.0172646518
H	-2.7612685730	-2.2858824521	0.0074244685
H	-2.7800046822	2.2656178387	-0.0078444947

R1: benzene, R2=R3 : phenyl

Ground state coordinates: M1

C	1.4888823682	0.7373076990	1.1982220806
C	-1.1889043364	1.1121832907	-1.0851730234
H	0.7616984110	0.5251237946	1.9759998157
H	-0.3989489523	0.8970237791	-1.7975717203
C	2.3656341417	1.8145188669	1.3390937271
C	3.2952558021	2.0719694176	0.3360109130
C	3.3472479490	1.2657335661	-0.8033894299
C	2.4636425975	0.1896601541	-0.9381078187
C	1.5181676660	-0.0928167892	0.0737480547
C	0.6067586565	-1.2744021994	-0.0240997084
C	-0.8021761048	-1.1529992572	-0.0399975884
C	-1.5053667363	0.1602678055	-0.1022990788

C	-1.8884000398	2.3147830203	-1.1636583007
C	-2.9173156969	2.5928259070	-0.2614427851
C	-2.5460828627	0.4500023710	0.7944861078
C	-3.2440364804	1.6553410214	0.7185877174
C	1.1759477205	-2.5575918129	-0.0198296083
C	-1.5814646770	-2.3230343319	-0.0238728013
C	0.3892409882	-3.7055885534	-0.0129257555
C	-1.0006710578	-3.5874531962	-0.0084491468
H	2.3219665850	2.4400783295	2.2250095850
H	3.9875225865	2.9038841434	0.4291646332
H	4.0729290825	1.4842888200	-1.5774873516
H	-1.6318665229	3.0358100842	-1.9348182778
H	-3.4601324918	3.5316270443	-0.3234849948
H	-2.7979082393	-0.2724426841	1.5659704553
H	-4.0407380776	1.8620120643	1.4277390298
H	2.2578174967	-2.6449410358	-0.0081774824
H	-2.6627527835	-2.2260903957	-0.0516788783
H	0.8590004792	-4.6849400209	-0.0054106396
H	-1.6291713449	-4.4733722816	-0.0041097536
H	2.5024243848	-0.4023035174	-1.7825657526

Ground state coordinates: M3

C	0.7062446835	-1.2585940797	-0.2957809354
C	-0.7064642885	-1.2584727322	0.2957774961
H	0.5856493316	-1.3658026674	-1.4020705772
H	-0.5858861226	-1.3657048007	1.4020668579
C	1.5041839571	-2.4561434314	0.1709847174
C	2.8500004129	-2.4271604122	0.2126121795
C	3.5559217127	-1.1961007361	-0.0554979724
C	2.8795619662	-0.0133251457	-0.1574806566
C	1.4498576554	0.0530271054	-0.0905190769
C	0.7336180504	1.2495749337	-0.0035060351
C	-0.7334009303	1.2497023061	0.0035072963
C	-1.4498492926	0.0532788108	0.0905189827
C	-1.5046113838	-2.4558828090	-0.1709886546
C	-2.8504229282	-2.4266667292	-0.2126111873
C	-2.8795648271	-0.0128259787	0.1574830441
C	-3.5561295978	-1.1954844875	0.0555019836
C	1.3999612253	2.5303818493	0.0450064119
C	-1.3995201738	2.5306258600	-0.0450060047
C	0.7155018654	3.7065088922	0.0326550266
C	-0.7148554874	3.7066335122	-0.0326569438
H	0.9682278652	-3.3664064404	0.4202155097
H	3.4157657272	-3.3124876542	0.4900488632
H	4.6411242730	-1.2029113472	-0.0944145955
H	-0.9688128043	-3.3662384007	-0.4202206161
H	-3.4163430053	-3.3118956119	-0.4900458406
H	-3.4556853103	0.9005322840	0.2529665608
H	-4.6413332899	-1.2021063458	0.0944209710
H	2.4815981475	2.5590044080	0.0946033167
H	-2.4811519986	2.5594385116	-0.0946024760
H	1.2522724048	4.6499826921	0.0654514990
H	-1.2514609175	4.6502011410	-0.0654550803
H	3.4558399838	0.8999338637	-0.2529624204

Ground state coordinates: M4

C	1.2014261950	-0.5986709990	0.3287514615
C	1.2014511024	0.5986215870	-0.3288542677
H	1.1146831136	-0.4004937525	1.4274674509
H	1.1146395433	0.4004514064	-1.4275648152
C	2.4741850265	-1.4193989355	0.2697357124
C	2.4813072734	-2.7631657353	0.1176804569
C	1.2561134777	-3.4726992932	-0.0809488893
C	0.0435401804	-2.8145500974	-0.1212098568
C	-0.0547102315	-1.4189363881	0.0252522759
C	-1.2996479763	-0.7210048558	-0.0296818469



C	-1.2996215406	0.7210821994	0.0296241873
C	-0.0546402579	1.4189578777	-0.0252593291
C	2.4742454415	1.4192879423	-0.2698842577
C	2.4814399625	2.7630393816	-0.1176936945
C	0.0436917715	2.8145376427	0.1214023741
C	1.2563047418	3.4726228829	0.0811448752
C	-2.5493625269	-1.3977001684	-0.0796323264
C	-2.5493058884	1.3978285793	0.0795762894
C	-3.7386733145	-0.7049903415	-0.0428409041
C	-3.7386447886	0.7051602705	0.0428047380
H	3.4077013107	-0.9052569621	0.4639226243
H	3.4160566156	-3.3133278889	0.1459195923
H	1.2817578328	-4.5497066141	-0.2131606527
H	3.4077248849	0.9051193164	-0.4641783703
H	3.4162137074	3.3131597350	-0.1459628994
H	-0.8478431513	3.3986927624	0.3123518052
H	1.2820292390	4.5496078738	0.2135159495
H	-2.5803004284	-2.4792270038	-0.1155987364
H	-2.5801837980	2.4793585303	0.1155147732
H	-4.6795511744	-1.2444230871	-0.0704961436
H	-4.6794998159	1.2446324847	0.0704764031
H	-0.8480197668	-3.3987160967	-0.3120089701

Ground state coordinates: M5=M6

C	-0.9312477470	0.7439291850	-0.5011210610
C	-0.8209342331	-0.6806568372	-1.1352248973
H	-0.4022586726	-0.4890849253	-2.1456055656
C	-2.0517210801	1.5809441140	-0.9019918462
C	-1.9871388038	2.9480771220	-0.8477615825
C	-0.7647409494	3.5588413869	-0.4955055040
C	0.3762933268	2.8109962534	-0.2466577562
C	0.3639745815	1.4069015785	-0.3213324976
C	1.5561302331	0.5984304700	-0.1075966193
C	1.4600361710	-0.8323690726	-0.0727520450
C	0.2074555061	-1.4931092699	-0.3748695070
C	-2.1293114552	-1.3928302953	-1.3359017532
C	-2.3150128182	-2.6863291294	-0.9666696625
C	-0.0633589312	-2.8116581648	-0.0248475208
C	-1.2851428551	-3.4203678290	-0.3081905349
C	2.8132723534	1.2007159337	0.1321373374
C	2.6263248418	-1.5706588313	0.2366967717
C	3.9383329587	0.4497597082	0.4202187115
C	3.8379134682	-0.9496501392	0.4810421465
H	-2.9960606406	1.0939857199	-1.1160918715
H	-2.8595447901	3.5551881322	-1.0655561741
H	-0.7087270698	4.6418534148	-0.4286749352
H	-2.9191239470	-0.8650469683	-1.8606254097
H	-3.2666123334	-3.1713079398	-1.1657086203
H	0.6748840186	-3.3745134992	0.5367390682
H	-1.4668710896	-4.4417273491	0.0083502613
H	2.9127515807	2.2788396673	0.0934101859
H	2.5794119906	-2.6534273339	0.2471302875
H	4.8896033522	0.9409409736	0.5985484373
H	4.7161315014	-1.5492063421	0.7020826902
H	1.2899747415	3.3398626252	-0.0060986915
H	-1.2253899797	0.5263267661	0.5362456639
Cl	-1.7138954052	0.0327120216	2.2105516457

Ground state coordinates: M7

C	-0.6469606618	0.3462821993	-0.9816637580
C	-0.0917610630	-1.0684369021	-1.2100607976
H	0.5029557623	-0.9802365707	-2.1454505358
C	-1.9665125892	0.6952029240	-1.2902319972
C	-2.4284327902	2.0032720331	-1.1101475935
C	-1.5669039696	2.9742491397	-0.5992151653
C	-0.2558245914	2.6333682412	-0.2777716483
C	0.2323750573	1.3292863264	-0.4732087506
C	1.6160601533	0.9556150525	-0.1049935583

C	1.9171385871	-0.4110917944	0.1515203680
C	0.8961680673	-1.4186834811	-0.1124715816
C	-1.1264875042	-2.1356563968	-1.4477700955
C	-1.1415290067	-3.3049773395	-0.7504826265
C	0.8163656565	-2.6282872761	0.5531167382
C	-0.1794874254	-3.5742932351	0.2640552761
C	2.6248506126	1.9151583993	0.0722176498
C	3.1995517107	-0.7496761562	0.6251781737
C	3.8907974086	1.5591996059	0.5276573769
C	4.1750753470	0.2206651965	0.8182738487
H	-2.6449969109	-0.0541293482	-1.6840185257
H	-3.4548815886	2.2545385918	-1.3613157392
H	-1.9183135263	3.9888047454	-0.4373034407
H	-1.8459628028	-1.9712661386	-2.2442903799
H	-1.8998403723	-4.0516814768	-0.9714487090
H	1.5272069074	-2.8396054056	1.3474616902
H	-0.2235561804	-4.5037237148	0.8217615346
H	2.4220933893	2.9556817880	-0.1599507237
H	3.4381908792	-1.7939009996	0.8019173576
H	4.6556523332	2.3204574574	0.6494690708
H	5.1626341937	-0.0653935141	1.1684838199
H	0.3903268233	3.3871578564	0.1595933251
H	-3.0331922687	0.4104192012	0.9646623163
Cl	-3.6979538019	0.2879822534	2.0686128108

Ground state coordinates: M8

C	1.3081948009	-0.5956212141	-0.1830897680
C	1.0417658184	0.8760154225	-0.4994772575
H	0.8131740492	0.8766651541	-1.5945731539
C	2.6145422871	-1.0756824759	-0.1364753943
C	2.8518132559	-2.4202206181	0.1357433056
C	1.7955471170	-3.2896246260	0.3710327451
C	0.4775807340	-2.8245339767	0.3286219460
C	0.1967556831	-1.4547916820	0.0105302208
C	-1.1652168098	-0.9050601878	-0.0680564916
C	-1.3700517791	0.5169059128	0.0470187175
C	-0.2498633154	1.4006278026	0.0484266120
C	2.2002480550	1.8123251845	-0.4518602561
C	2.0652288345	3.0992397123	-0.0473658803
C	-0.3170415762	2.7491413891	0.4521995824
C	0.7983878208	3.5610721623	0.4192438578
C	-2.3147595499	-1.7033052274	-0.2283458684
C	-2.6903128377	1.0423047161	0.0946490575
C	-3.5906171762	-1.1548995748	-0.2120721632
C	-3.7900218263	0.2220865080	-0.0268872698
H	3.4618247535	-0.4184272203	-0.2758573357
H	3.8713112141	-2.7877666248	0.1906393261
H	2.0009077149	-4.3268983708	0.5987119492
H	-0.5712997172	-3.6313066690	0.5980074250
H	3.1528146873	1.4615689947	-0.8299366050
H	2.9105982056	3.7783090997	-0.0629190322
H	-1.2411632504	3.1499530963	0.8492088989
H	0.7109857633	4.5863891169	0.7674357070
H	-2.2063435484	-2.7665415824	-0.3648977382
H	-2.8381987062	2.1131075902	0.1624429836
H	-4.4463338047	-1.8090392747	-0.3479963976
H	-4.7913545781	0.6381113255	-0.0132801999

Ground state coordinates: M9

C	0.6944957728	-1.2680251696	0.0048812888
C	-0.7715919345	-1.2188455999	0.0037188580
C	1.3928559864	-2.4964381540	0.0159560008
C	2.7751267106	-2.5502658095	0.0106515815
C	3.5139416682	-1.3600865930	-0.0076841956
C	2.8540967278	-0.1443083292	-0.0151921072
C	1.4435567730	-0.0601728831	-0.0058563433
C	0.7515878365	1.2333572750	-0.0035848327
C	-0.6687305163	1.2809115920	0.0020350030

C	-1.4429676709	0.0347334101	0.0007923141
C	-1.5528417941	-2.4003986730	-0.0006042008
C	-2.9395062277	-2.3629459087	-0.0053910824
C	-2.8565429219	0.0418398346	-0.0049997376
C	-3.5982221668	-1.1264859728	-0.0057057821
C	1.4654761917	2.4529138729	-0.0037714016
C	-1.3020983325	2.5440201109	0.0078437817
C	0.8210624851	3.6769252992	0.0011244992
C	-0.5791414779	3.7233282778	0.0072969155
H	0.8461966567	-3.4314997481	0.0305966044
H	3.2799880146	-3.5115835756	0.0206959639
H	4.5995282537	-1.3873303621	-0.0141999410
H	-1.0685947838	-3.3693691456	-0.0185219262
H	-3.5056625213	-3.2894508313	-0.0124270369
H	-3.3903536388	0.9839785075	-0.0062067688
H	-4.6828846962	-1.0815043444	-0.0075575852
H	2.5483782620	2.4458981769	-0.0059410984
H	-2.3831256089	2.6080623986	0.0153730022
H	1.4014379967	4.5948119152	0.0022874964
H	-1.0977752945	4.6774062185	0.0130522174
H	3.4495247032	0.7602413134	-0.0262142844

R1 : benzene, R2=R3 : 3-pyridine

Ground state coordinates: M1

C	1.2789869495	1.0405852716	1.0791220992
C	-1.2762722725	1.0403514960	-1.0756807063
H	0.4444171501	0.9163972039	1.7612141543
H	-0.4422919094	0.9152061970	-1.7583702038
N	2.0929341071	2.1674700332	1.1759795361
C	3.1732649255	2.3346635763	0.3069304423
C	3.4349515587	1.3624462102	-0.6587029957
C	2.6226610124	0.2322986149	-0.7523742327
C	1.5303769763	0.0539586699	0.1117588494
C	0.7065453321	-1.1879646405	0.0279160369
C	-0.7098748931	-1.1887018557	-0.0263399515
C	-1.5321453093	0.0536670525	-0.1094350358
N	-2.0866757636	2.1695275853	-1.1740206001
C	-3.1691107127	2.3387380133	-0.3083037355
C	-2.6277960929	0.2333129496	0.7504421945
C	-3.4371155150	1.3656243235	0.6547624054
C	1.3807466704	-2.4206770199	0.0408486438
C	-1.3822322708	-2.4225090150	-0.0397775637
C	0.6970628058	-3.6333444459	0.0161652245
C	-0.6963348741	-3.6341320274	-0.0176585925
H	3.8046893800	3.2151192076	0.3825761993
H	4.2701044962	1.4834100545	-1.3428613114
H	-3.7981319315	3.2208219792	-0.3849002994
H	-2.8335690369	-0.5166195165	1.5089755621
H	-4.2747330332	1.4876040884	1.3357087936
H	2.4649185941	-2.4163559852	0.1030079600
H	-2.4665292012	-2.4198322062	-0.1005454841
H	1.2492553940	-4.5683857711	0.0336000536
H	-1.2474144808	-4.5698227559	-0.0368994688
H	2.8231904325	-0.5164288654	-1.5132570003

Ground state coordinates: M2

C	1.1744935859	-0.6387051008	0.6219383274
C	1.1743558258	0.6388072030	-0.6218667223
H	1.0810636843	0.0510391135	1.4566107928
H	1.0809530396	-0.0510199361	-1.4564718394
N	2.4005502760	-1.3906844534	0.6441434790
C	2.5033855975	-2.6465516403	0.0718681611
C	1.3617657862	-3.2856139501	-0.4269274751
C	0.1167453451	-2.6503908445	-0.3136166954
C	-0.0181053683	-1.3950395144	0.2674292604

C	-1.3156280308	-0.6840356837	0.1970981022
C	-1.3157231658	0.6839418891	-0.1970448272
C	-0.0182795660	1.3950706292	-0.2673996327
N	2.4003884270	1.3908185489	-0.6440826389
C	2.5031371297	2.6467335198	-0.0718959938
C	0.1164775607	2.6504874587	0.3135342105
C	1.3614674702	3.2857762237	0.4268122953
C	-2.5359116210	-1.3257223779	0.4183625387
C	-2.5360727012	1.3254897100	-0.4183383843
C	-3.7505681460	-0.6612777755	0.2157275208
C	-3.7506542071	0.6609056801	-0.2157206162
H	3.4652894179	-3.1516329397	0.0440298527
H	1.4310892611	-4.2702427970	-0.8782030117
H	3.4650134423	3.1518673596	-0.0440495086
H	-0.7706678838	3.1453108033	0.6994943315
H	1.4307385848	4.2704406233	0.8780199914
H	-2.5352502805	-2.3554340059	0.7639026083
H	-2.5355060588	2.3551991060	-0.7638857717
H	-4.6870398741	-1.1824850024	0.3914166314
H	-4.6871911817	1.1819880623	-0.3914281201
H	-0.7703760409	-3.1452216133	-0.6996222533

Ground state coordinates: M3

C	0.7064974144	-1.2734660435	-0.2953942306
C	-0.7065351948	-1.2734469843	0.2953907362
H	0.5865154725	-1.3806833559	-1.4017497219
H	-0.5865549126	-1.3806703289	1.4017459454
N	1.5042677457	-2.4709576215	0.1718082180
C	2.8500591093	-2.4418771612	0.2141724293
C	3.5560379434	-1.2107663757	-0.0535512730
C	2.8796484928	-0.0280397584	-0.1559042494
C	1.4499029384	0.0382089769	-0.0897253620
C	0.7335291740	1.2347049434	-0.0031044731
C	-0.7334934317	1.2347260989	0.0031057495
C	-1.4499026936	0.0382507330	0.0897252493
N	-1.5043399447	-2.4709148436	-0.1718122435
C	-2.8501306134	-2.4417962049	-0.2141715245
C	-2.8796498829	-0.0279575729	0.1559066167
C	-3.5560730934	-1.2106650634	0.0535552313
C	1.3997529550	2.5155601009	0.0457727076
C	-1.3996787584	2.5156014204	-0.0457722489
C	0.7152153057	3.6916375836	0.0330465829
C	-0.7151060835	3.6916586415	-0.0330484154
H	3.4157365574	-3.3271634392	0.4919188249
H	4.6412621359	-1.2174984143	-0.0918738046
H	-3.4158346314	-3.3270660580	-0.4919159149
H	-3.4558886799	0.8853589740	0.2510746957
H	-4.6412974465	-1.2173654942	0.0918801271
H	2.4813604885	2.5442609732	0.0959617375
H	-2.4812853532	2.5443357587	-0.0959608444
H	1.2518994985	4.6351502448	0.0661368692
H	-1.2517617941	4.6351874160	-0.0661403389
H	3.4559125704	0.8852609736	-0.2510705509

Ground state coordinates: M4

C	1.2224914909	-0.6750862928	0.3844134512
C	1.2225004651	0.6750610810	-0.3844457210
H	1.1350144892	-0.4093718195	1.4613294529
H	1.1349928701	0.4093485167	-1.4613586979
N	2.4935938149	-1.4685241276	0.2897587403
C	2.4926162689	-2.8076360693	0.0995477380
C	1.2566668291	-3.5029210881	-0.1027853234
C	0.0459716545	-2.8395966554	-0.1281364148
C	-0.0407668264	-1.4445215813	0.0477094838
C	-1.2731727098	-0.7238551663	-0.0169869432
C	-1.2731553926	0.7238876228	0.0169827760
C	-0.0407309522	1.4445242071	-0.0477037194
N	2.4936239545	1.4684671985	-0.2898100890

C	2.4926844522	2.8075731465	-0.0995558747
C	0.0460468250	2.8395892349	0.1281939903
C	1.2567592403	3.5028834274	0.1028391619
C	-2.5263076744	-1.3972399762	-0.0525248435
C	-2.5262725684	1.3973044138	0.0525132199
C	-3.7158842477	-0.7058270790	-0.0280831106
C	-3.7158667224	0.7059214694	0.0280645143
H	3.4229738599	-3.3657301806	0.0955382152
H	1.2755372210	-4.5764534225	-0.2620798321
H	3.4230561310	3.3656439968	-0.0955568643
H	-0.8461265263	3.4149031525	0.3414369208
H	1.2756629560	4.5764086129	0.2621772112
H	-2.5572727627	-2.4792406521	-0.0608791949
H	-2.5572076468	2.4793061149	0.0608590315
H	-4.6562232598	-1.2466939875	-0.0421008708
H	-4.6561921136	1.2468123518	0.0420732457
H	-0.8462203973	-3.4148983472	-0.3413334848

Ground state coordinates: M5=M6

C	0.9646833808	-0.7803267836	-0.4927554067
C	0.9059368568	0.6584373065	-1.0886961538
H	0.5428215613	0.4837674716	-2.1240161614
N	2.0999009907	-1.6130093336	-0.7907360135
C	2.0398675218	-2.9816806945	-0.6610796815
C	0.8139305555	-3.5834129691	-0.3266475109
C	-0.3399035027	-2.8237995503	-0.1781970736
C	-0.3248739731	-1.4283865043	-0.3366179175
C	-1.5352756831	-0.6106557368	-0.2231735032
C	-1.4391828240	0.8166445910	-0.1809831514
C	-0.1606245684	1.4733859978	-0.3869972551
N	2.2279689879	1.3639879641	-1.2081857754
C	2.3977027601	2.6557954725	-0.8215360755
C	0.0948027210	2.7866550858	-0.0141314188
C	1.3358445373	3.3921125372	-0.2206233714
C	-2.8079191685	-1.2067384876	-0.0929302104
C	-2.6207401689	1.5614281679	0.0336809303
C	-3.9518434651	-0.4500124754	0.1039981303
C	-3.8527587282	0.9465819843	0.1790197001
H	2.9262541604	-3.5894221213	-0.8106907591
H	0.7603329610	-4.6603925949	-0.1959693150
H	3.3616329790	3.1367060974	-0.9635945037
H	-0.6742487188	3.3497274130	0.5046435402
H	1.5034384303	4.4111658892	0.1107748423
H	-2.9084791684	-2.2841312948	-0.1524409530
H	-2.5674255744	2.6441601652	0.0467718274
H	-4.9166505561	-0.9384926012	0.1977772854
H	-4.7430924984	1.5500631947	0.3294402565
H	-1.2643082586	-3.3356074185	0.0591267048
H	1.2391012154	-0.5396895996	0.7341062290
Cl	1.6075091829	-0.0612278037	2.6177966673

Ground state coordinates: M7

C	-0.7069856155	0.5191163911	-0.9604975083
C	-0.3135805006	-0.9338435320	-1.2679630311
H	0.2779673707	-0.8613250063	-2.2069847766
N	-1.9879948305	1.0239218201	-1.2110106967
C	-2.2958994508	2.3654841316	-0.9600038526
C	-1.3171833012	3.2109187188	-0.4390612583
C	-0.0430672288	2.7139014349	-0.1742863992
C	0.2904260435	1.3743470659	-0.4371441839
C	1.6296380127	0.8290086042	-0.1206219884
C	1.7742246093	-0.5724240712	0.0805001048
C	0.6413230837	-1.4454305323	-0.2060917924
N	-1.4599786823	-1.8686512209	-1.5448653087
C	-1.5933133660	-3.0662238355	-0.9109905103
C	0.4364981180	-2.6719428124	0.3994336933
C	-0.6574271713	-3.4897365164	0.0749497388
C	2.7460598143	1.6584993279	0.0667378005

C	3.0169605574	-1.0737045666	0.5137840117
C	3.9705624638	1.1417400179	0.4797536478
C	4.1020655212	-0.2303465290	0.7181047403
H	-3.2959433812	2.7376909044	-1.1619405768
H	-1.5484690985	4.2494649170	-0.2223152124
H	-2.4284972428	-3.7156498385	-1.1601327030
H	1.1277329892	-3.0007922757	1.1708366177
H	-0.7975961697	-4.4364965782	0.5856195175
H	2.6610567089	2.7237385716	-0.1228343514
H	3.1365205164	-2.1442583919	0.6489045279
H	4.8209812363	1.8044769785	0.6097036498
H	5.0558439854	-0.6417868363	1.0354647787
H	0.6946660771	3.3712294291	0.2734958288
H	-2.5829261305	0.5184417863	1.0795478106
Cl	-3.1216077535	0.1960113156	2.2130675088

Ground state coordinates: M8

C	1.4118793992	0.3884206479	-0.1662247149
C	0.2942015539	1.3857006124	-0.4451609155
H	0.1547316840	1.3119402302	-1.5558809760
N	2.7517181946	0.7822630461	-0.1281731620
C	3.7610507992	-0.1487525358	0.1021506644
C	3.4382267382	-1.4944700692	0.2914331462
C	2.1125928337	-1.8970925221	0.2433165753
C	1.0737195065	-0.9745636855	0.0006428744
C	-0.3302873802	-1.4015957208	-0.0539811203
C	-1.3891399426	-0.4349486050	-0.0073891394
C	-1.0730185527	0.9619052823	0.0003021899
N	0.6033126008	2.8373153635	-0.3244535263
C	-0.3443334750	3.7459531256	0.0177736883
C	-2.0070396028	1.9628475116	0.3322534707
C	-1.6551991432	3.2982603960	0.3511684659
C	-0.6867875061	-2.7599078517	-0.1152116048
C	-2.7403103580	-0.8766977689	0.0181708231
C	-2.0145596827	-3.1627149798	-0.0982248650
C	-3.0523214139	-2.2183905384	-0.0244993790
H	4.7937470301	0.1802432231	0.1523982618
H	4.2181375188	-2.2233141159	0.4842840047
H	1.8803612293	-2.9406699561	0.4153894678
H	-0.1121668161	4.8045814381	0.0531764724
H	-3.0078165439	1.6867926412	0.6386252010
H	-2.4016444442	4.0320522506	0.6417037159
H	0.0809920497	-3.5189039019	-0.1921251903
H	-3.5450138663	-0.1518122313	0.0250237505
H	-2.2509071228	-4.2208706768	-0.1501042990
H	-4.0876789267	-2.5408075616	-0.0232245454

Ground state coordinates: M9

C	0.7332237740	-1.2600024454	0.0011547749
C	-0.7335905887	-1.2601127333	0.0010182255
N	1.4726920546	-2.4641974715	0.0029181747
C	2.8555320717	-2.4737899265	0.0017969197
C	3.5558968323	-1.2607958600	-0.0012932486
C	2.8563161567	-0.0677299012	-0.0026159443
C	1.4440090685	-0.0292440749	-0.0010941540
C	0.7108103594	1.2414605031	-0.0010329480
C	-0.7103343772	1.2413493999	0.0005412595
C	-1.4440460460	-0.0289209801	0.0000032518
N	-1.4733132698	-2.4641801012	0.0009266651
C	-2.8562237822	-2.4729073875	-0.0006029045
C	-2.8564542182	-0.0667241119	-0.0019355159
C	-3.5562613974	-1.2596231131	-0.0022795247
C	1.3841358838	2.4837274005	-0.0016528930
C	-1.3832934795	2.4838750348	0.0026773862
C	0.7007843308	3.6861158341	-0.0002298385
C	-0.6998201575	3.6861724713	0.0022808025
H	3.3909078309	-3.4185358759	0.0032354236
H	4.6417649127	-1.2525759205	-0.0025061941

H	-3.3928870400	-3.4169241929	-0.0010262669
H	-3.4220260207	0.8568647242	-0.0036897215
H	-4.6421448020	-1.2509442513	-0.0040319050
H	2.4667789768	2.5114326180	-0.0029514367
H	-2.4659103236	2.5120943387	0.0052144191
H	1.2513009123	4.6221256792	-0.0007457207
H	-1.2498296635	4.6224536895	0.0041057440
H	3.4222871406	0.8555515416	-0.0049321123

R1 : benzene, R2=R3 : 2-thiophene

Ground state coordinates: M1

C	1.2796640953	-1.0564874891	1.2677588150
C	-1.2796640953	1.0564874891	1.2677588150
H	0.4140440763	-1.7036838104	1.3393163673
H	-0.4140440763	1.7036838104	1.3393163673
C	1.4988395270	-0.2328136010	0.1904132827
S	2.9960813655	0.6596137125	0.4128059344
C	3.2902015921	-0.0972184499	1.9441505169
C	2.2962997257	-0.9810793717	2.2632353565
C	0.7066370787	-0.0779671264	-1.0463970721
C	-0.7066370787	0.0779671264	-1.0463970721
C	-1.4988395270	0.2328136010	0.1904132827
S	-2.9960813655	-0.6596137125	0.4128059344
C	-3.2902015921	0.0972184499	1.9441505169
C	-2.2962997257	0.9810793717	2.2632353565
C	1.3771501903	-0.1250354408	-2.2813373188
C	0.6946721315	-0.0557225536	-3.4922303317
C	-0.6946721315	0.0557225536	-3.4922303317
C	-1.3771501903	0.1250354408	-2.2813373188
H	4.1733499746	0.1574739210	2.5132915113
H	2.2889700140	-1.5655847609	3.1761390236
H	-4.1733499746	-0.1574739210	2.5132915113
H	-2.2889700140	1.5655847609	3.1761390236
H	2.4550886420	-0.2533482660	-2.2803399327
H	1.2452229740	-0.1032986993	-4.4268343050
H	-1.2452229740	0.1032986993	-4.4268343050
H	-2.4550886420	0.2533482660	-2.2803399327

Ground state coordinates: M2

C	0.6228427711	-0.5922894176	1.2914971855
C	-0.6228427711	0.5922894176	1.2914971855
H	-0.0054511136	-1.4842762284	1.3324509831
H	0.0054511136	1.4842762284	1.3324509831
C	1.3556324864	-0.3580404785	0.0789039336
S	2.8267843458	0.5266276942	0.4076669322
C	2.6668646491	0.2673429972	2.1251132707
C	1.5220038160	-0.3862030713	2.4379382598
C	0.6842645874	-0.2282674081	-1.2174898799
C	-0.6842645874	0.2282674081	-1.2174898799
C	-1.3556324864	0.3580404785	0.0789039336
S	-2.8267843458	-0.5266276942	0.4076669322
C	-2.6668646491	-0.2673429972	2.1251132707
C	-1.5220038160	0.3862030713	2.4379382598
C	1.3068855935	-0.4766100126	-2.4357163537
C	0.6497386720	-0.2380038474	-3.6569528053
C	-0.6497386720	0.2380038474	-3.6569528053
C	-1.3068855935	0.4766100126	-2.4357163537
H	3.4595628044	0.5798285474	2.7919027159
H	1.2482362740	-0.6536848676	3.4526557160
H	-3.4595628044	-0.5798285474	2.7919027159
H	-1.2482362740	0.6536848676	3.4526557160
H	2.3173465371	-0.8750063751	-2.4361760043
H	1.1682144161	-0.4285106062	-4.5918221064
H	-1.1682144161	0.4285106062	-4.5918221064
H	-2.3173465371	0.8750063751	-2.4361760043

Ground state coordinates: M3

C	0.6564654044	-0.3892379264	1.3692535600
C	-0.6564654044	0.3892379264	1.3692535600
H	0.3952580487	-1.4698337718	1.3705674857
H	-0.3952580487	1.4698337718	1.3705674857
C	1.3999445523	-0.0911539385	0.0731886305
S	3.1504594480	-0.0042163406	0.3418094360
C	2.8979684241	0.0319250766	2.1024503036
C	1.6297460518	-0.1274799321	2.4914702070
C	0.7421696965	0.0388002097	-1.1156735731
C	-0.7421696965	-0.0388002097	-1.1156735731
C	-1.3999445523	0.0911539385	0.0731886305
S	-3.1504594480	0.0042163406	0.3418094360
C	-2.8979684241	-0.0319250766	2.1024503036
C	-1.6297460518	0.1274799321	2.4914702070
C	1.4050954395	0.1905743131	-2.3944297730
C	0.7136515355	0.1152113099	-3.5595170895
C	-0.7136515355	-0.1152113099	-3.5595170895
C	-1.4050954395	-0.1905743131	-2.3944297730
H	3.7657341408	0.1615750888	2.7377321790
H	1.3301451470	-0.1531995629	3.5338963366
H	-3.7657341408	-0.1615750888	2.7377321790
H	-1.3301451470	0.1531995629	3.5338963366
H	2.4813793083	0.3399648722	-2.4030483739
H	1.2320818803	0.2132445014	-4.5085521935
H	-1.2320818803	-0.2132445014	-4.5085521935
H	-2.4813793083	-0.3399648722	-2.4030483739

Ground state coordinates: M4

C	0.6584995341	-0.3998726593	1.3710500067
C	-0.6584995341	0.3998726593	1.3710500067
H	0.3858371092	-1.4732959118	1.3392004199
H	-0.3858371092	1.4732959118	1.3392004199
C	1.4003790163	-0.1002682225	0.0835751994
S	3.0965605661	0.0786329077	0.3474725251
C	2.8904096340	-0.0081676025	2.1137054124
C	1.6268657978	-0.2039318099	2.5023012313
C	0.7299610169	0.0087893976	-1.1416437781
C	-0.7299610169	-0.0087893976	-1.1416437781
C	-1.4003790163	0.1002682225	0.0835751994
S	-3.0965605661	-0.0786329077	0.3474725251
C	-2.8904096340	0.0081676025	2.1137054124
C	-1.6268657978	0.2039318099	2.5023012313
C	1.4083311003	0.0779224162	-2.3934442047
C	0.7090420818	0.0481717578	-3.5758769697
C	-0.7090420818	-0.0481717578	-3.5758769697
C	-1.4083311003	-0.0779224162	-2.3934442047
H	3.7741034597	0.0892922586	2.7315177831
H	1.3344789917	-0.3077925406	3.5409336178
H	-3.7741034597	-0.0892922586	2.7315177831
H	-1.3344789917	0.3077925406	3.5409336178
H	2.4930350703	0.1182547113	-2.4092620024
H	1.2421687565	0.0839548904	-4.5199516028
H	-1.2421687565	-0.0839548904	-4.5199516028
H	-2.4930350703	-0.1182547113	-2.4092620024

Ground state coordinates: M5=M6

C	1.1398750413	0.5564016377	-0.5460735764
C	-0.1192799352	1.2861766524	-1.0177692087
H	1.1811965017	0.8831356686	0.6794463311
H	-0.1725951399	1.1258793305	-2.1172610630
C	1.0135050971	-0.8641328213	-0.4516339877
S	2.5653761114	-1.6337832053	-0.5649063563
C	3.3548330384	-0.1149121703	-0.9519915836
C	2.4929333778	0.9253863087	-0.9566617808
C	-0.2255171406	-1.5319998080	-0.2031802956



C	-1.4231924993	-0.7213330701	-0.1128431876
C	-1.3466060149	0.6493449054	-0.4042766098
S	-2.5939591236	1.8364990337	-0.0859574501
C	-1.4566035935	3.1651071547	-0.4009527705
C	-0.2444944608	2.7712451232	-0.7989163349
C	-0.3153242329	-2.9218112837	0.0215987099
C	-1.5164961828	-3.5175304728	0.3590986697
C	-2.6779413223	-2.7250743521	0.4988680912
C	-2.6332847780	-1.3664781656	0.2765493040
H	4.4234366252	-0.1046222091	-1.1165925164
H	2.7977511539	1.9507397933	-1.1290912171
H	-1.8021755094	4.1789247249	-0.2455135068
H	0.5567807361	3.4617988576	-1.0349458539
H	0.5813603866	-3.5304455387	-0.0564030447
H	-1.5643589430	-4.5876408459	0.5311017333
H	-3.6168612049	-3.1929342617	0.7789847649
H	-3.5369125037	-0.7727971098	0.3760503627
Cl	1.2046866623	1.4740427767	2.1548204218

Ground state coordinates: M7

C	1.0811314267	0.4937773810	-0.9135530833
C	-0.1960038698	1.2682909731	-1.2007727491
H	1.3420362553	0.8793429145	1.4803817295
H	-0.3659137639	1.1746009287	-2.2987691140
C	0.9924204296	-0.8375512664	-0.5400883807
S	2.5868577716	-1.5510908799	-0.4256053208
C	3.3415289249	-0.0616386578	-0.8996126530
C	2.4251448379	0.9282675344	-1.1271522184
C	-0.2525479592	-1.5321625253	-0.2576819868
C	-1.4542241409	-0.7379259218	-0.1900865968
C	-1.3784339376	0.6398697308	-0.4983736592
S	-2.5785982843	1.8499488001	-0.0637796540
C	-1.4186615425	3.1560823483	-0.3877220382
C	-0.2536639639	2.7488636849	-0.9018430821
C	-0.3197999645	-2.9025782992	0.0218417692
C	-1.5194630271	-3.5074460263	0.3882292522
C	-2.6865679168	-2.7337290335	0.4962126981
C	-2.6548898656	-1.3780309731	0.2182724888
H	4.4188827785	-0.0037012826	-0.9676956733
H	2.6984148085	1.9322624238	-1.4309925953
H	-1.7179952775	4.1724996268	-0.1640034291
H	0.5470670589	3.4276620906	-1.1741116399
H	0.5843753786	-3.5027995312	-0.0383043506
H	-1.5473524679	-4.5719154476	0.5984076655
H	-3.6213825680	-3.2005326017	0.7922309915
H	-3.5662369985	-0.7910230750	0.2898148133
Cl	1.5800080243	1.3198437373	2.6763048608

Ground state coordinates: M8

C	0.7944362087	-1.3533556040	0.1392111712
C	-0.6744021293	-1.4020772893	0.4302287437
H	-0.7138251494	-1.3747070379	1.5478466411
C	1.3985404069	-0.1043888548	0.0369290968
S	3.1230195578	-0.2728884538	-0.1795313982
C	3.0001499650	-1.9932261696	-0.1086231795
C	1.7107443547	-2.4313193807	0.0711728370
C	0.6798194769	1.1405913181	0.0734085835
C	-0.7661175887	1.1195158760	0.1034113342
C	-1.4105827534	-0.1340213163	0.1196063643
S	-3.0600403225	-0.4453344169	-0.2207770865
C	-2.8176256130	-2.2040443436	-0.1928389068
C	-1.5594690407	-2.5625974475	0.0893845978
C	1.3213610342	2.3940053458	0.0267741725
C	0.5881922166	3.5681730385	-0.0014708280
C	-0.8251468232	3.5500295546	0.0104306591
C	-1.4884080446	2.3465315678	0.0560890503
H	3.8919732660	-2.5955781580	-0.2199564480
H	1.4442446818	-3.4793103356	0.1344348571

H	-3.6711618000	-2.8384008862	-0.3954097259
H	-1.2287520978	-3.5914051898	0.1669171468
H	2.4054458540	2.4404549115	0.0107610876
H	1.1091122003	4.5200028101	-0.0360107209
H	-1.3797597312	4.4816436575	-0.0095253884
H	-2.5738950089	2.3259683903	0.0835961294

Ground state coordinates: M9

C	0.7203905805	-1.3709539284	0.0103922910
C	-0.7160951612	-1.3717007892	0.0165494034
C	1.3900792664	-0.1430413507	0.0022375811
S	3.1253258776	-0.3825472435	-0.0096710313
C	2.9266781636	-2.1127345636	-0.0016725844
C	1.6187045976	-2.4903143117	0.0087234541
C	0.7164197566	1.1228348799	0.0030471996
C	-0.7167673873	1.1236076829	0.0108602330
C	-1.3900630188	-0.1428479044	0.0152850430
S	-3.1264889070	-0.3843345350	-0.0113410941
C	-2.9254503258	-2.1146838062	-0.0132108866
C	-1.6171613321	-2.4922860929	0.0025731592
C	1.3974371857	2.3629918308	-0.0044850161
C	0.7037725608	3.5568962734	-0.0060571829
C	-0.7056782265	3.5570367392	0.0017506850
C	-1.3989837883	2.3629110203	0.0111491183
H	3.8020796437	-2.7475504915	-0.0052104337
H	1.2981212711	-3.5254395737	0.0141076320
H	-3.8000047300	-2.7506735172	-0.0207203053
H	-1.2973565998	-3.5275733994	0.0037119100
H	2.4837940378	2.3693714550	-0.0081397265
H	1.2453963631	4.4979061275	-0.0119011336
H	-1.2476999574	4.4978149049	0.0022839502
H	-2.4854187846	2.3699588738	0.0192071273

R1: benzene, R2=R3 : 2-pyrrole

Ground state coordinates: M1

C	1.3404771575	1.3375456643	0.9781887196
C	-1.3404597289	1.3375619721	-0.9781853748
H	0.5150466832	1.4091092399	1.6759199965
H	-0.5150290732	1.4091083965	-1.6759171704
C	1.5100701147	0.2602024216	0.1428993602
N	2.9513518126	0.4825870411	-0.8373448558
C	3.2901417206	2.0139292863	-0.0994277773
C	2.3507985416	2.3330238904	0.8422090335
C	0.7100256950	-0.9766069529	0.0356324091
C	-0.7100344642	-0.9765954107	-0.0356319529
C	-1.5100655829	0.2602152148	-0.1428980377
N	-2.9513467168	0.4826105953	0.8373445661
C	-3.2901225768	2.0139583501	0.0994262187
C	-2.3507785887	2.3330437460	-0.8422129053
C	1.3821522817	-2.2115477799	0.0425798777
C	0.6967434818	-3.4224370140	0.0141389495
C	-0.6967787826	-3.4224353497	-0.0141404274
C	-1.3821743472	-2.2115345837	-0.0425803014
H	4.1565115218	2.5830670751	-0.4063976580
H	2.3783855270	3.2459259719	1.4261079722
H	-4.1564907688	2.5831005612	0.4064019721
H	-2.3783630931	3.2459416645	-1.4261084634
H	2.4658205261	-2.2105589229	0.1062926240
H	1.2491513700	-4.3570476614	0.0287556201
H	-1.2491892069	-4.3570347023	-0.0287603213
H	-2.4658425891	-2.2105334407	-0.1062930550
H	-3.3940189117	-0.0536863174	1.5342480730
H	3.3940128151	-0.0537160462	-1.5342343101

## Ground state coordinates: M3

C	-0.3860297166	-0.6531401640	1.4990821555
C	0.3860297166	0.6531401640	1.4990821555
H	-1.4685697690	-0.3976154686	1.5323499571
H	1.4685697690	0.3976154686	1.5323499571
C	-0.1155308041	-1.3875640322	0.1882556569
N	-0.0596850059	-2.7486924202	0.4877280267
C	0.0568752064	-2.8984876636	1.8804800368
C	-0.0827985130	-1.7280011648	2.5245688227
C	0.0176460918	-0.7436452246	-1.0099724362
C	-0.0176460918	0.7436452246	-1.0099724362
C	0.1155308041	1.3875640322	0.1882556569
N	0.0596850059	2.7486924202	0.4877280267
C	-0.0568752064	2.8984876636	1.8804800368
C	0.0827985130	1.7280011648	2.5245688227
C	0.1298836179	-1.4103697022	-2.2882426633
C	0.0795378102	-0.7186118916	-3.4567595917
C	-0.0795378102	0.7186118916	-3.4567595917
C	-0.1298836179	1.4103697022	-2.2882426633
H	0.1993792098	-3.8900640011	2.2916153057
H	-0.1213007507	-1.5973043894	3.5971384094
H	-0.1993792098	3.8900640011	2.2916153057
H	0.1213007507	1.5973043894	3.5971384094
H	0.2155227438	-2.4946666983	-2.3104410968
H	0.1446777578	-1.2433746943	-4.4053739039
H	-0.1446777578	1.2433746943	-4.4053739039
H	-0.2155227438	2.4946666983	-2.3104410968
H	-0.3684679113	3.4090291082	-0.1438567446
H	0.3684679113	-3.4090291082	-0.1438567446

## Ground state coordinates: M4

C	-0.3940180750	-0.6569391385	1.4984487365
C	0.3940180750	0.6569391385	1.4984487365
H	-1.4712711769	-0.4001747881	1.4952719216
H	1.4712711769	0.4001747881	1.4952719216
C	-0.0960627631	-1.3815365924	0.1980202910
N	0.0654793006	-2.6875151710	0.5024106562
C	0.0520494314	-2.8881375471	1.9003293174
C	-0.1536107834	-1.7246002171	2.5369104023
C	0.0065455044	-0.7281457654	-1.0402574745
C	-0.0065455044	0.7281457654	-1.0402574745
C	0.0960627631	1.3815365924	0.1980202910
N	-0.0654793006	2.6875151710	0.5024106562
C	-0.0520494314	2.8881375471	1.9003293174
C	0.1536107834	1.7246002171	2.5369104023
C	0.0628790581	-1.4083063917	-2.2900206339
C	0.0388740483	-0.7098537884	-3.4730412773
C	-0.0388740483	0.7098537884	-3.4730412773
C	-0.0628790581	1.4083063917	-2.2900206339
H	0.1887887042	-3.8858510850	2.2929625937
H	-0.2493166437	-1.5912841111	3.6046932107
H	-0.1887887042	3.8858510850	2.2929625937
H	0.2493166437	1.5912841111	3.6046932107
H	0.0852141309	-2.4938733238	-2.3137461786
H	0.0661033034	-1.2434042387	-4.4170539691
H	-0.0661033034	1.2434042387	-4.4170539691
H	-0.0852141309	2.4938733238	-2.3137461786
H	-0.3039415453	3.4111046504	-0.1613383407
H	0.3039415453	-3.4111046504	-0.1613383407

## Ground state coordinates: M5=M6

C	-1.0535592427	0.3322808012	-0.9356018178
C	-0.6475624332	-1.0997195824	-1.2541146344
H	-0.3031063035	-1.1130311642	-2.3103160919
C	0.0280588342	1.2286934673	-0.6640157603
N	-0.4216580299	2.4856650122	-0.9133385947

C	-1.7139240423	2.4466257552	-1.4349202165
C	-2.1028259363	1.1453772342	-1.5357405169
C	1.3110356652	0.8313487474	-0.1550797370
C	1.5104062316	-0.5860429726	0.0659232025
C	0.5116047936	-1.4781298057	-0.3536754035
N	0.3396498342	-2.7963773363	0.0209797170
C	-0.9550376743	-3.2120059964	-0.3496562976
C	-1.5895765447	-2.2683070894	-1.0622654590
C	2.3212209385	1.7371365235	0.2069125522
C	3.4963327664	1.3038950142	0.8053630957
C	3.6776172612	-0.0708741274	1.0687893946
C	2.7123921735	-0.9920520902	0.7155753434
H	-2.2382535078	3.3628425909	-1.6623310760
H	-3.0648100879	0.7938908654	-1.8796292637
H	-1.2909968102	-4.2007112641	-0.0669860013
H	-2.5639409918	-2.3631566804	-1.5196368468
H	2.1807273859	2.8009474825	0.0288326495
H	4.2660000805	2.0185914512	1.0774329088
H	4.5938450001	-0.4099049628	1.5436078303
H	2.8897191057	-2.0491402545	0.8934142921
H	0.7774161150	-3.1586882398	0.8571207941
H	0.0659066784	3.3337307653	-0.6671648470
H	-1.5363735083	0.2259417149	0.3206157688
Cl	-2.1288502061	0.0104369197	1.7575284438

Ground state coordinates: M7

C	-0.8872472880	-0.0273870849	-1.0612063411
C	-0.2896386566	-1.4057156688	-1.1205994445
H	0.0020771216	-1.5931309758	-2.1795574943
C	-0.0851305012	1.0508389236	-0.7081846436
N	-0.8568711284	2.1911126033	-0.8246478070
C	-2.1240572023	1.8576465452	-1.2305274847
C	-2.1755035516	0.4808851061	-1.3943012839
C	1.2877075815	0.9656411418	-0.2482337091
C	1.7873509985	-0.3606829885	0.0317995704
C	0.9546698012	-1.4609486623	-0.2591800762
N	1.0256761987	-2.7342687394	0.2936606027
C	-0.2212546906	-3.3665038001	0.1225294984
C	-1.0427912985	-2.6394852224	-0.6532496379
C	2.0981372690	2.0722574282	0.0171884166
C	3.3685629542	1.9245737465	0.5778746612
C	3.8445349723	0.6417949809	0.8919135808
C	3.0718440892	-0.4785324846	0.6277441357
H	-2.8824923501	2.6123837366	-1.3766443876
H	-3.0243506043	-0.0779990946	-1.7653706018
H	-0.3853081629	-4.3381145324	0.5706197773
H	-2.0180525787	-2.9436387159	-1.0068847731
H	1.7346573643	3.0725632870	-0.2091857598
H	3.9811517943	2.7994266262	0.7718150590
H	4.8313551932	0.5227172614	1.3302874106
H	3.4710406621	-1.4675001010	0.8386403117
H	1.5661727151	-2.8927984619	1.1335996128
H	-0.5707267991	3.1140514700	-0.5396740897
H	-3.1045116920	0.5035116214	0.6984204257
Cl	-3.6650444128	0.5273134746	1.8758494993

Ground state coordinates: M8

C	1.4995246369	-0.7147349835	-0.1931344476
C	1.5259719804	0.7390512032	-0.5755788498
H	1.6476151813	0.7865877994	-1.6821728629
C	0.2782283534	-1.3608087811	-0.0461513728
N	0.5470117781	-2.6915320061	0.2113375493
C	1.9030263338	-2.8966244642	0.2407501944
C	2.5275789612	-1.6843854866	-0.0148494764
C	-1.0240317123	-0.7244846276	-0.0981525157
C	-1.0295482700	0.7199655299	-0.1250615010
C	0.2092001851	1.3890479878	-0.2054408022
N	0.4802242715	2.6981060461	0.1752547265

C	1.8664529299	2.8234514974	0.3908960040
C	2.5284054483	1.7168115090	0.0134395998
C	-2.2383747838	-1.4122410118	-0.0334074791
C	-3.4557333176	-0.7317958056	0.0386381901
C	-3.4671387615	0.6718649251	0.0554727926
C	-2.2809174746	1.3851673215	-0.0223337789
H	2.3177567117	-3.8751627016	0.4322343154
H	3.5942043553	-1.5345944107	-0.1171393661
H	2.2569190688	3.7544901733	0.7813103586
H	3.6022811088	1.5939095461	-0.0066305128
H	-2.2415446635	-2.5003457658	-0.0318941969
H	-4.3865622347	-1.2883055615	0.0846791446
H	-4.4118732412	1.2050140092	0.1137209820
H	-2.3089676512	2.4716069684	-0.0496510995
H	-0.1737697601	3.2018518862	0.7594535338
H	-0.1425782776	-3.3827791044	0.4594244304

Ground state coordinates: M9

C	1.5139682108	-0.7140051443	0.0023389617
C	1.5068417062	0.7158718340	0.0005829068
C	0.2738616108	-1.3779203544	0.0012355502
N	0.5404538693	-2.7322054873	0.0007425291
C	1.9027921170	-2.9333681525	-0.0021473145
C	2.5354039049	-1.7116801849	0.0008714978
C	-0.9988963074	-0.7203092386	0.0007211807
C	-1.0041512910	0.7152790429	0.0004159618
C	0.2671670216	1.3767317506	0.0020113819
N	0.5285639094	2.7355322033	0.0056938709
C	1.8840226922	2.9472493774	-0.0015744011
C	2.5264879391	1.7226452648	-0.0090345738
C	-2.2368890867	-1.4012328312	0.0003123823
C	-3.4358690029	-0.7112883131	-0.0000601652
C	-3.4401787043	0.6962019095	0.0002156726
C	-2.2441855862	1.3915042958	0.0005262484
H	2.3129852314	-3.9326703942	-0.0065653339
H	3.6041410936	-1.5527566182	-0.0000394972
H	2.2902663622	3.9481147939	0.0020588256
H	3.5959236078	1.5712747276	0.0373913352
H	-2.2520006345	-2.4885085347	-0.0007157325
H	-4.3748163741	-1.2568800475	-0.0003056215
H	-4.3819645222	1.2366901249	-0.0001501772
H	-2.2645985552	2.4788457123	0.0022379485
H	-0.1656796448	3.4629774616	-0.0436348420
H	-0.1496323601	-3.4644497742	-0.0138234426

R1 : benzene, R2=R3 : 3-pyridine

Ground state coordinates: M1

C	1.2789869495	1.0405852716	1.0791220992
C	-1.2762722725	1.0403514960	-1.0756807063
H	0.4444171501	0.9163972039	1.7612141543
H	-0.4422919094	0.9152061970	-1.7583702038
N	2.0929341071	2.1674700332	1.1759795361
C	3.1732649255	2.3346635763	0.3069304423
C	3.4349515587	1.3624462102	-0.6587029957
C	2.6226610124	0.2322986149	-0.7523742327
C	1.5303769763	0.0539586699	0.1117588494
C	0.7065453321	-1.1879646405	0.0279160369
C	-0.7098748931	-1.1887018557	-0.0263399515
C	-1.5321453093	0.0536670525	-0.1094350358
N	-2.0866757636	2.1695275853	-1.1740206001
C	-3.1691107127	2.3387380133	-0.3083037355
C	-2.6277960929	0.2333129496	0.7504421945
C	-3.4371155150	1.3656243235	0.6547624054
C	1.3807466704	-2.4206770199	0.0408486438
C	-1.3822322708	-2.4225090150	-0.0397775637

C	0.6970628058	-3.6333444459	0.0161652245
C	-0.6963348741	-3.6341320274	-0.0176585925
H	3.8046893800	3.2151192076	0.3825761993
H	4.2701044962	1.4834100545	-1.3428613114
H	-3.7981319315	3.2208219792	-0.3849002994
H	-2.8335690369	-0.5166195165	1.5089755621
H	-4.2747330332	1.4876040884	1.3357087936
H	2.4649185941	-2.4163559852	0.1030079600
H	-2.4665292012	-2.4198322062	-0.1005454841
H	1.2492553940	-4.5683857711	0.0336000536
H	-1.2474144808	-4.5698227559	-0.0368994688
H	2.8231904325	-0.5164288654	-1.5132570003

Ground state coordinates: M2

C	1.1744935859	-0.6387051008	0.6219383274
C	1.1743558258	0.6388072030	-0.6218667223
H	1.0810636843	0.0510391135	1.4566107928
H	1.0809530396	-0.0510199361	-1.4564718394
N	2.4005502760	-1.3906844534	0.6441434790
C	2.5033855975	-2.6465516403	0.0718681611
C	1.3617657862	-3.2856139501	-0.4269274751
C	0.1167453451	-2.6503908445	-0.3136166954
C	-0.0181053683	-1.3950395144	0.2674292604
C	-1.3156280308	-0.6840356837	0.1970981022
C	-1.3157231658	0.6839418891	-0.1970448272
C	-0.0182795660	1.3950706292	-0.2673996327
N	2.4003884270	1.3908185489	-0.6440826389
C	2.5031371297	2.6467335198	-0.0718959938
C	0.1164775607	2.6504874587	0.3135342105
C	1.3614674702	3.2857762237	0.4268122953
C	-2.5359116210	-1.3257223779	0.4183625387
C	-2.5360727012	1.3254897100	-0.4183383843
C	-3.7505681460	-0.6612777755	0.2157275208
C	-3.7506542071	0.6609056801	-0.2157206162
H	3.4652894179	-3.1516329397	0.0440298527
H	1.4310892611	-4.2702427970	-0.8782030117
H	3.4650134423	3.1518673596	-0.0440495086
H	-0.7706678838	3.1453108033	0.6994943315
H	1.4307385848	4.2704406233	0.8780199914
H	-2.5352502805	-2.3554340059	0.7639026083
H	-2.5355060588	2.3551991060	-0.7638857717
H	-4.6870398741	-1.1824850024	0.3914166314
H	-4.6871911817	1.1819880623	-0.3914281201
H	-0.7703760409	-3.1452216133	-0.6996222533

Ground state coordinates: M3

C	0.7064974144	-1.2734660435	-0.2953942306
C	-0.7065351948	-1.2734469843	0.2953907362
H	0.5865154725	-1.3806833559	-1.4017497219
H	-0.5865549126	-1.3806703289	1.4017459454
N	1.5042677457	-2.4709576215	0.1718082180
C	2.8500591093	-2.4418771612	0.2141724293
C	3.5560379434	-1.2107663757	-0.0535512730
C	2.8796484928	-0.0280397584	-0.1559042494
C	1.4499029384	0.0382089769	-0.0897253620
C	0.7335291740	1.2347049434	-0.0031044731
C	-0.7334934317	1.2347260989	0.0031057495
C	-1.4499026936	0.0382507330	0.0897252493
N	-1.5043399447	-2.4709148436	-0.1718122435
C	-2.8501306134	-2.4417962049	-0.2141715245
C	-2.8796498829	-0.0279575729	0.1559066167
C	-3.5560730934	-1.2106650634	0.0535552313
C	1.3997529550	2.5155601009	0.0457727076
C	-1.3996787584	2.5156014204	-0.0457722489
C	0.7152153057	3.6916375836	0.0330465829
C	-0.7151060835	3.6916586415	-0.0330484154
H	3.4157365574	-3.3271634392	0.4919188249
H	4.6412621359	-1.2174984143	-0.0918738046

H	-3.4158346314	-3.3270660580	-0.4919159149
H	-3.4558886799	0.8853589740	0.2510746957
H	-4.6412974465	-1.2173654942	0.0918801271
H	2.4813604885	2.5442609732	0.0959617375
H	-2.4812853532	2.5443357587	-0.0959608444
H	1.2518994985	4.6351502448	0.0661368692
H	-1.2517617941	4.6351874160	-0.0661403389
H	3.4559125704	0.8852609736	-0.2510705509

Ground state coordinates: M4

C	1.2224914909	-0.6750862928	0.3844134512
C	1.2225004651	0.6750610810	-0.3844457210
H	1.1350144892	-0.4093718195	1.4613294529
H	1.1349928701	0.4093485167	-1.4613586979
N	2.4935938149	-1.4685241276	0.2897587403
C	2.4926162689	-2.8076360693	0.0995477380
C	1.2566668291	-3.5029210881	-0.1027853234
C	0.0459716545	-2.8395966554	-0.1281364148
C	-0.0407668264	-1.4445215813	0.0477094838
C	-1.2731727098	-0.7238551663	-0.0169869432
C	-1.2731553926	0.7238876228	0.0169827760
C	-0.0407309522	1.4445242071	-0.0477037194
N	2.4936239545	1.4684671985	-0.2898100890
C	2.4926844522	2.8075731465	-0.0995558747
C	0.0460468250	2.8395892349	0.1281939903
C	1.2567592403	3.5028834274	0.1028391619
C	-2.5263076744	-1.3972399762	-0.0525248435
C	-2.5262725684	1.3973044138	0.0525132199
C	-3.7158842477	-0.7058270790	-0.0280831106
C	-3.7158667224	0.7059214694	0.0280645143
H	3.4229738599	-3.3657301806	0.0955382152
H	1.2755372210	-4.5764534225	-0.2620798321
H	3.4230561310	3.3656439968	-0.0955568643
H	-0.8461265263	3.4149031525	0.3414369208
H	1.2756629560	4.5764086129	0.2621772112
H	-2.5572727627	-2.4792406521	-0.0608791949
H	-2.5572076468	2.4793061149	0.0608590315
H	-4.6562232598	-1.2466939875	-0.0421008708
H	-4.6561921136	1.2468123518	0.0420732457
H	-0.8462203973	-3.4148983472	-0.3413334848

Ground state coordinates: M5=M6

C	0.9646833808	-0.7803267836	-0.4927554067
C	0.9059368568	0.6584373065	-1.0886961538
H	0.5428215613	0.4837674716	-2.1240161614
N	2.0999009907	-1.6130093336	-0.7907360135
C	2.0398675218	-2.9816806945	-0.6610796815
C	0.8139305555	-3.5834129691	-0.3266475109
C	-0.3399035027	-2.8237995503	-0.1781970736
C	-0.3248739731	-1.4283865043	-0.3366179175
C	-1.5352756831	-0.6106557368	-0.2231735032
C	-1.4391828240	0.8166445910	-0.1809831514
C	-0.1606245684	1.4733859978	-0.3869972551
N	2.2279689879	1.3639879641	-1.2081857754
C	2.3977027601	2.6557954725	-0.8215360755
C	0.0948027210	2.7866550858	-0.0141314188
C	1.3358445373	3.3921125372	-0.2206233714
C	-2.8079191685	-1.2067384876	-0.0929302104
C	-2.6207401689	1.5614281679	0.0336809303
C	-3.9518434651	-0.4500124754	0.1039981303
C	-3.8527587282	0.9465819843	0.1790197001
H	2.9262541604	-3.5894221213	-0.8106907591
H	0.7603329610	-4.6603925949	-0.1959693150
H	3.3616329790	3.1367060974	-0.9635945037
H	-0.6742487188	3.3497274130	0.5046435402
H	1.5034384303	4.4111658892	0.1107748423
H	-2.9084791684	-2.2841312948	-0.1524409530
H	-2.5674255744	2.6441601652	0.0467718274

H	-4.9166505561	-0.9384926012	0.1977772854
H	-4.7430924984	1.5500631947	0.3294402565
H	-1.2643082586	-3.3356074185	0.0591267048
H	1.2391012154	-0.5396895996	0.7341062290
Cl	1.6075091829	-0.0612278037	2.6177966673

Ground state coordinates: M7

C	-0.7069856155	0.5191163911	-0.9604975083
C	-0.3135805006	-0.9338435320	-1.2679630311
H	0.2779673707	-0.8613250063	-2.2069847766
N	-1.9879948305	1.0239218201	-1.2110106967
C	-2.2958994508	2.3654841316	-0.9600038526
C	-1.3171833012	3.2109187188	-0.4390612583
C	-0.0430672288	2.7139014349	-0.1742863992
C	0.2904260435	1.3743470659	-0.4371441839
C	1.6296380127	0.8290086042	-0.1206219884
C	1.7742246093	-0.5724240712	0.0805001048
C	0.6413230837	-1.4454305323	-0.2060917924
N	-1.4599786823	-1.8686512209	-1.5448653087
C	-1.5933133660	-3.0662238355	-0.9109905103
C	0.4364981180	-2.6719428124	0.3994336933
C	-0.6574271713	-3.4897365164	0.0749497388
C	2.7460598143	1.6584993279	0.0667378005
C	3.0169605574	-1.0737045666	0.5137840117
C	3.9705624638	1.1417400179	0.4797536478
C	4.1020655212	-0.2303465290	0.7181047403
H	-3.2959433812	2.7376909044	-1.1619405768
H	-1.5484690985	4.2494649170	-0.2223152124
H	-2.4284972428	-3.7156498385	-1.1601327030
H	1.1277329892	-3.0007922757	1.1708366177
H	-0.7975961697	-4.4364965782	0.5856195175
H	2.6610567089	2.7237385716	-0.1228343514
H	3.1365205164	-2.1442583919	0.6489045279
H	4.8209812363	1.8044769785	0.6097036498
H	5.0558439854	-0.6417868363	1.0354647787
H	0.6946660771	3.3712294291	0.2734958288
H	-2.5829261305	0.5184417863	1.0795478106
Cl	-3.1216077535	0.1960113156	2.2130675088

Ground state coordinates: M8

C	1.4118793992	0.3884206479	-0.1662247149
C	0.2942015539	1.3857006124	-0.4451609155
H	0.1547316840	1.3119402302	-1.5558809760
N	2.7517181946	0.7822630461	-0.1281731620
C	3.7610507992	-0.1487525358	0.1021506644
C	3.4382267382	-1.4944700692	0.2914331462
C	2.1125928337	-1.8970925221	0.2433165753
C	1.0737195065	-0.9745636855	0.0006428744
C	-0.3302873802	-1.4015957208	-0.0539811203
C	-1.3891399426	-0.4349486050	-0.0073891394
C	-1.0730185527	0.9619052823	0.0003021899
N	0.6033126008	2.8373153635	-0.3244535263
C	-0.3443334750	3.7459531256	0.0177736883
C	-2.0070396028	1.9628475116	0.3322534707
C	-1.6551991432	3.2982603960	0.3511684659
C	-0.6867875061	-2.7599078517	-0.1152116048
C	-2.7403103580	-0.8766977689	0.0181708231
C	-2.0145596827	-3.1627149798	-0.0982248650
C	-3.0523214139	-2.2183905384	-0.0244993790
H	4.7937470301	0.1802432231	0.1523982618
H	4.2181375188	-2.2233141159	0.4842840047
H	1.8803612293	-2.9406699561	0.4153894678
H	-0.1121668161	4.8045814381	0.0531764724
H	-3.0078165439	1.6867926412	0.6386252010
H	-2.4016444442	4.0320522506	0.6417037159
H	0.0809920497	-3.5189039019	-0.1921251903
H	-3.5450138663	-0.1518122313	0.0250237505
H	-2.2509071228	-4.2208706768	-0.1501042990



H -4.0876789267 -2.5408075616 -0.0232245454

Ground state coordinates: M9

C 0.7332237740 -1.2600024454 0.0011547749  
C -0.7335905887 -1.2601127333 0.0010182255  
N 1.4726920546 -2.4641974715 0.0029181747  
C 2.8555320717 -2.4737899265 0.0017969197  
C 3.5558968323 -1.2607958600 -0.0012932486  
C 2.8563161567 -0.0677299012 -0.0026159443  
C 1.4440090685 -0.0292440749 -0.0010941540  
C 0.7108103594 1.2414605031 -0.0010329480  
C -0.7103343772 1.2413493999 0.0005412595  
C -1.4440460460 -0.0289209801 0.0000032518  
N -1.4733132698 -2.4641801012 0.0009266651  
C -2.8562237822 -2.4729073875 -0.0006029045  
C -2.8564542182 -0.0667241119 -0.0019355159  
C -3.5562613974 -1.2596231131 -0.0022795247  
C 1.3841358838 2.4837274005 -0.0016528930  
C -1.3832934795 2.4838750348 0.0026773862  
C 0.7007843308 3.6861158341 -0.0002298385  
C -0.6998201575 3.6861724713 0.0022808025  
H 3.3909078309 -3.4185358759 0.0032354236  
H 4.6417649127 -1.2525759205 -0.0025061941  
H -3.3928870400 -3.4169241929 -0.0010262669  
H -3.4220260207 0.8568647242 -0.0036897215  
H -4.6421448020 -1.2509442513 -0.0040319050  
H 2.4667789768 2.5114326180 -0.0029514367  
H -2.4659103236 2.5120943387 0.0052144191  
H 1.2513009123 4.6221256792 -0.0007457207  
H -1.2498296635 4.6224536895 0.0041057440  
H 3.4222871406 0.8555515416 -0.0049321123

R1: benzene R2=R3 : 3-thiophene

Ground state coordinates: M1

C 1.3828514938 0.9019605344 -0.9809488365  
C -1.3828514938 -0.9019605344 -0.9809488365  
H 0.6349755234 1.6745551268 -1.0842100853  
H -0.6349755234 -1.6745551268 -1.0842100853  
C 1.5359009278 0.0127345428 0.0550723966  
C 2.6546140237 -0.8637931309 -0.1682057109  
C 3.3030690408 -0.6280885518 -1.3463306650  
S 2.5709463940 0.6802634429 -2.2193242075  
C 0.7086327234 -0.0167119097 1.2893732695  
C -0.7086327234 0.0167119097 1.2893732695  
C -1.5359009278 -0.0127345428 0.0550723966  
C -2.6546140237 0.8637931309 -0.1682057109  
C -3.3030690408 0.6280885518 -1.3463306650  
S -2.5709463940 -0.6802634429 -2.2193242075  
C 1.3811332557 -0.0501024765 2.5226811387  
C 0.6963223360 -0.0295320799 3.7346745613  
C -0.6963223360 0.0295320799 3.7346745613  
C -1.3811332557 0.0501024765 2.5226811387  
H 4.1571884458 -1.1471504155 -1.7576940606  
H -4.1571884458 1.1471504155 -1.7576940606  
H 2.4671243503 -0.0616568626 2.5209692510  
H 1.2482479924 -0.0490588671 4.6697452651  
H -1.2482479924 0.0490588671 4.6697452651  
H -2.4671243503 0.0616568626 2.5209692510  
H 2.9398991207 -1.6494479116 0.5224829798  
H -2.9398991207 1.6494479116 0.5224829798

Ground state coordinates: M2

C -0.5626925218 -0.7036888839 1.0550459839  
C 0.5626925218 0.7036888839 1.0550459839

H	-1.5052225304	-0.1679383472	1.1302219128
H	1.5052225304	0.1679383472	1.1302219128
C	-0.1817192664	-1.4030607941	-0.1478448732
C	0.5096962134	-2.6028954265	0.1190851633
C	0.5465566883	-2.9554425592	1.4503841572
S	-0.3326456756	-1.8259584539	2.4356468589
C	-0.1452782339	-0.6999322715	-1.4454653163
C	0.1452782339	0.6999322715	-1.4454653163
C	0.1817192664	1.4030607941	-0.1478448732
C	-0.5096962134	2.6028954265	0.1190851633
C	-0.5465566883	2.9554425592	1.4503841572
S	0.3326456756	1.8259584539	2.4356468589
C	-0.3158679837	-1.3545810074	-2.6613424792
C	-0.1606129693	-0.6738486349	-3.8816250729
C	0.1606129693	0.6738486349	-3.8816250729
C	0.3158679837	1.3545810074	-2.6613424792
H	1.0710678266	-3.7855113321	1.9020925357
H	-1.0710678266	3.7855113321	1.9020925357
H	-0.5849615581	-2.4068901937	-2.6619562818
H	-0.2905205605	-1.2103573676	-4.8167926479
H	0.2905205605	1.2103573676	-4.8167926479
H	0.5849615581	2.4068901937	-2.6619562818
H	1.0183355196	-3.1709045849	-0.6526356484
H	-1.0183355196	3.1709045849	-0.6526356484

Ground state coordinates: M3

C	-0.3791703824	-0.6504009993	1.0666982515
C	0.3791703824	0.6504009993	1.0666982515
H	-1.4618786533	-0.4364982718	1.1112056669
H	1.4618786533	0.4364982718	1.1112056669
C	-0.0754759734	-1.4237885383	-0.2111658094
C	-0.0052801074	-2.8327234499	0.0413492642
C	0.0226267350	-3.1667220057	1.3564791854
S	-0.0067028532	-1.8058776367	2.4712668892
C	0.0236127239	-0.7356172361	-1.4095845233
C	-0.0236127239	0.7356172361	-1.4095845233
C	0.0754759734	1.4237885383	-0.2111658094
C	0.0052801074	2.8327234499	0.0413492642
C	-0.0226267350	3.1667220057	1.3564791854
S	0.0067028532	1.8058776367	2.4712668892
C	0.1224143364	-1.4055019704	-2.6835903512
C	0.0731607884	-0.7151132315	-3.8552650230
C	-0.0731607884	0.7151132315	-3.8552650230
C	-0.1224143364	1.4055019704	-2.6835903512
H	0.0714842765	-4.1699395601	1.7611191561
H	-0.0714842765	4.1699395601	1.7611191561
H	0.2119857768	-2.4869484362	-2.6982824150
H	0.1323234845	-1.2435344356	-4.8020921350
H	-0.1323234845	1.2435344356	-4.8020921350
H	-0.2119857768	2.4869484362	-2.6982824150
H	0.0490942401	-3.5803095120	-0.7417464665
H	-0.0490942401	3.5803095120	-0.7417464665

Ground state coordinates: M4

C	-0.3913157366	-0.6504321398	1.0603556708
C	0.3913157366	0.6504321398	1.0603556708
H	-1.4704638004	-0.4283511608	1.0772902911
H	1.4704638004	0.4283511608	1.0772902911
C	-0.0766325422	-1.4236920658	-0.2061042107
C	0.0887461901	-2.7979150459	0.0448773107
C	0.0951125847	-3.1219388623	1.3838997372
S	-0.0956863772	-1.7993916686	2.4783648677
C	-0.0005323122	-0.7253760854	-1.4380594410
C	0.0005323122	0.7253760854	-1.4380594410
C	0.0766325422	1.4236920658	-0.2061042107
C	-0.0887461901	2.7979150459	0.0448773107
C	-0.0951125847	3.1219388623	1.3838997372
S	0.0956863772	1.7993916686	2.4783648677

C	0.0330669414	-1.4056536471	-2.6854255727
C	0.0209523572	-0.7076389192	-3.8726774586
C	-0.0209523572	0.7076389192	-3.8726774586
C	-0.0330669414	1.4056536471	-2.6854255727
H	0.2211598153	-4.1198086234	1.7883082299
H	-0.2211598153	4.1198086234	1.7883082299
H	0.0354188290	-2.4896644295	-2.7036528710
H	0.0332737987	-1.2446059708	-4.8152426684
H	-0.0332737987	1.2446059708	-4.8152426684
H	-0.0354188290	2.4896644295	-2.7036528710
H	0.2506709813	-3.5455513913	-0.7217370800
H	-0.2506709813	3.5455513913	-0.7217370800

Ground state coordinates: M5=M6

C	0.9474270616	-0.5734615284	-0.2681218691
C	0.8540173357	0.8462434811	-0.7843185882
H	1.0521834599	-0.4532747159	1.0079573232
H	0.8239153962	0.8287310525	-1.8858845694
C	-0.2555243710	-1.3516883814	-0.4005173759
C	0.0210763247	-2.7371423067	-0.5362023151
C	1.3584645056	-3.0046724587	-0.6824350028
S	2.3565836944	-1.6022552327	-0.6756183024
C	-1.5459797506	-0.7143593568	-0.2985733224
C	-1.6083098275	0.7181452916	-0.1731657705
C	-0.4118255181	1.4925513983	-0.2550158174
C	-0.2045289858	2.8288364345	0.1316121744
C	1.1087559909	3.2322152113	0.1189718492
S	2.2483443581	2.0051336495	-0.3734892176
C	-2.7411798815	-1.4624145769	-0.2599330938
C	-3.9675852900	-0.8475489503	-0.0810514973
C	-4.0295752144	0.5506159500	0.0765476699
C	-2.8787679642	1.3131459534	0.0352289516
H	1.8133895826	-3.9847079390	-0.7525404555
H	1.4816329061	4.2016141541	0.4230290068
H	-2.6976467389	-2.5420280423	-0.3578823765
H	-4.8755969577	-1.4409046318	-0.0518639095
H	-4.9902398219	1.0349198628	0.2240177683
H	-2.9484235034	2.3907497405	0.1386201571
H	-0.7279863524	-3.5185797984	-0.5202913380
H	-0.9944760599	3.4811508862	0.4857473195
Cl	1.1891896878	-0.2122324171	2.5873309249

Ground state coordinates: M7

C	0.8916627631	-0.5392730647	-0.7620659276
C	0.7911109537	0.9264155296	-1.0463996925
H	0.9778154990	-0.6034262198	1.7221073334
H	0.7100111694	1.0717619012	-2.1376269506
C	-0.2344325276	-1.3064219345	-0.5116092722
C	0.0837977357	-2.7068608784	-0.4344898324
C	1.4040577151	-2.9671308876	-0.6532365363
S	2.3152884747	-1.5197784124	-0.9591276366
C	-1.5560424394	-0.6843255263	-0.3661077762
C	-1.6350413433	0.7410566951	-0.2683604624
C	-0.4271329587	1.5208602895	-0.3666971936
C	-0.1779529393	2.8001366547	0.1532909094
C	1.1418626710	3.1958784096	0.1223301556
S	2.2364859264	2.0077365339	-0.5601343580
C	-2.7298726849	-1.4423213025	-0.2690077663
C	-3.9660168231	-0.8352984007	-0.0606253206
C	-4.0453792124	0.5576913613	0.0616742258
C	-2.8974570992	1.3313272057	-0.0381723837
H	1.9102878966	-3.9218056965	-0.6187825476
H	1.5480861151	4.1151274988	0.5239109366
H	-2.6769779214	-2.5232610779	-0.3537401699
H	-4.8627706678	-1.4432504559	0.0101992461
H	-5.0066215080	1.0365769247	0.2246522375
H	-2.9723807384	2.4122165168	0.0328536808
H	-0.6361954849	-3.4823563610	-0.2032480560

H	-0.9419979341	3.4098090084	0.6234367335
Cl	1.1331394289	-0.6723015816	3.0071347475

Ground state coordinates: M8

C	1.0679118891	-0.7320306701	-0.1238880582
C	1.0632210222	0.7145560817	-0.4550628451
H	1.1200956269	0.8080568372	-1.5585928170
C	-0.1243834731	-1.4253065612	0.0169066983
C	0.1041580044	-2.8322630303	0.2022773858
C	1.4264377455	-3.1559260195	0.1831503540
S	2.4450640968	-1.7662516104	-0.0663771229
C	-1.4029896136	-0.7302404770	-0.0288693526
C	-1.4381180563	0.7085961871	-0.0922386088
C	-0.2113033707	1.4286668607	-0.1060212426
C	0.0176980277	2.7829899107	0.1873263713
C	1.3591734289	3.0989138349	0.2941091319
S	2.4635623311	1.8180040620	0.0432825187
C	-2.6245689401	-1.4182272398	0.0321548731
C	-3.8328563047	-0.7321690774	0.0347449175
C	-3.8700705143	0.6744886100	-0.0164598553
C	-2.6885051949	1.3832976313	-0.0704365161
H	1.8818906731	-4.1272286401	0.3189431171
H	1.7485208354	4.0867039169	0.5192311234
H	-2.6306842602	-2.5011119695	0.0757426322
H	-4.7623619265	-1.2914330348	0.0782160864
H	-4.8216977985	1.1945940531	-0.0190979307
H	-2.7139193939	2.4662240358	-0.1284971058
H	-0.6751466239	-3.5674675357	0.3570923105
H	-0.7595478792	3.5115468639	0.3803167318

Ground state coordinates: M9

C	1.0630858930	-0.7088868337	-0.0038514313
C	1.0640901568	0.7056833066	-0.0071977664
C	-0.1444957452	-1.4200777181	0.0000415857
C	0.0826801400	-2.8397451901	0.0027907558
C	1.4023235949	-3.1713564908	0.0010171682
S	2.4471808715	-1.7746598252	-0.0045630000
C	-1.4045254920	-0.7142100009	0.0006235905
C	-1.4060948860	0.7166517897	-0.0050544003
C	-0.1434512516	1.4226354935	-0.0119994565
C	0.0892216354	2.8442738292	-0.0045684765
C	1.4104680800	3.1708390800	0.0050898593
S	2.4498140191	1.7693028898	0.0091089601
C	-2.6451331951	-1.3940022190	0.0064731060
C	-3.8408820907	-0.7023537645	0.0061967184
C	-3.8417786763	0.7054058288	0.0002791148
C	-2.6461210565	1.3976380088	-0.0047567973
H	1.8393157600	-4.1603176991	0.0007921736
H	1.8514910516	4.1579349449	0.0071344633
H	-2.6561952182	-2.4791472146	0.0105406286
H	-4.7811392929	-1.2456382219	0.0091456149
H	-4.7822880768	1.2481268533	-0.0005950604
H	-2.6568054465	2.4829222098	-0.0089058010
H	-0.7056466309	-3.5823974498	0.0056193297
H	-0.6969730351	3.5892568270	-0.0069681335

R1: benzene, R2=R3 : 3-pyrrole

Ground state coordinates: M1

C	1.3278190570	1.2881320501	0.9811618372
C	-1.3278417277	1.2881177680	-0.9811587058
H	0.5361141297	1.3913879735	1.7087762189
H	-0.5361278901	1.3913818447	-1.7087731517
C	1.5325348621	0.2521130088	0.1023846813
C	2.7005170406	0.4753990593	-0.7073251844

C	3.3340912035	1.6535324398	-0.4341681759
N	2.5268270875	2.5265183550	0.8292151197
C	0.7084084094	-0.9821913500	0.0246900114
C	-0.7083971239	-0.9821988318	-0.0246862890
C	-1.5325366367	0.2520968093	-0.1023912995
C	-2.7005211354	0.4753607588	0.7073285045
C	-3.3341177655	1.6534873783	0.4341612066
N	-2.5268628254	2.5264814630	-0.8292123301
C	1.3817204248	-2.2154977968	0.0306236583
C	0.6968829173	-3.4274914127	0.0111715036
C	-0.6968358649	-3.4274987690	-0.0111771419
C	-1.3816861256	-2.2155123849	-0.0306196312
H	4.2170608565	2.0648970337	-0.9024671848
H	-4.2170817234	2.0648427845	0.9024700661
H	2.4665327519	-2.2137720662	0.0824966005
H	1.2490169014	-4.3625584979	0.0239082676
H	-1.2489499465	-4.3625716837	-0.0239036836
H	-2.4664984707	-2.2138081155	-0.0824925739
H	3.0311890007	-0.2152893020	-1.4749818834
H	-3.0311858074	-0.2153208798	1.4749853941
H	-2.6874331580	3.3863405535	-1.2809914325
H	2.6873883111	3.3863792645	1.2809839849

Ground state coordinates: M3

C	1.4277238021	-0.6409588620	0.3901608344
C	1.4277246038	0.6409586264	-0.3901583953
H	1.4317993738	-0.3840852207	1.4706325287
H	1.4318024672	0.3840868876	-1.4706302579
C	0.1371218003	-1.4047474027	0.0920529298
C	0.5216933844	-2.7829267432	-0.0259732884
C	1.8820704670	-2.8560981662	-0.0534973309
N	2.5032730103	-1.6196215779	0.1464074057
C	-1.0676236525	-0.7387426156	-0.0047969247
C	-1.0676232909	0.7387425351	0.0047989273
C	0.1371219662	1.4047466179	-0.0920521575
C	0.5216934966	2.7829268235	0.0259665501
C	1.8820698980	2.8560994081	0.0534912854
N	2.5032757679	1.6196201508	-0.1464032266
C	-2.3410890661	-1.4121066580	-0.0774886953
C	-3.5120176933	-0.7185714720	-0.0496948386
C	-3.5120174391	0.7185716354	0.0496953923
C	-2.3410888829	1.4121067664	0.0774899953
H	2.4932369125	-3.7422771987	-0.1795641092
H	2.4932355883	3.7422799062	0.1795511998
H	-2.3512881898	-2.4972641543	-0.1295292102
H	-4.4602788502	-1.2466766357	-0.0906868435
H	-4.4602785199	1.2466770157	0.0906871206
H	-2.3512879770	2.4972641873	0.1295310410
H	-0.1432797754	-3.6307175916	-0.1214756604
H	-0.1432801861	3.6307181357	0.1214618447
H	3.2196022965	1.3557602671	0.5230475182
H	3.2196190517	-1.3557585673	-0.5230201289

Ground state coordinates: M4

C	-0.3994987757	-0.6446394803	1.4308391362
C	0.3994987757	0.6446394803	1.4308391362
H	-1.4754911806	-0.3957085723	1.4509751117
H	1.4754911806	0.3957085723	1.4509751117
C	-0.0829205344	-1.4077637710	0.1517462301
C	0.0940970828	-2.7551920327	0.5049068135
C	0.0427383792	-2.8490712039	1.8877083030
N	-0.1063600824	-1.6309670255	2.4729130881
C	0.0067066040	-0.7245263980	-1.0838145634
C	-0.0067066040	0.7245263980	-1.0838145634
C	0.0829205344	1.4077637710	0.1517462301
C	-0.0940970828	2.7551920327	0.5049068135

C	-0.0427383792	2.8490712039	1.8877083030
N	0.1063600824	1.6309670255	2.4729130881
C	0.0578598480	-1.4071169497	-2.3284841407
C	0.0356098284	-0.7079678441	-3.5145642985
C	-0.0356098284	0.7079678441	-3.5145642985
C	-0.0578598480	1.4071169497	-2.3284841407
H	0.1262110034	-3.7416575268	2.4955182080
H	-0.1262110034	3.7416575268	2.4955182080
H	0.0801263964	-2.4918082350	-2.3403208335
H	0.0606595865	-1.2428011509	-4.4581680322
H	-0.0606595865	1.2428011509	-4.4581680322
H	-0.0801263964	2.4918082350	-2.3403208335
H	0.3005764233	-3.5832380635	-0.1575164560
H	-0.3005764233	3.5832380635	-0.1575164560
H	0.4775773093	1.5402979829	3.4090949198
H	-0.4775773093	-1.5402979829	3.4090949198

Ground state coordinates: M5=M6

C	1.2295938586	0.0575881233	-0.5207103233
C	0.6478030098	1.4365841388	-0.7406061417
H	0.5091764864	1.5952905349	-1.8312267506
C	0.2879479411	-1.0270558959	-0.7407852063
C	1.0067655501	-2.1111295850	-1.2841040634
C	2.3066110809	-1.6748616377	-1.4995206934
N	2.4262656986	-0.3617468703	-1.1937592778
C	-1.1070169468	-0.8864760340	-0.4147812502
C	-1.5855921511	0.4095721656	-0.0070586568
C	-0.6989265982	1.5197957700	-0.0351780501
C	-0.7678900314	2.7894811578	0.5755573156
C	0.4590679492	3.4067563438	0.4440150410
N	1.3680553727	2.5876000194	-0.1887679568
C	-1.9923054733	-1.9822564412	-0.4211063126
C	-3.3119547743	-1.8386000514	-0.0263403011
C	-3.7803609250	-0.5768664176	0.3943027842
C	-2.9387868391	0.5185288164	0.4100154240
H	3.1641344334	-2.2451404615	-1.8327904149
H	0.7689418776	4.3740888499	0.8176755403
H	-1.6216516816	-2.9594440211	-0.7177982372
H	-3.9782188093	-2.6948666732	-0.0272188408
H	-4.8151787153	-0.4639912580	0.7047101207
H	-3.3192838253	1.4864185245	0.7215718922
H	0.6354344435	-3.0998301909	-1.5115797720
H	-1.5976193871	3.1818641427	1.1465295169
H	2.1422810613	2.9874066790	-0.6982791816
H	3.3239059251	0.0379684441	-0.9482220249
H	1.5921756128	-0.0216868688	0.7189212673
Cl	2.3890147472	-0.1073960392	2.1906235061

Ground state coordinates: M7

C	1.1026988481	-0.3118854839	-0.9356430445
C	0.8526765919	1.1465177275	-1.1301891579
H	0.6843804962	1.3373421630	-2.2135506430
C	0.0853462362	-1.2150220778	-0.6403173382
C	0.6551359741	-2.5266363693	-0.7430228009
C	1.9747632977	-2.3752243756	-1.0996515266
N	2.2335850822	-1.0275492707	-1.2454419785
C	-1.2711126637	-0.7634602504	-0.3295772366
C	-1.4888560457	0.6441542150	-0.1592941253
C	-0.3896213673	1.5487591372	-0.3515944530
C	-0.1358418967	2.8267363840	0.1869725565
C	1.1830402016	3.1567633199	-0.0377606230
N	1.8724762439	2.1068244212	-0.6553186064
C	-2.3360580567	-1.6492304642	-0.1344462153
C	-3.5993443882	-1.1893588532	0.2357490253
C	-3.8120611962	0.1819335300	0.4282752762
C	-2.7718648526	1.0821700944	0.2382334509
H	2.7564136391	-3.1082230550	-1.2325484940
H	1.7201383136	4.0419978729	0.2765410413

H	-2.1698085658	-2.7146557825	-0.2671837335
H	-4.4124695998	-1.8948126674	0.3783828767
H	-4.7936606260	0.5452655710	0.7189982425
H	-2.9478643265	2.1459494989	0.3717342880
H	0.1605904060	-3.4690140146	-0.5563967885
H	-0.8231401566	3.4144199146	0.7814010275
H	2.5802061545	2.3719891577	-1.3298174253
H	3.1469021678	-0.6285192162	-1.3945837917
H	1.3597554370	-0.6537203278	1.3995119259
Cl	1.9825131343	-0.7223673159	2.5415548731

Ground state coordinates: M8

C	1.4020327169	-0.7142725748	-0.1241794398
C	1.4640284635	0.7153671907	-0.5479538714
H	1.5629025476	0.7542427755	-1.6557047077
C	0.2002687822	-1.3987446694	0.0343724076
C	0.5341455640	-2.7795671710	0.2277777592
C	1.9044191758	-2.8832863057	0.1720614924
N	2.4255161904	-1.6291048404	-0.0728204670
C	-1.0876306716	-0.7082714734	-0.0363218844
C	-1.0799790423	0.7250322963	-0.0943684055
C	0.1792349012	1.4152228272	-0.1346434755
C	0.5399464322	2.7109239014	0.2881345788
C	1.9139893219	2.8026371860	0.3377311907
N	2.5174333131	1.5777373725	0.0302569527
C	-2.3110922545	-1.3846902394	0.0123583445
C	-3.5203690321	-0.6904075255	0.0196893282
C	-3.5190423485	0.7102331415	-0.0112851985
C	-2.3178446516	1.4052388615	-0.0625859465
H	2.5520844268	-3.7353542380	0.3150258371
H	2.5234613277	3.6374685247	0.6579161272
H	-2.3146980975	-2.4703857038	0.0529104567
H	-4.4584231595	-1.2363337162	0.0542862226
H	-4.4582338949	1.2560507874	-0.0033659665
H	-2.3240625801	2.4908873927	-0.1044742886
H	-0.1493633883	-3.5968074110	0.4078028510
H	-0.1395552324	3.4805854229	0.6301798144
H	3.3863289389	1.6248564635	-0.4883389297
H	3.4062684444	-1.3981306941	-0.0530140940

Ground state coordinates: M9

C	1.4275267064	-0.7105957735	-0.0021128797
C	1.4302760223	0.7043968305	-0.0030731020
C	0.2102141705	-1.4141908714	-0.0008391419
C	0.5451356901	-2.8072034273	0.0007228149
C	1.9141519169	-2.9045489965	-0.0010050512
N	2.4524955108	-1.6306497528	-0.0004372520
C	-1.0525982618	-0.7152074191	-0.0009465603
C	-1.0530524703	0.7170697517	-0.0063934942
C	0.2132950591	1.4135704051	-0.0132557354
C	0.5557198696	2.8101670554	-0.0040278200
C	1.9259146086	2.9005766388	0.0085969816
N	2.4564818876	1.6228735748	0.0165333012
C	-2.2917447247	-1.3928107291	0.0062476413
C	-3.4888652550	-0.6993363101	0.0061965733
C	-3.4882895216	0.7077311921	0.0003512307
C	-2.2896722417	1.3988552396	-0.0056751175
H	2.5561769555	-3.7729018232	-0.0020858369
H	2.5718886077	3.7657543708	0.0112953154
H	-2.2979044177	-2.4790914444	0.0109397991
H	-4.4298324337	-1.2419841212	0.0106710964
H	-4.4282520306	1.2520469255	0.0001780941
H	-2.2931826252	2.4853247758	-0.0086683440
H	-0.1398683434	-3.6426111448	0.0020119173
H	-0.1269693408	3.6476860658	0.0014729321
H	3.4400400942	1.4140225182	-0.0270468474
H	3.4369923362	-1.4246543945	-0.0201585074

R1 : benzene, R2 : Phenyl, R3 : 2-methoxyphenyl

Ground state coordinates: M1

C	0.6912166487	-0.9458091091	-1.6873652309
C	-1.4529039302	-0.9720445137	1.1281286623
H	-0.1587799536	-0.6600711598	-2.2994326786
H	-0.5083581968	-0.8417159807	1.6464581887
C	1.3903368870	-2.1205101198	-1.9705827214
C	2.4804085713	-2.4719682462	-1.1800864839
C	2.8679994983	-1.6621014575	-0.1101115207
C	2.1607659298	-0.4878105546	0.1686136716
C	1.0562209333	-0.1097538957	-0.6280315462
C	0.3258462500	1.1720815451	-0.3834295206
C	-1.0506898580	1.2175427157	-0.0622167656
C	-1.8661968394	-0.0028875912	0.1995417071
C	-2.2489368545	-2.0828033454	1.4006341114
C	-3.4733979499	-2.2500253111	0.7504900736
C	-3.1022368913	-0.1802530667	-0.4423218362
C	-3.8976369366	-1.2939477010	-0.1725669162
C	1.0206035195	2.3792065470	-0.5587544468
C	-1.6789181884	2.4708252382	0.0433379559
C	0.3847100534	3.6116041034	-0.4417594076
C	-0.9774243634	3.6577852619	-0.1446261936
H	1.0859891509	-2.7485168263	-2.8018840721
H	3.0384266482	-3.3807458145	-1.3867852437
H	3.7150267382	-1.9540387224	0.4989310691
O	2.4572538929	0.3476995642	1.2112921255
H	-1.9137849406	-2.8185076510	2.1264335313
H	-4.0915069977	-3.1174999803	0.9632758320
H	-3.4327306544	0.5563020606	-1.1695030571
H	-4.8470754927	-1.4150166166	-0.6866136745
H	2.0770620813	2.3384716268	-0.8046393938
H	-2.7323791893	2.5021772542	0.3052402030
H	0.9483193526	4.5286764509	-0.5872795876
H	-1.4886819282	4.6113728665	-0.0488037836
C	3.5576198592	0.0267149648	2.0454222166
H	3.6062712849	0.8180486478	2.7948920926
H	4.5005330670	0.0029191150	1.4837460337
H	3.4193198559	-0.9385245684	2.5497326826

Ground state coordinates: M3

C	-0.0984355381	-1.3797966904	-0.2336292380
C	-1.5192037997	-1.0371593333	0.1562178999
H	-0.2117744512	-1.3780535842	-1.3165654194
H	-1.4551742032	-1.1903488597	1.2331606208
C	0.2877811295	-2.6743311342	-0.0395931197
C	1.6950869984	-3.0812263012	-0.0179117613
C	2.6473845194	-2.1597533358	-0.0160011511
C	2.2989257492	-0.7114246608	-0.0058620845
C	0.9770739463	-0.3193267756	-0.0895339805
C	0.5061445283	1.1234096242	-0.0737184227
C	-0.8918121823	1.3983309997	0.0323714931
C	-1.9055294171	0.2811620665	0.1337269868
C	-2.6091067601	-2.0432602984	-0.1590268865
C	-3.9066411683	-1.7239125561	-0.1303445235
C	-3.3781635991	0.6031258586	0.2576614009
C	-4.3093231060	-0.3471290097	0.1470156178
C	1.3927155467	2.2330188142	-0.1801580911
C	-1.3197384818	2.7522247900	0.0314047405
C	0.9317919167	3.5439295382	-0.1730694419
C	-0.4189839696	3.8029128002	-0.0662139830
H	-0.4108428163	-3.4871046372	0.0890147375
H	1.9547127521	-4.1347870685	0.0219749726
H	3.6790619345	-2.4920349439	0.0204252215



O	3.3006922873	0.1961311803	0.1221766149
H	-2.3878812805	-3.0737415611	-0.3985465597
H	-4.6629032249	-2.4773280649	-0.3285993325
H	-3.7539705174	1.6005133585	0.4173298463
H	-5.3633558230	-0.0954576174	0.2159817259
H	2.4528113075	2.1584197245	-0.2911922716
H	-2.3487978822	3.0480206409	0.1002870794
H	1.6311283774	4.3665106062	-0.2584996626
H	-0.7739667514	4.8259497586	-0.0654591767
C	4.6502981371	-0.0695642218	0.2282508152
H	5.2004906402	0.8892549580	0.3192891136
H	5.0108893749	-0.5972681638	-0.6802024129
H	4.8524475687	-0.6789750345	1.1346709781

Ground state coordinates: M4

C	-0.1292291870	-1.2618125092	-0.5917906294
C	-1.3593197239	-1.0418304381	0.3308700561
H	-0.4695071910	-0.9959830979	-1.6136541097
H	-0.9582044161	-1.0492286419	1.3700888973
C	0.3315372670	-2.6809710855	-0.6840359985
C	1.6305037884	-3.0127175036	-0.5030761955
C	2.5926254627	-2.0271063228	-0.1404098577
C	2.2597561170	-0.6799684477	0.0118315126
C	0.9229880547	-0.2293081314	-0.2039452137
C	0.4725583237	1.1275556662	-0.1272926802
C	-0.9563359212	1.4109636486	-0.0730704218
C	-1.8945592257	0.3559091497	0.1162399900
C	-2.3866508229	-2.1348532228	0.3299480781
C	-3.7113089087	-1.8686470733	0.3485491961
C	-3.2943223809	0.5497615180	0.1706600164
C	-4.1667458274	-0.5102438866	0.2812607377
C	1.3602780680	2.2409605337	-0.1846461358
C	-1.3868899328	2.7675248083	-0.1346705999
C	0.8933619891	3.5362753540	-0.2339695241
C	-0.4915055225	3.8070207348	-0.2114018984
H	-0.3921470666	-3.4294723681	-0.9858879828
H	1.9617441384	-4.0386219267	-0.6278664009
H	3.6129317777	-2.3464945510	0.0276670030
O	3.1665546734	0.2353441648	0.4152287403
H	-2.0304569762	-3.1549175962	0.4187478115
H	-4.4384832889	-2.6710557020	0.4140872989
H	-3.7104448287	1.5445597447	0.0800911921
H	-5.2344534971	-0.3140616938	0.2995728483
H	2.4214396167	2.0612593195	-0.2357059665
H	-2.4437261541	2.9979689567	-0.1036458565
H	1.6013813500	4.3556408288	-0.3059161572
H	-0.8482784341	4.8307588965	-0.2509941863
C	4.4957145159	-0.1701697362	0.7667154466
H	4.9928645867	0.7374901406	1.1062175126
H	5.0276739514	-0.5760671432	-0.0996746827
H	4.4804922438	-0.9045868196	1.5784475838

Ground state coordinates: M5=M6

C	-0.0812153131	-1.2626500430	-0.6880530683
C	-1.3630000068	-1.0587068864	0.1858187827
H	-0.4154339409	-0.9808966739	-1.7068707170
C	0.3986072159	-2.6773988875	-0.7636764972
C	1.6806871176	-3.0071579572	-0.4691751134
C	2.6211494303	-2.0322790681	-0.0371207780
C	2.2598222159	-0.6814811069	0.0616428054
C	0.9629658017	-0.2462633617	-0.2646365404
C	0.4955837739	1.1278923411	-0.2222392988
C	-0.9069789757	1.4004105569	-0.0654687178
C	-1.8427009407	0.3149530651	0.2085525893
C	-2.3524378601	-2.1137270810	0.2351324665
C	-3.6574097050	-1.8558505804	0.5740374963
C	-3.1764095008	0.5364878589	0.5955749710
C	-4.0573977400	-0.5199982850	0.7786133946

C	1.3644787662	2.2331227878	-0.3882068655
C	-1.3587241163	2.7362997315	-0.1299547356
C	0.8877360504	3.5331338262	-0.4361404997
C	-0.4842558104	3.7931995843	-0.3156834110
H	-0.2919678166	-3.4328458005	-1.1237276257
H	2.0105812301	-4.0383756360	-0.5612057242
H	3.6208511553	-2.3502655244	0.2261256306
O	3.1434298271	0.2618982773	0.4988847095
H	-2.0107160758	-3.1375787187	0.1354565882
H	-4.3698320723	-2.6654144424	0.6931400754
H	-3.5421865708	1.5440431280	0.7497103148
H	-5.0806799905	-0.3079313287	1.0759080864
H	2.4219324884	2.0485061966	-0.5063543905
H	-2.4179594437	2.9491825693	-0.0456510416
H	1.5851493599	4.3525103710	-0.5858425715
H	-0.8607814496	4.8100461512	-0.3671826164
C	4.3512168382	-0.1565285175	1.1231142253
H	4.8106328938	0.7524243539	1.5144468302
H	5.0390172966	-0.6243793992	0.4074569689
H	4.1519663245	-0.8487045884	1.9483319030
H	-0.9512372993	-1.1749216854	1.2564985515
Cl	-0.2503531575	-1.4005052269	2.8372038229

Ground state coordinates: M7

C	0.2814735574	0.7224867001	1.0109672846
C	1.4952203292	-0.1982357785	1.2165294303
H	1.2575584454	-0.7575123962	2.1468522733
C	0.3615598183	2.0946613251	1.2761385175
C	-0.7611196579	2.9054884497	1.1232097625
C	-1.9567749309	2.3602920361	0.6703899376
C	-2.0400806714	0.9943613847	0.3765671637
C	-0.9239921042	0.1323442191	0.5651019531
C	-0.9385382195	-1.3177965266	0.2380910019
C	0.2960514406	-1.9503413421	-0.0945924211
C	1.5419360121	-1.2227240810	0.1033217941
C	2.8084291186	0.5009369914	1.4415534023
C	3.9158364257	0.2242060096	0.7005392157
C	2.7028997021	-1.4458233380	-0.6120266336
C	3.8857880207	-0.7403432954	-0.3454136309
C	-2.1103149121	-2.0935098591	0.1928200504
C	0.2926456847	-3.2858479031	-0.5367151067
C	-2.0864464728	-3.4226729892	-0.2206762608
C	-0.8848664336	-4.0174538179	-0.6105932732
H	1.2943395631	2.5274340982	1.6168298758
H	-0.7017812171	3.9671014097	1.3427688193
H	-2.8179820617	3.0013357583	0.5346859544
O	-3.1828440199	0.4381262103	-0.1204794615
H	2.8672627792	1.2115780077	2.2603658223
H	4.8457456105	0.7459224526	0.9108192448
H	2.6919419727	-2.1691710753	-1.4227763917
H	4.7738138488	-0.9237522209	-0.9405006681
H	-3.0519290652	-1.6491179175	0.4783559918
H	1.2386358906	-3.7627553557	-0.7731713310
H	-3.0102539007	-3.9933300076	-0.2387616790
H	-0.8629727090	-5.0525337520	-0.9385018729
C	-4.2767835606	1.2806744038	-0.4555488095
H	-5.0262868871	0.6265072038	-0.9025791899
H	-3.9853254240	2.0485984969	-1.1815939785
H	-4.7041871970	1.7638724208	0.4317587388
H	0.8544090571	2.4235817699	-1.0106883575
Cl	1.1871896809	2.7860597584	-2.2110592840

Ground state coordinates: M8

C	-0.1795078889	-1.3069034834	0.3995307949
C	-1.5856240288	-0.7713596990	0.7148070734
H	-1.5181515905	-0.4333410291	1.7711977261
C	0.0671403126	-2.6818356528	0.3096144564
C	1.3555876240	-3.1487407428	0.0578816232

C	2.3964739001	-2.2480971329	-0.1371299031
C	2.1558081003	-0.8708185177	-0.0723935243
C	0.8595154685	-0.3636174277	0.2230554563
C	0.5313064820	1.0859249763	0.2655352449
C	-0.8095659476	1.4856067887	-0.0130523523
C	-1.8464946022	0.4681112710	-0.1138915429
C	-2.6960834486	-1.7841945947	0.6419636358
C	-3.8146349593	-1.5845194756	-0.1073502908
C	-3.0045801911	0.5988735110	-0.8565306758
C	-3.9881348090	-0.4014392684	-0.8794754725
C	1.4799463396	2.0922006095	0.5198055559
C	-1.1179355287	2.8546797570	-0.1118688104
C	1.1458404143	3.4417756037	0.4447818212
C	-0.1520235726	3.8282613286	0.1040946037
H	-0.7423743862	-3.3880880638	0.4489003337
H	1.5481976950	-4.2157310485	-0.0001283303
H	3.3902006506	-2.6193019523	-0.3513182072
O	3.1441825383	0.0390543190	-0.3124310612
H	-2.6054043223	-2.6763606032	1.2542098099
H	-4.5960457218	-2.3398673481	-0.1162113157
H	-3.1452718094	1.4905365212	-1.4614785330
H	-4.8756609776	-0.2771045165	-1.4904454634
H	2.4922788524	1.8150418540	0.7728178091
H	-2.1440364660	3.1485753977	-0.3097311835
H	1.9031790859	4.1920889502	0.6520711531
H	-0.4151237356	4.8799688499	0.0393773201
C	4.4179212765	-0.4183919754	-0.7447903102
H	5.0013681241	0.4809891130	-0.9457063944
H	4.3414622396	-1.0141795194	-1.6619396879
H	4.9221924085	-1.0087564091	0.0303091527

Ground state coordinates: M9

C	-0.0589293812	-1.3634375986	-0.1100379066
C	-1.4959677951	-1.0656485616	-0.0409049560
C	0.3704622572	-2.7051407142	-0.2148428900
C	1.7081488020	-3.0325562631	-0.2060839817
C	2.6690636099	-2.0301162216	-0.0645856845
C	2.2811170513	-0.6983600353	0.0296982603
C	0.8998683798	-0.3092072724	-0.0383590913
C	0.4330322511	1.0899363401	-0.0493238484
C	-0.9667033215	1.3673333044	0.0008734488
C	-1.9412985987	0.2761077444	0.0539780707
C	-2.4646882180	-2.0964929370	-0.0262235045
C	-3.8166522501	-1.8305384050	0.0845390072
C	-3.3281655427	0.5213522682	0.1825049133
C	-4.2539541163	-0.5046717365	0.1962746463
C	1.3096274060	2.1996939693	-0.1567662819
C	-1.4019480573	2.7102733311	-0.0286219877
C	0.8513703733	3.5053607238	-0.1841792882
C	-0.5187896155	3.7699490636	-0.1114263865
H	-0.3528004291	-3.5033452940	-0.3057474628
H	2.0201189218	-4.0690321280	-0.2926567763
H	3.7160652380	-2.3002601597	-0.0274455012
O	3.2153585641	0.2846300442	0.2095062566
H	-2.1573231532	-3.1320994922	-0.0878647616
H	-4.5304075334	-2.6489187195	0.0948151897
H	-3.6911577735	1.5362732835	0.2827422394
H	-5.3115724503	-0.2801185576	0.2981605016
H	2.3685659672	2.0274401535	-0.2307830134
H	-2.4615494949	2.9301695381	-0.0050841750
H	1.5654459843	4.3194757343	-0.2697644996
H	-0.8913498247	4.7899003944	-0.1335081637
C	4.5848397511	-0.0632445808	0.3328317445
H	5.1143846680	0.8771627404	0.4929857076
H	4.9676453029	-0.5412443854	-0.5773720029
H	4.7584681512	-0.7259979735	1.1894069635

R1: Benzene, R2 : phenyl , R3: 3-methoxyphenyl

Ground state coordinates: M1e

C	1.5550211284	0.6287473135	0.7021118255
C	-1.1602997019	0.9757192006	-1.4348130067
O	0.6453062939	0.6519094996	1.7175677117
H	-0.3877950746	0.6121149536	-2.1039959013
C	2.5890536649	1.5615816398	0.5664743207
C	3.5056210287	1.4461350192	-0.4813255438
C	3.4009016006	0.4033882730	-1.3962036334
C	2.3641437139	-0.5220571945	-1.2577427131
C	1.4213109308	-0.4280970463	-0.2282384042
C	0.3617441994	-1.4725660013	-0.0939376090
C	-1.0257323500	-1.1924253541	-0.1369200361
C	-1.5815117894	0.1719028940	-0.3636810030
C	-1.7343417743	2.2275925153	-1.6560830772
C	-2.7404110358	2.7018354134	-0.8128012284
C	-2.5967112738	0.6607954705	0.4750080562
C	-3.1698281471	1.9122933562	0.2551423185
C	0.7786249170	-2.8016515915	0.0788377760
C	-1.9303456061	-2.2554440743	0.0172416645
C	-0.1340304725	-3.8444798388	0.2230951835
C	-1.4993811081	-3.5676101768	0.1974973175
H	2.6944180923	2.3725532131	1.2769468940
H	4.3031364240	2.1781435405	-0.5715249511
H	4.1120143224	0.3083679965	-2.2108380715
H	2.2673897631	-1.3366062065	-1.9701638990
H	-1.3987758371	2.8301647746	-2.4954942099
H	-3.1868209311	3.6765106613	-0.9878849551
H	-2.9242134470	0.0562979531	1.3157749052
H	-3.9505032657	2.2720337794	0.9198078392
H	1.8442498970	-3.0069345207	0.1229452336
H	-2.9939201051	-2.0423114454	-0.0358645051
H	0.2208871331	-4.8617709673	0.3602313536
H	-2.2267878140	-4.3668668113	0.3070729756
C	0.6747467406	1.7373180864	2.6295283317
H	-0.1566920911	1.5737954778	3.3163465397
H	0.5367515296	2.6979486121	2.1179868986
H	1.6127630611	1.7634155666	3.1989689243

Ground state coordinates: M2e

C	0.8919073305	0.8291155717	0.1754143734
C	-0.4663225413	1.0440414436	-0.7774483128
O	0.3405125698	0.8531018962	1.5005318569
H	-0.0314963159	0.7938334517	-1.7467554422
C	1.8988009918	1.8408315797	-0.1168459218
C	2.9944543936	1.5958612405	-0.9228439657
C	3.2677542670	0.3079465931	-1.3906852275
C	2.4163307537	-0.7411346283	-0.9990505743
C	1.3198228262	-0.5453071346	-0.1813299160
C	0.3522862417	-1.6473458951	0.0045275160
C	-1.0272749671	-1.3636994838	-0.1930927980
C	-1.4369227732	0.0532415048	-0.2737476690
C	-0.9622162062	2.4186493389	-0.7672692165
C	-2.1497672110	2.7871719241	-0.1772928687
C	-2.6114509563	0.4687809483	0.3405635101
C	-2.9916461529	1.8131861472	0.3856005201
C	0.7448706766	-2.9601214893	0.2617188863
C	-1.9393924574	-2.4200434848	-0.2200936242
C	-0.1867719031	-4.0070088706	0.2616331390
C	-1.5252908020	-3.7396820138	0.0031750815
H	1.7209256497	2.8538037069	0.2245351360

H	3.6631285854	2.4171554470	-1.1678935928
H	4.1292384882	0.1116162712	-2.0197051339
H	2.6139553524	-1.7477877435	-1.3573681195
H	-0.3368111426	3.1791038976	-1.2271308880
H	-2.4498657824	3.8317448759	-0.1724073014
H	-3.2507611834	-0.2787575680	0.8003077122
H	-3.9246264259	2.1000699713	0.8601914082
H	1.7911094400	-3.1667695833	0.4672731801
H	-2.9845055705	-2.2157746937	-0.4336056194
H	0.1440647424	-5.0232485792	0.4547596692
H	-2.2538139805	-4.5446832189	-0.0203679902
C	0.5527771221	1.9883086567	2.3158922687
H	0.0423269880	1.7674038042	3.2566338462
H	0.1162453153	2.9046711893	1.8957532923
H	1.6184072535	2.1634689083	2.5174961073

Ground state coordinates: M3e

C	1.1826181766	-0.3763992638	0.0575428498
C	0.7755126021	1.0078477524	-0.4588520333
O	1.0182943268	-0.1529231177	1.4028804596
H	0.7595304298	0.7955557536	-1.5288948616
C	2.6176247396	-0.7954295853	-0.2431260997
C	2.9382768778	-2.0282580360	-0.6487554698
C	1.8921376275	-3.0284204536	-0.8576027933
C	0.6124947957	-2.7019084467	-0.6699346468
C	0.2105139575	-1.3174394668	-0.2408324558
C	-1.2580833963	-0.9934067116	-0.0950184144
C	-1.6868134816	0.3576608826	-0.0735383295
C	-0.6628773141	1.4344410921	-0.2533556585
C	1.7056652436	2.0100459439	-0.4362532672
C	1.3276483285	3.4360295588	-0.5107821898
C	-0.9894378532	2.7539731364	-0.2771697521
C	0.0449563425	3.7887258732	-0.4452346865
C	-2.2276695713	-2.0166625025	0.0272917652
C	-3.0663024595	0.6380123758	0.0797079709
C	-3.5786632385	-1.7136578609	0.1769152989
C	-3.9963452613	-0.3907353027	0.2047893076
H	3.4484027000	-0.1184201110	-0.0967768541
H	3.9761347150	-2.2922636100	-0.8274182939
H	2.1604685112	-4.0289010145	-1.1828581636
H	-0.1154225092	-3.4744272730	-0.8727993467
H	2.7676296947	1.8272285669	-0.3951212178
H	2.0972912805	4.1967859066	-0.5958354287
H	-2.0004480711	3.1140186317	-0.1646610530
H	-0.2358339239	4.8366123496	-0.4823356810
H	-1.9676591653	-3.0619060024	0.0325645054
H	-3.4585831140	1.6406265747	0.1002462775
H	-4.3048332096	-2.5104841854	0.2761436042
H	-5.0476608055	-0.1596717091	0.3208799218
C	1.9950059481	-0.0058160713	2.3731748420
H	2.6470367460	0.8606736142	2.1350452590
H	2.6037603566	-0.9312245446	2.4533486319
H	1.5062593663	0.1775645098	3.3516315976

Ground state coordinates: M4e

C	1.1744870887	0.3384747147	-0.2202433322
C	0.1129629882	1.3610493374	-0.5392908003
O	1.2215432033	0.6836929911	1.6078511299
H	0.1184822426	1.3875307348	-1.6609632194
C	2.5267267053	0.6647679000	-0.6709021307
C	3.4632652866	-0.3028331730	-0.8534071371
C	3.1112296703	-1.6847710187	-0.7382699834
C	1.8101703120	-2.0437410470	-0.5082814172
C	0.7732825320	-1.0747390262	-0.3494785771
C	-0.5939370383	-1.4250830262	-0.2325615258
C	-1.6333346595	-0.4082063991	-0.1338960888
C	-1.3077708889	0.9531338686	-0.2319658680
C	0.4445612112	2.7759029907	-0.1463269803

C	-0.5219002941	3.7072874271	-0.0286968613
C	-2.2741151837	2.0048593368	-0.1973838483
C	-1.9060412268	3.3205062808	-0.1286633702
C	-1.0172509956	-2.7966795347	-0.2078207099
C	-2.9958729125	-0.8395149008	0.0339864097
C	-2.3279759245	-3.1537912440	-0.0624047163
C	-3.3391892877	-2.1586824431	0.0707183395
H	2.7961835968	1.7059142025	-0.8027315980
H	4.4793190962	-0.0320170277	-1.1276457961
H	3.8713292012	-2.4474646981	-0.8743959987
H	1.5668097611	-3.0989975833	-0.4852157586
H	1.4844849084	3.0397492683	-0.0064748545
H	-0.2736222706	4.7405667233	0.1936279013
H	-3.3300853603	1.7645483416	-0.1766130996
H	-2.6742208944	4.0870961927	-0.0819648030
H	-0.2769213893	-3.5812966596	-0.2936829905
H	-3.7756946083	-0.0961192392	0.1423897620
H	-2.6017776595	-4.2046125976	-0.0385251108
H	-4.3759585424	-2.4529065984	0.2005861248
C	2.0866516929	-0.1534679580	2.3079063950
H	2.1087788529	0.1938628500	3.3531849498
H	3.1271937281	-0.1269476374	1.9378581462
H	1.7663810545	-1.2106366471	2.3201741289

Ground state coordinates: M5e

C	0.8036979690	-1.4203972161	0.2547608193
C	-0.4890951618	-0.8762634342	0.6842432219
C	1.0349734018	-2.8126548649	0.1903447566
C	2.2511981099	-3.3334156376	-0.2122967165
C	3.2913080096	-2.4659253614	-0.5695428280
C	3.0905187999	-1.0987585846	-0.5167171167
C	1.8578653501	-0.5399621688	-0.1106153117
C	1.6523987680	0.9114440583	-0.0612589242
C	0.3988899608	1.4388030308	0.3515102442
C	-0.6885335851	0.5299840793	0.7294157841
C	-1.5584748604	-1.7212256636	1.0600653228
C	-2.7829565270	-1.2198127674	1.4621629998
C	-1.9497791219	1.0178783215	1.1444981036
C	-2.9819568204	0.1674714169	1.5063483006
C	2.6769967861	1.8158757335	-0.4197866969
C	0.2356881696	2.8416520748	0.3867312889
C	2.4911362945	3.1855187732	-0.3768761607
C	1.2558940456	3.7048124658	0.0311304239
H	0.2471675991	-3.5051154229	0.4599993676
H	2.3944509534	-4.4090635091	-0.2505560646
H	4.2517026998	-2.8605218587	-0.8874203031
H	3.9110336200	-0.4504472192	-0.7978480458
H	-1.4300363189	-2.7961551232	1.0377914349
H	-3.5820272061	-1.8985392359	1.7438113526
H	-2.1273208689	2.0850399180	1.1926355202
H	-3.9359004371	0.5769268822	1.8242053191
H	3.6409168589	1.4411582859	-0.7407308253
H	-0.7092770903	3.2691562041	0.6981435391
H	3.3008641889	3.8513861167	-0.6597147103
H	1.0956792387	4.7780323594	0.0693448025
O	-4.1637243690	0.5316372050	-1.6215971588
H	-3.5456640802	0.5452585530	-0.8782056424
C	-3.7783530593	-0.5291923717	-2.4766607868
H	-3.7912197413	-1.5082205786	-1.9734551955
H	-2.7780143161	-0.3846304190	-2.9130121810
H	-4.5010593215	-0.5623538947	-3.2969514439
	-0.7382699834		
C	1.8101703120	-2.0437410470	-0.5082814172
C	0.7732825320	-1.0747390262	-0.3494785771
C	-0.5939370383	-1.4250830262	-0.2325615258
C	-1.6333346595	-0.4082063991	-0.1338960888
C	-1.3077708889	0.9531338686	-0.2319658680
C	0.4445612112	2.7759029907	-0.1463269803

C	-0.5219002941	3.7072874271	-0.0286968613
C	-2.2741151837	2.0048593368	-0.1973838483
C	-1.9060412268	3.3205062808	-0.1286633702
C	-1.0172509956	-2.7966795347	-0.2078207099
C	-2.9958729125	-0.8395149008	0.0339864097
C	-2.3279759245	-3.1537912440	-0.0624047163
C	-3.3391892877	-2.1586824431	0.0707183395
H	2.7961835968	1.7059142025	-0.8027315980
H	4.4793190962	-0.0320170277	-1.1276457961
H	3.8713292012	-2.4474646981	-0.8743959987
H	1.5668097611	-3.0989975833	-0.4852157586
H	1.4844849084	3.0397492683	-0.0064748545
H	-0.2736222706	4.7405667233	0.1936279013
H	-3.3300853603	1.7645483416	-0.1766130996
H	-2.6742208944	4.0870961927	-0.0819648030
H	-0.2769213893	-3.5812966596	-0.2936829905
H	-3.7756946083	-0.0961192392	0.1423897620
H	-2.6017776595	-4.2046125976	-0.0385251108
H	-4.3759585424	-2.4529065984	0.2005861248
C	2.0866516929	-0.1534679580	2.3079063950
H	2.1087788529	0.1938628500	3.3531849498
H	3.1271937281	-0.1269476374	1.9378581462
H	1.7663810545	-1.2106366471	2.3201741289

Ground state coordinates: M5e

C	0.8036979690	-1.4203972161	0.2547608193
C	-0.4890951618	-0.8762634342	0.6842432219
C	1.0349734018	-2.8126548649	0.1903447566
C	2.2511981099	-3.3334156376	-0.2122967165
C	3.2913080096	-2.4659253614	-0.5695428280
C	3.0905187999	-1.0987585846	-0.5167171167
C	1.8578653501	-0.5399621688	-0.1106153117
C	1.6523987680	0.9114440583	-0.0612589242
C	0.3988899608	1.4388030308	0.3515102442
C	-0.6885335851	0.5299840793	0.7294157841
C	-1.5584748604	-1.7212256636	1.0600653228
C	-2.7829565270	-1.2198127674	1.4621629998
C	-1.9497791219	1.0178783215	1.1444981036
C	-2.9819568204	0.1674714169	1.5063483006
C	2.6769967861	1.8158757335	-0.4197866969
C	0.2356881696	2.8416520748	0.3867312889
C	2.4911362945	3.1855187732	-0.3768761607
C	1.2558940456	3.7048124658	0.0311304239
H	0.2471675991	-3.5051154229	0.4599993676
H	2.3944509534	-4.4090635091	-0.2505560646
H	4.2517026998	-2.8605218587	-0.8874203031
H	3.9110336200	-0.4504472192	-0.7978480458
H	-1.4300363189	-2.7961551232	1.0377914349
H	-3.5820272061	-1.8985392359	1.7438113526
H	-2.1273208689	2.0850399180	1.1926355202
H	-3.9359004371	0.5769268822	1.8242053191
H	3.6409168589	1.4411582859	-0.7407308253
H	-0.7092770903	3.2691562041	0.6981435391
H	3.3008641889	3.8513861167	-0.6597147103
H	1.0956792387	4.7780323594	0.0693448025
O	-4.1637243690	0.5316372050	-1.6215971588
H	-3.5456640802	0.5452585530	-0.8782056424
C	-3.7783530593	-0.5291923717	-2.4766607868
H	-3.7912197413	-1.5082205786	-1.9734551955
H	-2.7780143161	-0.3846304190	-2.9130121810
H	-4.5010593215	-0.5623538947	-3.2969514439