

Experimental and theoretical study on the absorption and fluorescence properties of substituted aryl hydrazones of 1,8-naphthalimide

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Table S1. PBE0/6-31G(d,p) computed and experimental absorption and emission maxima [nm] in acetonitrile solution for the series of substituted aryl hydrazones.

PBE0 6-31+G(d)				Substituent	PBE0 6-31G(d,p)		A_{exp}	PBE0 6-31G(d,p)		F_{exp}
A_{calc}	A_{cor}^a	F_{calc}	F_{cor}^a		A_{calc}	A_{cor}^a		F_{calc}	F_{cor}^a	
solvent acetonitrile										
514	570	631	737	4-N(CH ₃) ₂	494	547	476	604	706	
464	476	557	624	3,4-(OCH ₃) ₂	449	461	455	538	602	549
466	487	566		3,4-(OCH ₂ O)	453	477	453	548	659	547
464	475	557	613	4-OCH ₃	449	460	453	537	590	546
453	457	533	564	4-CH ₃	438	441	446	514	540	530
447	449	523	541	H	432	434	442	505	520	526
448	449	523	540	4-Cl	433	433	441	505	516	523
448	441	523	499	4-CN	435	427	438	508	479	512
486	521	597	660	4-NO ₂	461	485	455	559	618	

^a With correction for state-specific solvation.

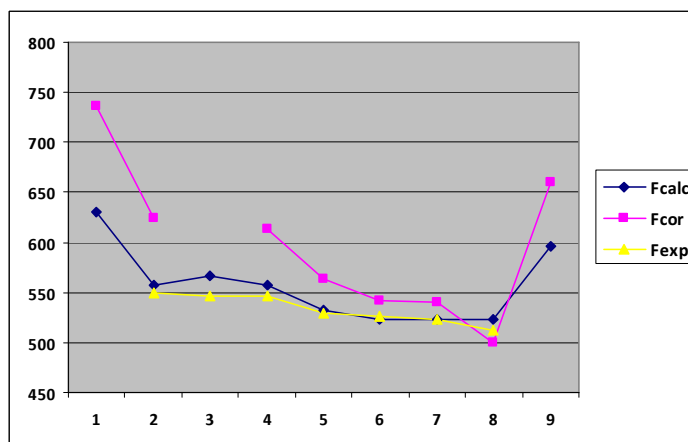
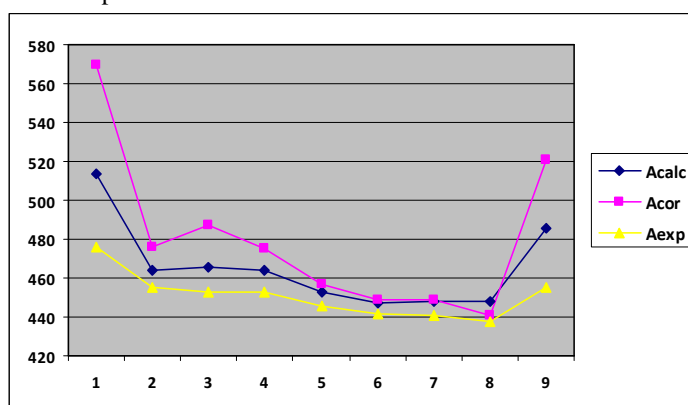


Figure S1. Graphical representation of the data in Table S1 for PBE0/6-31+G(d) calculations.

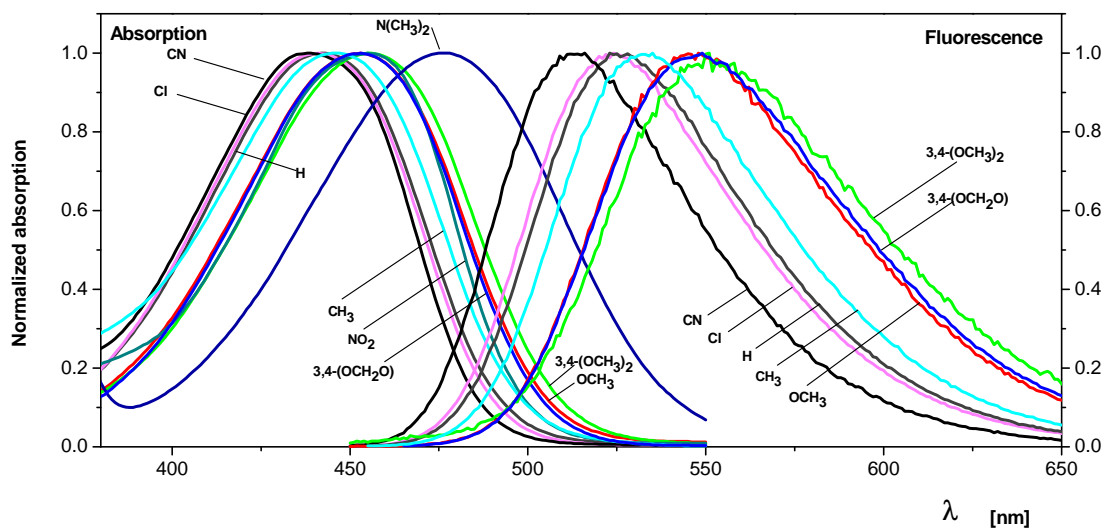


Figure S2. Normalized absorption and fluorescence spectra in acetonitrile solution for the series of substituted aryl hydrazones of *N*-hexyl-1,8-naphthalimide.

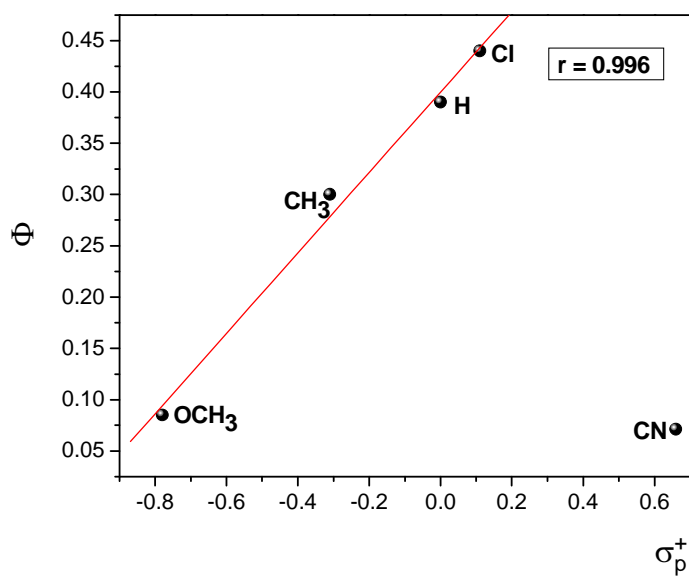


Figure S3. Dependence between experimental fluorescence quantum yield and σ_p^+ constants.

Table S2. Theoretical absorption maxima [nm] calculated with TDDFT method (three different functionals, two basis sets) in gas-phase and acetonitrile for the series of substituted aryl hydrazones.

Substituent	B3LYP	PBE0	PBE0	M06	B3LYP	CAM-B3LYP	B3LYP	PBE0	PBE0	M06	B3LYP	A _{exp}
	6-31G(d,p)			6-31+G(d)			6-31G(d,p)			6-31+G(d)		
solvent acetonitrile							gas phase					
4-N(CH ₃) ₂	520	494	514	497	544	418	470	450	463	454	486	476
3,4-(OCH ₃) ₂	467	449	464	456	485	401	441	424	436	432	454	455
3,4-(OCH ₂ O)	473	453	466	458	487	400	443	426	436	431	454	453
4-OCH ₃	467	449	464	457	485	402	439	423	435	431	453	453
4-CH ₃	454	438	453	448	472	397	430	415	426	424	443	446
H	448	432	447	443	465	395	425	410	422	419	438	442
4-Cl	448	433	448	444	465	395	425	410	422	420	438	441
4-CN	451	435	448	445	467	396	427	412	422	422	439	438
4-NO ₂	495	461	486	488	530	406	453	427	442	444	473	455

Table S3. Theoretical emission maxima [nm] calculated with TDDFT method (three different functionals, two basis sets) in gas-phase and acetonitrile for the series of substituted aryl hydrazones.

Substituent	B3LYP	PBE0	PBE0	M06	B3LYP	CAM-B3LYP	F _{exp}
	6-31G(d,p)			6-31+G(d)			
solvent acetonitrile							
4-N(CH ₃) ₂	636	604	631	608		513	
3,4-(OCH ₃) ₂	565	538	557	544	587	478	549
3,4-(OCH ₂ O)	576	548	566	553	597	478	547
4-OCH ₃	563	537	557	545	586	479	546
4-CH ₃	535	514	533	526	558	471	530
H	524	505	523	516	545	468	526
4-Cl	522	504	523	517	544	468	523
4-CN	526	508	523	521	543	470	512
4-NO ₂	614	559	597	605	668	501	

Table S4. PBE0/6-31+G(d) computed EPN and Hirshfeld charges at the bridge atoms for the **ground state** of substituted aryl hydrazones.

Substituent	EPN [a.u.]				σ_p	Hirshfeld [a.u.]				λ_{\max}^{abs} (exp.) [nm]
	C ₇	N ₁₇	N ₁₈	C ₁₉		C ₇	N ₁₇	N ₁₈	C ₁₉	
4-N(CH ₃) ₂	-14.6595	-18.2370	-18.2974	-14.6774	-0.83	0.0606	0.1267	-0.1023	0.0743	476
3,4-(OCH ₃) ₂	-14.6500	-18.2258	-18.2811	-14.6658		0.0615	0.1311	-0.0881	0.0820	455
3,4-(OCH ₂ O)	-14.6482	-18.2231	-18.2777	-14.6615		0.0616	0.1320	-0.0856	0.0823	453
4-OCH ₃	-14.6503	-18.2264	-18.2817	-14.6654	-0.27	0.0615	0.1300	-0.0903	0.0809	453
4-CH ₃	-14.6488	-18.2244	-18.2791	-14.6649	-0.17	0.0617	0.1319	-0.0850	0.0817	446
H	-14.6464	-18.2213	-18.2749	-14.6620	0	0.0619	0.1333	-0.0812	0.0827	442
4-Cl	-14.6416	-18.2148	-18.2661	-14.6528	0.23	0.0618	0.1352	-0.0783	0.0849	441
4-CN	-14.6324	-18.2023	-18.2504	-14.6407	0.66	0.0619	0.1418	-0.0680	0.0865	438
4-NO ₂	-14.6290	-18.1972	-18.2447	-14.6368	0.78	0.0619	0.1458	-0.0634	0.0876	455
r (with σ_p)	0.995	0.990	0.995	0.990		0.836	0.970	0.996	0.975	

Table S5. PBE0/6-31+G(d) computed EPN and Hirshfeld charges at the bridge atoms for the **excited state** of substituted aryl hydrazones.

Substituent	EPN [a.u.]				σ_p^+	Hirshfeld [a.u.]				λ_{\max}^{fl} (exp.) [nm]
	C ₇	N ₁₇	N ₁₈	C ₁₉		C ₇	N ₁₇	N ₁₈	C ₁₉	
4-N(CH ₃) ₂	-14.6875	-18.2151	-18.2601	-14.6470	-1.70	0.0248	0.1733	-0.0614	0.0735	570
3,4-(OCH ₃) ₂	-14.6595	-18.1827	-18.2421	-14.6286		0.0348	0.2041	-0.0597	0.0984	549
3,4-(OCH ₂ O)	-14.6637	-18.1858	-18.2408	-14.6269		0.0318	0.1993	-0.0569	0.0926	547
4-OCH ₃	-14.6582	-18.1818	-18.2418	-14.6272	-0.78	0.0356	0.2040	-0.0615	0.0985	546
4-CH ₃	-14.6474	-18.1727	-18.2401	-14.6252	-0.31	0.0423	0.2133	-0.0626	0.1064	533
H	-14.6405	-18.1672	-18.2375	-14.6228	0	0.0464	0.2170	-0.0631	0.1096	526
4-Cl	-14.6364	-18.1620	-18.2325	-14.6171	0.11	0.0465	0.2193	-0.0636	0.1080	523
4-CN	-14.6151	-18.1468	-18.2313	-14.6171	0.66	0.0570	0.2289	-0.0729	0.1019	512
4-NO ₂	-14.5734	-18.1315	-18.2325	-14.6167	0.79	0.0862	0.2231	-0.0870	0.1208	-
r (with σ_p^+)	0.924	0.986	0.946	0.943		0.869	0.958	0.714	0.873	0.998
r (with λ_{\max}^{fl})	0.987	0.986	0.930	0.932	0.998	0.981	0.976	0.702	0.842	

Table S6. MO6/6-31+G(d) computed EPN and Hirshfeld charges at the bridge atoms for the **ground state** of substituted aryl hydrazones.

Substituent	EPN [a.u.]				σ_p	Hirshfeld [a.u.]				A_{exp} [nm]	A_{MO6} [nm]
	C ₇	N ₁₇	N ₁₈	C ₁₉		C ₇	N ₁₇	N ₁₈	C ₁₉		
4-N(CH ₃) ₂	-14.6436	-18.2440	-18.3005	-14.6599	-0.83	0.0692	0.1110	-0.1113	0.0809	476	497
3,4-(OCH ₃) ₂	-14.6342	-18.2327	-18.2844	-14.6483	–	0.0699	0.1161	-0.0968	0.0881	455	456
3,4-(OCH ₂ O)	-14.6326	-18.2299	-18.2814	-14.6445	–	0.0699	0.1177	-0.0928	0.0886	453	458
4-OCH ₃	-14.6350	-18.2338	-18.2854	-14.6483	-0.27	0.0699	0.1144	-0.1000	0.0871	453	457
4-CH ₃	-14.6338	-18.2321	-18.2833	-14.6482	-0.17	0.0701	0.1162	-0.0949	0.0875	446	448
H	-14.6313	-18.2284	-18.2792	-14.6453	0	0.0700	0.1191	-0.0884	0.0889	442	443
4-Cl	-14.6265	-18.2223	-18.2696	-14.6358	0.23	0.0701	0.1196	-0.0878	0.0907	441	444
4-CN	-14.6175	-18.2100	-18.2538	-14.6236	0.66	0.0700	0.1256	-0.0775	0.0920	438	445
4-NO ₂	-14.6137	-18.2043	-18.2470	-14.6191	0.78	0.0699	0.1297	-0.0721	0.0930	455	488
r (with σ_p)	0.993	0.989	0.992	0.986		0.635	0.974	0.990	0.972		

Table S7. MO6/6-31+G(d) computed EPN and Hirshfeld charges at the bridge atoms for the **excited state** of substituted aryl hydrazones.

Substituent	EPN [a.u.]				σ_p^+	Hirshfeld [a.u.]				Fl_{exp} [nm]	Fl_{MO6} [nm]
	C ₇	N ₁₇	N ₁₈	C ₁₉		C ₇	N ₁₇	N ₁₈	C ₁₉		
4-N(CH ₃) ₂	-14.6714	-18.2185	-18.2625	-14.6296	-1.7	0.0297	0.1645	-0.0709	0.0786	570	608
3,4-(OCH ₃) ₂	-14.6427	-18.1889	-18.2479	-14.6142	–	0.0414	0.1920	-0.0719	0.1010	549	544
3,4-(OCH ₂ O)	-14.6475	-18.1914	-18.2465	-14.6124	–	0.0376	0.1889	-0.0666	0.0960	547	553
4-OCH ₃	-14.6426	-18.1892	-18.2477	-14.6133	-0.78	0.0418	0.1901	-0.0740	0.1008	546	545
4-CH ₃	-14.6331	-18.1822	-18.2474	-14.6127	-0.31	0.0483	0.1975	-0.0753	0.1067	530	526
H	-14.6261	-18.1764	-18.2452	-14.6105	0	0.0523	0.2024	-0.0731	0.1105	526	516
4-Cl	-14.6214	-18.1717	-18.2402	-14.6056	0.11	0.0531	0.2028	-0.0768	0.1071	523	517
4-CN	-14.6002	-18.1570	-18.2394	-14.6062	0.66	0.0637	0.2120	-0.0861	0.0989	512	521
4-NO ₂	-14.5555	-18.1391	-18.2374	-14.6020	0.79	0.0956	0.2071	-0.0981	0.1240	–	–
r (with σ_p^+)	0.913	0.976	0.962	0.952		0.865	0.964	-0.772	0.805	-0.995	-0.910
r (with Fl_{exp})	-0.978	-0.975	-0.903	-0.897	-0.995	-0.979	-0.967	0.741	-0.750		0.914

Cartesian coordinates of the optimized structures of the ground and excited states for the substituted aryl hydrazones of 1,8-naphthalimide calculated at M06/6-31+G(d) level of theory

4-N(CH₃)₂

Ground state S₀

C,0,-4.182842502,3.0264893621,0.
C,0,-2.8968981659,3.5792751189,0.
C,0,-1.7905352823,2.7535787252,0.
C,0,-1.9177715297,1.3482065057,0.
C,0,-3.2275983324,0.789142525,0.
C,0,-4.3480143965,1.6536973987,0.
C,0,-0.7900523661,0.4502687719,0.
C,0,-1.0070050771,-0.930674642,0.
C,0,-2.2985988926,-1.4415416414,0.
C,0,-3.4149405179,-0.6133071666,0.
C,0,-4.7502461687,-1.1942236248,0.
N,0,-5.8291723874,-0.2909403453,0.
C,0,-5.7092621367,1.0941961486,0.
C,0,-7.1894332401,-0.8185137292,0.
O,0,-4.9605393205,-2.4048007476,0.
O,0,-6.7171232153,1.79506833,0.
N,0,0.4731470375,0.9594370367,0.
N,0,1.5691533644,0.1537237962,0.
C,0,2.7075022933,0.7569684593,0.
C,0,3.9748601283,0.0593085359,0.
C,0,5.166409139,0.7989252484,0.
C,0,6.4064080262,0.184492658,0.
C,0,6.5145486441,-1.2253880848,0.
C,0,5.3079299969,-1.9718168301,0.
C,0,4.0794519856,-1.341941796,0.
N,0,7.7342722899,-1.8460690784,0.
C,0,7.8166611049,-3.2924700281,0.
C,0,8.9476727377,-1.0551483207,0.
H,0,-5.0649554294,3.6633297241,0.
H,0,-2.7676570401,4.6589510095,0.
H,0,-0.8105622973,3.227323564,0.
H,0,-0.1502308625,-1.5972340728,0.
H,0,-2.44991328,-2.5194546885,0.
H,0,-7.7259192776,-0.4716624698,0.8887686112
H,0,-7.1316265668,-1.9064656903,0.
H,0,-7.7259192776,-0.4716624698,-0.8887686112
H,0,0.6223340504,1.9665008705,0.
H,0,2.7578471634,1.8583402939,0.
H,0,5.1163076813,1.8888088262,0.
H,0,7.2981938291,0.8053440661,0.
H,0,5.3372861219,-3.0582334917,0.
H,0,3.1708836373,-1.9432376638,0.
H,0,8.8671187892,-3.5920294184,0.
H,0,7.3397253989,-3.7268703035,-0.8913154869
H,0,7.3397253989,-3.7268703035,0.8913154869
H,0,9.8123510024,-1.7224385481,0.
H,0,9.0139978213,-0.4126785328,0.8910316082
H,0,9.0139978213,-0.4126785328,-0.8910316082

4-N(CH₃)₂

Excited state S₁

C,0,-4.1654783547,3.0355221121,0.
C,0,-2.8902483774,3.57716099,0.
C,0,-1.7597591344,2.7575348334,0.
C,0,-1.8903499927,1.3470003778,0.
C,0,-3.2047190254,0.780955793,0.
C,0,-4.3365240962,1.6367873322,0.
C,0,-0.7889703463,0.4402201691,0.
C,0,-0.9762930244,-0.9475146507,0.
C,0,-2.2546748041,-1.4758638865,0.
C,0,-3.3731244787,-0.6263187852,0.
C,0,-4.7076826474,-1.2126431574,0.
N,0,-5.7786199373,-0.3212704203,0.
C,0,-5.6686711374,1.078844651,0.
C,0,-7.1340051701,-0.8563199434,0.
O,0,-4.8982548904,-2.4365922477,0.
O,0,-6.7059038826,1.7606606102,0.
N,0,0.5001835976,0.9648954792,0.
N,0,1.5785926781,0.2129077432,0.
C,0,2.7359791095,0.8370925287,0.
C,0,3.9649771093,0.1267471731,0.
C,0,5.1840618375,0.8480691624,0.
C,0,6.3989258097,0.2110073593,0.
C,0,6.4724454404,-1.2117410933,0.
C,0,5.2454060482,-1.9397831498,0.
C,0,4.0386573665,-1.2909749782,0.
N,0,7.6652152737,-1.8522207945,0.
C,0,7.7223311507,-3.3059304022,0.
C,0,8.9084708512,-1.096473583,0.
H,0,-5.0475144115,3.6717625666,0.
H,0,-2.7610793744,4.6584805196,0.
H,0,-0.7847471146,3.2405748239,0.
H,0,-0.1052038945,-1.5972469617,0.
H,0,-2.4100253105,-2.5517057994,0.
H,0,-7.674926913,-0.51236875,0.8875856688
H,0,-7.0704914119,-1.9442740737,0.
H,0,-7.674926913,-0.51236875,-0.8875856688
H,0,0.6144567015,1.9803214518,0.
H,0,2.7759467029,1.9356880416,0.
H,0,5.1522676299,1.9372469217,0.
H,0,7.3062127326,0.8072950698,0.
H,0,5.2565068108,-3.0256291531,0.
H,0,3.1159874157,-1.8675613447,0.
H,0,8.7660021272,-3.6227558193,0.
H,0,7.2356140739,-3.7210121204,-0.8925041117
H,0,7.2356140739,-3.7210121204,0.8925041117
H,0,9.7497635459,-1.7908232589,0.
H,0,8.9847531683,-0.4616693115,0.8926662417
H,0,8.9847531683,-0.4616693115,-0.8926662417

3,4-(OCH₃)₂
Ground state S₀

C,0,-4.1170499735,3.1536951626,2.0428082037
C,0,-4.2357037819,1.7602857891,2.1161647054
C,0,-3.1947651385,0.9549051133,1.7007054135
C,0,-1.9949065403,1.501999548,1.1960441855
C,0,-1.8778377173,2.9198960271,1.1240950948
C,0,-2.9574311417,3.7265909359,1.5555221196
C,0,-0.8832514814,0.7030995736,0.7489141507
C,0,0.2684046585,1.3272654959,0.2663636529
C,0,0.3491333804,2.7137785588,0.2109212233
C,0,-0.69864665,3.5235784053,0.6283016566
C,0,-0.5696742593,4.9735279427,0.5487015285
N,0,-1.6721470385,5.7279090035,0.9874482974
C,0,-2.8543224537,5.193608179,1.4882445611
C,0,-1.5989353283,7.1838980736,0.929058643
O,0,0.4354591629,5.5380808072,0.1255171027
O,0,-3.7572511215,5.9412961344,1.8513294626
N,0,-0.9665569719,-0.659879896,0.8007427552
N,0,0.0586057381,-1.444357661,0.3877668349
C,0,-0.1199296219,-2.714003097,0.4724794914
C,0,0.8947778912,-3.6746551223,0.0698675636
C,0,0.6178361964,-5.0426494585,0.2086958162
C,0,1.5446077247,-6.0036433526,-0.1559204177
C,0,2.7949832586,-5.6156402456,-0.6765832552
C,0,3.0783021499,-4.252095595,-0.812511986
C,0,2.1398867317,-3.2966682942,-0.444737908
O,0,1.2223349072,-7.3292633639,-0.0452689639
O,0,3.6386504387,-6.6122287484,-1.0175118549
C,0,4.9056990369,-6.2621447115,-1.5502322022
C,0,1.808209861,-7.9698327824,1.0836455993
H,0,-4.9305171033,3.7998240917,2.3660148976
H,0,-5.1482613489,1.3109667375,2.500345677
H,0,-3.3324705616,-0.1220826146,1.7769327758
H,0,1.1010928776,0.7157038819,-0.0664995196
H,0,1.253199462,3.1857766352,-0.1691510487
H,0,-2.4071787816,7.573056813,0.302058185
H,0,-0.632709819,7.4596085168,0.507973677
H,0,-1.7034309398,7.6049315622,1.934039382
H,0,-1.806049527,-1.1149383674,1.1529574817
H,0,-1.0630750523,-3.1285606198,0.8620002295
H,0,-0.3399027553,-5.3793589839,0.6072539405
H,0,4.0353098196,-3.927632183,-1.2129011654
H,0,2.3752007496,-2.2401636911,-0.5598841035
H,0,5.4173629489,-7.2042656982,-1.7557316054
H,0,5.4898095532,-5.6783774992,-0.8263047186
H,0,4.7976926176,-5.6936550303,-2.4834471317
H,0,1.4648519909,-9.0075178623,1.0721287647
H,0,1.4750050436,-7.4838350796,2.0121588373
H,0,2.9044859095,-7.9443860304,1.0263439711

3,4-(OCH₃)₂
Excited state S₁

C,0,-4.822786356,-2.469613621,-0.0554365697
C,0,-3.6139231844,-3.1436053703,-0.0969696852
C,0,-2.39955099,-2.4496660809,-0.0944482166
C,0,-2.3788966252,-1.0379444031,-0.0500266247
C,0,-3.6240937567,-0.3354075972,-0.0054241362
C,0,-4.8412183867,-1.0615965891,-0.0084326173
C,0,-1.1869077775,-0.2461552514,-0.0460640016
C,0,-1.22904027,1.1603213802,0.0039453657
C,0,-2.4416172548,1.8148737128,0.0471673752
C,0,-3.6415652004,1.0803350146,0.0419765635
C,0,-4.908847287,1.807803584,0.0840688713
N,0,-6.0677830242,1.0394220282,0.0770536927
C,0,-6.1072737273,-0.3639658032,0.0361404449
C,0,-7.3582052571,1.7162840014,0.1166548938
O,0,-4.9572963682,3.0428355003,0.1242702239
O,0,-7.2082048927,-0.9325426585,0.0397195431
N,0,0.0373014064,-0.8824465874,-0.0934759632
N,0,1.1825358921,-0.2311960807,-0.0844705354
C,0,2.2740118491,-0.9619458106,-0.1387262963
C,0,3.5676139694,-0.3665660964,-0.1325284083
C,0,4.707452063,-1.2015847249,-0.185648717
C,0,5.9778879515,-0.6735865983,-0.1800463359
C,0,6.159342347,0.7337052817,-0.121577055
C,0,5.0322250692,1.5709601511,-0.0614144124
C,0,3.7614465729,1.0327844535,-0.067970131
O,0,7.0583420037,-1.4979144497,-0.2805515997
O,0,7.4234366328,1.1654487199,-0.1381362154
C,0,7.6714892839,2.5664843375,-0.088479229
C,0,7.7516605485,-1.7064368581,0.9490714559
H,0,-5.7673744697,-3.0084990813,-0.0583227481
H,0,-3.6011713399,-4.2315563713,-0.1323958953
H,0,-1.4827091063,-3.0349722671,-0.1264965466
H,0,-0.2953001217,1.7154432288,0.0063287275
H,0,-2.4899430407,2.8998338053,0.084283741
H,0,-7.9493574117,1.4467968867,-0.7643058386
H,0,-7.1795077698,2.7910146838,0.1329127255
H,0,-7.9132895535,1.4152515919,1.0109507712
H,0,0.0571073946,-1.9046733739,-0.137658278
H,0,2.2097963499,-2.0579921666,-0.1879917953
H,0,4.5974255262,-2.2847873723,-0.2343168508
H,0,5.1549134163,2.6495524065,-0.015948361
H,0,2.8951307048,1.6891758934,-0.0257739446
H,0,8.7561888986,2.6776235409,-0.1166042556
H,0,7.2791494263,2.996904472,0.8412305253
H,0,7.2254500498,3.069962623,-0.9547840871
H,0,8.5737463024,-2.3921239505,0.7313363213
H,0,7.0785274769,-2.1609110266,1.6894185792
H,0,8.1530395622,-0.7631965991,1.3411643924

3,4-(OCH₂O)

Ground state S₀

C,0,-3.2472564939,3.4387171986,2.3254582646
C,0,-3.3770726797,2.0454857905,2.3861878308
C,0,-2.3491140015,1.2352858344,1.9485917293
C,0,-1.1513860373,1.7772890987,1.4332313366
C,0,-1.0228752526,3.1950774292,1.3747322487
C,0,-2.0896430022,4.0066817436,1.8281109427
C,0,-0.0517593341,0.9744341329,0.9655686537
C,0,1.0989839835,1.5937929396,0.4754998329
C,0,1.191275619,2.9800781234,0.4331977559
C,0,0.1554854906,3.7937342007,0.8713594838
C,0,0.2970665508,5.2434996249,0.806779165
N,0,-0.7922617079,6.0027967358,1.2684856768
C,0,-1.9746849432,5.4735172728,1.7741288031
C,0,-0.7055070358,7.4585471102,1.2268752268
O,0,1.3020661072,5.8030550455,0.3769733935
O,0,-2.868087782,6.225116744,2.1521631341
N,0,-0.1424124165,-0.389815567,1.0050922285
N,0,0.8819185586,-1.1689977472,0.5858641024
C,0,0.7090118158,-2.4403351388,0.6441414624
C,0,1.7399476095,-3.383623511,0.232654761
C,0,1.446718038,-4.762079987,0.3208076404
C,0,2.4290614184,-5.6381051458,-0.0742714163
C,0,3.6654976917,-5.2007513128,-0.5354478661
C,0,3.9788070948,-3.859334165,-0.6246567922
C,0,2.9901752196,-2.9533144223,-0.2340911728
C,0,3.569625184,-7.3998884258,-0.7837526849
O,0,2.4170834335,-7.0050079072,-0.0460364101
O,0,4.4527388918,-6.2797723982,-0.8103286622
H,0,-4.050240114,4.0883407775,2.6672969076
H,0,-4.2879863994,1.6002580948,2.7789048763
H,0,-2.4945112211,0.158707588,2.0160675017
H,0,1.9219789902,0.9787173939,0.1256098906
H,0,2.0946853231,3.448603479,0.0473559569
H,0,-1.5059499767,7.8631419242,0.5994915987
H,0,0.2655957651,7.7299079193,0.8142558678
H,0,-0.8124383405,7.8683744219,2.236119145
H,0,-0.9847130308,-0.8457230356,1.3494752824
H,0,-0.2350596425,-2.8692746975,1.0145588986
H,0,0.4843555125,-5.1130185059,0.6892737356
H,0,4.9505294531,-3.5261315415,-0.9804452635
H,0,3.1894363449,-1.885387771,-0.2935723856
H,0,4.057938679,-8.2379795003,-0.2827220343
H,0,3.2759576373,-7.6534078432,-1.8136076462

3,4-(OCH₂O)

Excited state S₁

C,0,-3.2780165158,3.4232325745,2.2861072379
C,0,-3.4059777384,2.0445804686,2.3237483551
C,0,-2.3658347526,1.211951965,1.9007082365
C,0,-1.1528158618,1.7597529176,1.4265057278
C,0,-1.016356009,3.1838578443,1.3796621151
C,0,-2.0862332701,4.0058489347,1.813382156
C,0,-0.0363827911,0.9859930006,0.9803719135
C,0,1.1417632325,1.5889699482,0.5050112385
C,0,1.2484519203,2.963577472,0.4645026624
C,0,0.1809470122,3.7693115557,0.8991432272
C,0,0.3292765247,5.2206357554,0.8445552947
N,0,-0.7544490691,5.9739177296,1.2868195964
C,0,-1.9615552927,5.446762661,1.7720763835
C,0,-0.6569441871,7.4278807962,1.2543145804
O,0,1.3598182463,5.7647310971,0.4290116671
O,0,-2.8525392592,6.2268130551,2.1376372846
N,0,-0.1190746483,-0.395477555,1.019350452
N,0,0.8492997524,-1.1733555572,0.5899541222
C,0,0.6677435502,-2.4713418564,0.6899795394
C,0,1.6647620136,-3.3846752265,0.2391223284
C,0,1.4225015716,-4.7788214114,0.3609645222
C,0,2.4019702648,-5.6183249413,-0.0923377129
C,0,3.5943826928,-5.140147517,-0.6528456089
C,0,3.8597025772,-3.7852084279,-0.7814620853
C,0,2.8800670148,-2.9150430538,-0.3287647191
C,0,3.6511688624,-7.3706029012,-0.6959108279
O,0,2.4250400501,-6.9750035013,-0.0914244937
O,0,4.3732808738,-6.1752212452,-1.0105209312
H,0,-4.0866178616,4.0719728526,2.6143569653
H,0,-4.3294156717,1.5957670272,2.685760363
H,0,-2.5277513154,0.1368618316,1.9462750148
H,0,1.96175145,0.956959551,0.176019814
H,0,2.1537935154,3.4424576932,0.1010736571
H,0,-1.4464853735,7.8429741458,0.6197035488
H,0,0.3216509673,7.6954160385,0.8564000197
H,0,-0.7752493631,7.8348549809,2.2636930841
H,0,-0.96283503,-0.8283031595,1.4032237946
H,0,-0.2576896316,-2.8777908407,1.1196690384
H,0,0.498292058,-5.1548545998,0.7940452786
H,0,4.7897210726,-3.4307610893,-1.2169424311
H,0,3.033971215,-1.8415339621,-0.4063088934
H,0,4.2366295106,-7.9674635227,0.0107316554
H,0,3.4492186932,-7.9199395278,-1.6219821715

4-OCH₃
Ground state S₀

C,0,-4.2562702015,3.185034702,2.0021845846
C,0,-4.3599529723,1.7899923739,2.057131462
C,0,-3.3004818141,1.002063193,1.6554436202
C,0,-2.0967296694,1.5693160317,1.1835693224
C,0,-1.9947690765,2.9884484272,1.1290873325
C,0,-3.0936964407,3.7772247688,1.5459867518
C,0,-0.9661139551,0.7867553445,0.7542828442
C,0,0.1875706515,1.4291438785,0.3010201526
C,0,0.2530094227,2.81714951,0.2610455669
C,0,-0.8124824749,3.6117595415,0.6649920362
C,0,-0.6996659482,5.063828576,0.6060504966
N,0,-1.820155346,5.7998004941,1.0317766637
C,0,-3.007509443,5.2456718814,1.4969871965
C,0,-1.76169353,7.257344559,0.9938537657
O,0,0.306705002,5.6463251229,0.210637698
O,0,-3.9285163946,5.9781653952,1.8455027663
N,0,-1.0396095502,-0.5756601437,0.7969442241
N,0,-0.0036038678,-1.3580656082,0.404228343
C,0,-0.1895864009,-2.6272487369,0.4895338634
C,0,0.8199327895,-3.6004618345,0.1090727852
C,0,0.5253863347,-4.9675828023,0.2375342559
C,0,1.4524247471,-5.9332941766,-0.1110368521
C,0,2.7074795403,-5.5528837821,-0.6007838637
C,0,3.0194026791,-4.1935517071,-0.7359448359
C,0,2.0793336873,-3.2348913747,-0.382257652
O,0,3.5495686684,-6.5629748234,-0.9160506517
C,0,4.8349003648,-6.2360736177,-1.4170878154
H,0,-5.0832459638,3.8189032966,2.31546444
H,0,-5.2752536502,1.3258396809,2.4163221839
H,0,-3.4280495424,-0.0770813285,1.7162644425
H,0,1.0336673233,0.8293171498,-0.0200943545
H,0,1.1605553111,3.3007964812,-0.0952276622
H,0,-2.5501911423,7.6460414742,0.341736292
H,0,-0.7836486215,7.5488576909,0.6124425243
H,0,-1.9088787967,7.6633996439,1.9996003479
H,0,-1.884917963,-1.0350247763,1.1290474774
H,0,-1.1434450596,-3.0324266179,0.8629538883
H,0,-0.4499877538,-5.2719348949,0.6182469451
H,0,1.2278295574,-6.9937872998,-0.0128971438
H,0,3.9873813844,-3.8750162996,-1.1139883637
H,0,2.3252814073,-2.1794332119,-0.4886589832
H,0,5.3388767509,-7.1864940447,-1.6022228529
H,0,5.4085963359,-5.6550797966,-0.6826148756
H,0,4.7604066205,-5.6726503397,-2.3568433666

4-OCH₃
Excited state S₁

C,0,-4.2672261105,3.1520265884,2.0066675702
C,0,-4.3521657477,1.7712120105,2.0540607066
C,0,-3.2817395326,0.967279413,1.6483167378
C,0,-2.0836763507,1.5507909862,1.178595799
C,0,-1.9888467269,2.9760528855,1.1268976996
C,0,-3.0877375037,3.76897662,1.543768539
C,0,-0.9403860288,0.8076595582,0.7440341041
C,0,0.2285802674,1.4433308097,0.2850165803
C,0,0.296524731,2.8202426604,0.2442166209
C,0,-0.802130001,3.5947511181,0.6611798418
C,0,-0.696145257,5.0522022137,0.604823145
N,0,-1.8071470726,5.773595642,1.0271404504
C,0,-3.0060943124,5.2112799155,1.4969967612
C,0,-1.7525253319,7.2300579752,0.9906800148
O,0,0.3252554166,5.6222348024,0.2035804559
O,0,-3.9252160328,5.9662145378,1.8447123735
N,0,-0.99604139,-0.5703129659,0.7800756858
N,0,0.001034693,-1.3454626188,0.4023579913
C,0,-0.2066077956,-2.6407529277,0.4963634013
C,0,0.7852122896,-3.5895313119,0.122488219
C,0,0.4986022538,-4.9713092494,0.2481664572
C,0,1.4288285662,-5.9201508445,-0.1018483408
C,0,2.6878029413,-5.5233201165,-0.5934708756
C,0,2.9942795965,-4.1559806344,-0.7267012198
C,0,2.0544419435,-3.2093707379,-0.3729407678
O,0,3.5267766815,-6.5182452752,-0.9076547628
C,0,4.819083665,-6.200147267,-1.4114448333
H,0,-5.0982451589,3.7787547519,2.3216350217
H,0,-5.2643350783,1.2968628382,2.4120130832
H,0,-3.4100600078,-0.1113734691,1.7093070762
H,0,1.0684468811,0.8321384563,-0.0335193823
H,0,1.192381091,3.3246028235,-0.10774474
H,0,-2.5426909531,7.6185826172,0.3402256023
H,0,-0.7754108824,7.5258634126,0.6094590338
H,0,-1.9018536417,7.6359966626,1.9963225555
H,0,-1.8542640817,-1.0137858804,1.1168953822
H,0,-1.16609827,-3.0233224506,0.8717479179
H,0,-0.4746827315,-5.2800810119,0.6282446561
H,0,1.219531747,-6.9836954332,-0.0094921233
H,0,3.9610177803,-3.8347473572,-1.1043939349
H,0,2.2870160759,-2.1511699151,-0.4742656268
H,0,5.3126599945,-7.1558969312,-1.5923019456
H,0,5.3914096749,-5.6222503171,-0.6752811999
H,0,4.7422927093,-5.6402405837,-2.3516947309

4-CH₃

Ground state S₀

C,0,-3.8117796585,3.4189974351,2.4641713411
C,0,-3.9159378211,2.0240865209,2.5309463903
C,0,-2.8761341182,1.2313108791,2.0895552408
C,0,-1.6918636947,1.7932051429,1.5643988851
C,0,-1.5903123759,3.2122756105,1.497296722
C,0,-2.6684450654,4.0058816876,1.9559258955
C,0,-0.5813624111,1.00783355482,1.0920145734
C,0,0.5519159197,1.6448866348,0.5848365029
C,0,0.6174793967,3.0327229599,0.5334590545
C,0,-0.4282806052,3.8300495204,0.9788252456
C,0,-0.3149038245,5.2819700653,0.9061418335
N,0,-1.4137989718,6.0229452416,1.3755541667
C,0,-2.5811734383,5.4741197718,1.8950726169
C,0,-1.3546262222,7.4799707882,1.3270356231
O,0,0.6748391354,5.8585772703,0.4636677592
O,0,-3.4845189676,6.2105972189,2.2792293404
N,0,-0.6499355153,-0.3562794697,1.1457974517
N,0,0.3689593817,-1.1333628086,0.706456401
C,0,0.2033751271,-2.4035024152,0.8071353426
C,0,1.2078655163,-3.3630578378,0.3740711231
C,0,0.9399280502,-4.7277639381,0.5261094973
C,0,1.8682482408,-5.6836883803,0.1259761204
C,0,3.0880813124,-5.3064114933,-0.4382312108
C,0,3.3531095065,-3.9358763877,-0.586063805
C,0,2.4348962125,-2.9775110124,-0.1902063507
C,0,4.0903305348,-6.3248247925,-0.8886534639
H,0,-4.6239139766,4.0557565312,2.8086686331
H,0,-4.8163778847,1.5638437615,2.9304199508
H,0,-3.0030774864,0.1526750641,2.1608331349
H,0,1.3830871499,1.0427988496,0.2312200446
H,0,1.5083743221,3.5149414768,0.1356610124
H,0,-2.1705490836,7.8667515777,0.7084366113
H,0,-0.3941260068,7.7678497533,0.9010607519
H,0,-1.4561933872,7.8920028815,2.3359621266
H,0,-1.4753948781,-0.8178798016,1.5218176609
H,0,-0.7235028877,-2.8202694476,1.2320225035
H,0,-0.0078864394,-5.042126253,0.9644170196
H,0,1.6417915807,-6.7424696415,0.2535174027
H,0,4.3030105882,-3.6235906146,-1.0222068938
H,0,2.6574237148,-1.9184712264,-0.312495663
H,0,5.0855100134,-6.1177545053,-0.4733308213
H,0,4.1958882602,-6.3183643982,-1.9825069212
H,0,3.7995257569,-7.3380847678,-0.58782985

4-CH₃

Excited state S₁

C,0,-3.835709679,3.3864589588,2.4504410046
C,0,-3.9237600498,2.006343781,2.5014020086
C,0,-2.8692972545,1.1977181655,2.0609412422
C,0,-1.6854949128,1.7759271365,1.5559975366
C,0,-1.5896063734,3.2007914386,1.4953707063
C,0,-2.6702578261,3.9980878101,1.9461202243
C,0,-0.5549788719,1.0292512904,1.089133807
C,0,0.5984116607,1.6641946517,0.579757671
C,0,0.6637710497,3.0383947687,0.5281336239
C,0,-0.4197461085,3.814708025,0.9836651324
C,0,-0.3127778847,5.2728575843,0.9158988899
N,0,-1.4044066657,5.9988491632,1.375299414
C,0,-2.5863732438,5.4413825931,1.8912055806
C,0,-1.3477905546,7.4550554836,1.3301853157
O,0,0.6951536265,5.8349643601,0.4736405356
O,0,-3.4901173771,6.1984864026,2.2701714175
N,0,-0.5967741341,-0.3428989301,1.1417888798
N,0,0.3868421098,-1.1116525523,0.7071412092
C,0,0.208287757,-2.4057343079,0.8360132969
C,0,1.1883749279,-3.3478466504,0.4007996459
C,0,0.9304486057,-4.724494924,0.569396995
C,0,1.8527288397,-5.6705088909,0.1575569975
C,0,3.0625572558,-5.2858483708,-0.4372312059
C,0,3.320278711,-3.9118141917,-0.6022105431
C,0,2.4108221049,-2.9572926219,-0.1964156851
C,0,4.0590060188,-6.2981976378,-0.8997758176
H,0,-4.6543286589,4.0153930779,2.7918014324
H,0,-4.8255497428,1.534668045,2.8876969779
H,0,-3.0012385481,0.1193078141,2.1192366487
H,0,1.4265482273,1.0510777813,0.2364548491
H,0,1.5447387747,3.5428533126,0.1409083775
H,0,-2.1620158972,7.8423937265,0.7095610497
H,0,-0.3858624643,7.7468140887,0.909419793
H,0,-1.4559003939,7.8656322407,2.3391247662
H,0,-1.4248263592,-0.7924291521,1.5416684499
H,0,-0.7148699597,-2.7975532965,1.2862165215
H,0,-0.0064352116,-5.0384798278,1.0292978883
H,0,1.6395495638,-6.7302504444,0.2945766373
H,0,4.2596429414,-3.6020930614,-1.0610301184
H,0,2.6227894781,-1.8982278468,-0.3301221453
H,0,5.0577942636,-6.0872044436,-0.4943036216
H,0,4.1555646969,-6.2802641788,-1.9948441066
H,0,3.7743525584,-7.3140573714,-0.6039022825

H

Ground state S_0

C,0,-3.3151639658,3.0402156414,1.9362350421
C,0,-3.4413950187,1.6459702134,1.9851959049
C,0,-2.3817560911,0.8419790639,1.6179338231
C,0,-1.1541284642,1.3915450358,1.1872560431
C,0,-1.0301913204,2.810176805,1.1389003359
C,0,-2.1295602376,3.6153347532,1.5201169912
C,0,-0.0210524946,0.5963312075,0.7942946854
C,0,1.1552259339,1.2222641523,0.3810251884
C,0,1.2423483514,2.609438279,0.3455648091
C,0,0.1754747247,3.4160170552,0.7154756587
C,0,0.3129597235,4.8672231152,0.6621294622
N,0,-0.8085017244,5.6196710289,1.0512940991
C,0,-2.0191459155,5.0830049659,1.4763538133
C,0,-0.7270405022,7.0760536409,1.017509757
H,0,-1.4874654222,7.4773741822,0.3402897804
H,0,0.2672596823,7.3532625775,0.6689826769
H,0,-0.9009526594,7.4835232181,2.018338671
O,0,1.3413265122,5.432222468,0.3007834098
O,0,-2.9396168623,5.8290055649,1.7954365568
N,0,-0.1046500691,-0.7701420887,0.8285028099
H,0,-0.9596553902,-1.2330304616,1.1298100368
N,0,0.9459023179,-1.5383054851,0.4635233748
C,0,0.7929606956,-2.8116429639,0.5221197032
H,0,-0.1559313661,-3.2589801549,0.8563839783
C,0,1.8624762462,-3.7304446501,0.1508795655
C,0,1.6300197792,-5.108625153,0.238070541
C,0,2.6263735646,-6.0174435732,-0.1077671206
C,0,3.8661034532,-5.5572631226,-0.5445981981
C,0,4.1059126305,-4.1837146347,-0.6343104726
C,0,3.114854599,-3.2755148303,-0.2903219183
H,0,5.074619536,-3.8225032178,-0.9756533603
H,0,2.4332652015,-7.0863473101,-0.0356924663
H,0,3.2994933201,-2.2047420583,-0.3594821599
H,0,0.6584665645,-5.4665029777,0.5803501532
H,0,-4.3750809332,1.1953227941,2.3128272389
H,0,2.1666605624,3.0834940278,0.0209144654
H,0,2.0035012361,0.6123638075,0.0868852949
H,0,-4.1433389904,3.6847245373,2.2232254756
H,0,-2.5259776056,-0.2354865628,1.67205338
H,0,4.6470003978,-6.2657288902,-0.8157370299

H

Excited state S_1

C,0,-3.3952683192,2.499247261,0.0004048835
C,0,-2.1826985775,3.1656918978,0.0005776978
C,0,-0.9709248424,2.4633045827,0.0002894723
C,0,-0.9600583218,1.0537803787,-0.0001157434
C,0,-2.2094586804,0.3584108324,-0.0001884722
C,0,-3.421743256,1.0899494359,0.0000834356
C,0,0.2285068151,0.2512312963,-0.0003307232
C,0,0.172765106,-1.1622385403,-0.0005636228
C,0,-1.0423785799,-1.8054732025,-0.0005058004
C,0,-2.2370157425,-1.0579864442,-0.0003927297
C,0,-3.5110631114,-1.7795230986,-0.0005224732
N,0,-4.6641623889,-1.0057563218,0.0000949233
C,0,-4.6938579941,0.3984962757,0.0001559056
C,0,-5.9590078666,-1.6761172061,0.0003329243
H,0,-6.5297573714,-1.3874766897,0.8885726328
H,0,-5.7864155912,-2.7520098375,0.000225528
H,0,-6.5300862399,-1.3874903748,-0.8876894498
O,0,-3.5619413072,-3.0140131211,-0.0010163516
O,0,-5.7892014688,0.9749684636,0.0001972759
N,0,1.4549703694,0.8648530038,-0.0003392258
H,0,1.4978302313,1.8874750289,-0.0008084333
N,0,2.5899116851,0.1843335393,-0.0001521686
C,0,3.6980874771,0.8836219876,-0.0006867445
H,0,3.67172831,1.9823068873,-0.0012911636
C,0,4.9759834958,0.2372058949,-0.000240977
C,0,6.1456126231,1.0256158826,-0.0007050518
C,0,7.3956537877,0.4264382079,-0.0002214068
C,0,7.502603957,-0.9667297207,0.0007230457
C,0,6.3494588319,-1.759791998,0.0012333667
C,0,5.0975522732,-1.1713471141,0.0007606575
H,0,6.4376937975,-2.8444603001,0.0020271314
H,0,8.2927514054,1.0422605646,-0.000546563
H,0,4.1965952522,-1.7816376904,0.0011344631
H,0,6.0556923782,2.1117544308,-0.0014258265
H,0,-2.1621355992,4.2539705895,0.0009275967
H,0,-1.1017823362,-2.8902357616,-0.0006352174
H,0,1.1027822268,-1.72265803,-0.0006753526
H,0,-4.3364228432,3.0436151116,0.0006898117
H,0,-0.0499578106,3.0427338707,0.0005520688
H,0,8.484554408,-1.4362894296,0.0011234136

4-C1

Ground state S_0

C,0,-3.2633859198,3.0249018637,2.0405859847
C,0,-3.358322626,1.6295172459,2.1136771066
C,0,-2.3011364476,0.8423099146,1.7060535054
C,0,-1.1073256324,1.410968587,1.209466396
C,0,-1.0146632498,2.8299427862,1.1367049323
C,0,-2.1114177916,3.6178213679,1.5603066232
C,0,0.021200509,0.6323853439,0.7727871328
C,0,1.1634295103,1.2734887842,0.2952292966
C,0,1.2208519503,2.6622772887,0.2374772649
C,0,0.1569669325,3.4537181639,0.6477149153
C,0,0.260632235,4.9071446636,0.56966879
N,0,-0.8568118839,5.6416663086,1.0028655847
C,0,-2.0341721976,5.0863538327,1.4925405967
C,0,-0.8076573094,7.0990066607,0.9465450714
O,0,1.2580620834,5.4883903301,0.1521975227
O,0,-2.9538160213,5.8175399906,1.8460151082
N,0,-0.0433654106,-0.7338069849,0.8329160077
N,0,0.9888219422,-1.5092480664,0.4350937914
C,0,0.8238564331,-2.7791946634,0.5333074461
C,0,1.854583276,-3.7298882217,0.1404686231
C,0,1.5917880273,-5.0979859272,0.2807203684
C,0,2.5392520722,-6.0496314175,-0.0784425386
C,0,3.7600496335,-5.6185232398,-0.5824782913
C,0,4.0501901612,-4.2631542684,-0.7334690585
C,0,3.0964078431,-3.324657899,-0.3714298042
Cl,0,4.9651808757,-6.8023686155,-1.0399840009
H,0,-4.0894193099,3.6575567394,2.3586511944
H,0,-4.265690902,1.1650047584,2.4919111104
H,0,-2.4220401526,-0.2366414087,1.7817680867
H,0,2.0084907156,0.6751818465,-0.0314043139
H,0,2.1198242386,3.1472642875,-0.1378929664
H,0,-1.6081835114,7.4749941428,0.3017514804
H,0,0.1626171447,7.3919183556,0.5469379759
H,0,-0.9419977207,7.516262341,1.9494508105
H,0,-0.8808353825,-1.1945386413,1.1827275572
H,0,-0.1150237711,-3.2011543631,0.923166546
H,0,0.6302679093,-5.4233923708,0.6773522689
H,0,2.3332410836,-7.1120944448,0.0312526037
H,0,5.0141262639,-3.9523296999,-1.1307304376
H,0,3.3089813997,-2.263102371,-0.4837682909

4-C1

Excited state S_1

C,0,-3.281666905,2.9957522797,2.0486990236
C,0,-3.3568598829,1.6154681199,2.1134426632
C,0,-2.2854453903,0.8140855278,1.7003888452
C,0,-1.101915738,1.3971461143,1.2075678058
C,0,-1.017463453,2.8220567733,1.1379720785
C,0,-2.1132793586,3.6118155425,1.5611720086
C,0,0.0442194506,0.6557625699,0.7628206891
C,0,1.206004095,1.3014082574,0.2772281298
C,0,1.2596117504,2.67430746,0.2213997384
C,0,0.1570719505,3.4439693376,0.6478232084
C,0,0.2524656698,4.9028565834,0.5729703691
N,0,-0.8557319177,5.6226776095,1.0028910834
C,0,-2.0417085717,5.058038064,1.4962505511
C,0,-0.8110322456,7.0794583318,0.9485618736
O,0,1.2649567953,5.4699846541,0.1496917274
O,0,-2.9617260174,5.8054191508,1.8494667968
N,0,0.0101183484,-0.7115612327,0.8106349631
N,0,1.0176810721,-1.4773803065,0.4225554067
C,0,0.8278407778,-2.7710586419,0.531510231
C,0,1.8328511448,-3.7118717001,0.1488219639
C,0,1.5648544952,-5.0902559185,0.291460596
C,0,2.5064732888,-6.0387345257,-0.0654092189
C,0,3.7342386288,-5.6109100412,-0.5721973594
C,0,4.0311548308,-4.2535491763,-0.7259980837
C,0,3.0865876524,-3.3112010916,-0.3677870718
Cl,0,4.92781895,-6.7957208135,-1.0249992081
H,0,-4.1115243341,3.6212646696,2.3685091522
H,0,-4.2595586559,1.1383034602,2.4901342704
H,0,-2.4056140838,-0.264640952,1.7757980284
H,0,2.0455087897,0.693405551,-0.0469231002
H,0,2.1438019081,3.1859409715,-0.1486685872
H,0,-1.6131840427,7.4543521584,0.3050767807
H,0,0.1582771455,7.3769603073,0.5494187962
H,0,-0.9476987143,7.4953560842,1.9517688334
H,0,-0.8357272189,-1.1673919085,1.1638397274
H,0,-0.1197159026,-3.1653705594,0.9242589878
H,0,0.6019592156,-5.4098214442,0.6885239427
H,0,2.300104377,-7.1009741103,0.0444478274
H,0,4.9971989054,-3.9504726348,-1.1239189142
H,0,3.3026101904,-2.2509715207,-0.4814925557

4-CN

Ground state S_0

C,0,-4.0922411604,3.078810998,2.0460192906
C,0,-4.1976870623,1.6834780879,2.1133822762
C,0,-3.147780851,0.8895903135,1.7014059868
C,0,-1.9498697415,1.4515203575,1.2054517417
C,0,-1.8467145229,2.870026658,1.138752234
C,0,-2.9366367837,3.6647520857,1.5669390097
C,0,-0.827885525,0.6686918369,0.7638845808
C,0,0.3179418448,1.3008991273,0.2880510769
C,0,0.3864787112,2.690377222,0.2360245153
C,0,-0.6708817016,3.4864424676,0.6510250092
C,0,-0.5562532036,4.9408877076,0.5791112833
N,0,-1.6668352973,5.6817113378,1.0164653606
C,0,-2.8481063408,5.1331497432,1.5052252878
C,0,-1.6066955218,7.1390122525,0.9664985762
O,0,0.4454665386,5.5144898327,0.1628631508
O,0,-3.7614755513,5.8695697468,1.8627671302
N,0,-0.9038213326,-0.7006951191,0.8185097053
N,0,0.1166096906,-1.4807486481,0.4187488093
C,0,-0.0555375665,-2.750880545,0.510139359
C,0,0.9747725085,-3.6982972644,0.109406969
C,0,0.7061298096,-5.0674363311,0.2417263828
C,0,1.6503741786,-6.0138142997,-0.124140293
C,0,2.8852956821,-5.5925877692,-0.6312211071
C,0,3.1655533853,-4.2232309884,-0.7682605755
C,0,2.216768935,-3.2869536354,-0.4003823756
C,0,3.8663008628,-6.559706708,-1.0116065881
N,0,4.6661533271,-7.3468288644,-1.3217744589
H,0,-4.913179025,3.7161314216,2.3678353844
H,0,-5.1082015497,1.2246378136,2.4909087164
H,0,-3.277451001,-0.1885627893,1.7731333249
H,0,1.1581051591,0.6976667531,-0.0423227826
H,0,1.2884623935,3.1703779347,-0.1382709361
H,0,-2.4050081832,7.5236539211,0.3241352278
H,0,-0.6346670009,7.4264594408,0.5672625575
H,0,-1.7369620662,7.5525749928,1.9714255248
H,0,-1.7459341754,-1.1544021941,1.1670200385
H,0,-0.995012179,-3.1720051625,0.8975818036
H,0,-0.2562111964,-5.3903263441,0.6367976791
H,0,1.4391418365,-7.0758054054,-0.0203361049
H,0,4.1283692578,-3.9063350827,-1.1634271082
H,0,2.4270894177,-2.2246019017,-0.5038236626

4-CN

Excited state S_1

C,0,-4.1092055513,3.0491290967,2.052859529
C,0,-4.194461895,1.6667604068,2.1116683423
C,0,-3.1276458313,0.8663800601,1.6931712301
C,0,-1.9446066329,1.4405490108,1.2034327138
C,0,-1.8516332123,2.8648510004,1.140778106
C,0,-2.9422888922,3.6550839294,1.569123049
C,0,-0.7990886085,0.6897374526,0.7521436216
C,0,0.366172337,1.3399221811,0.2683299758
C,0,0.4205302872,2.711136759,0.2222775266
C,0,-0.6761588063,3.4852319673,0.653340721
C,0,-0.5731372205,4.9435489629,0.5860257259
N,0,-1.6798657641,5.6696598112,1.0220062962
C,0,-2.863562722,5.110045173,1.5117106685
C,0,-1.6276498661,7.1271839356,0.975308738
O,0,0.4382494506,5.5092033177,0.1660716789
O,0,-3.7812163163,5.8502021147,1.8707838191
N,0,-0.8306168784,-0.6663577497,0.7886930608
N,0,0.1813234452,-1.4314040821,0.3918210904
C,0,-0.0257100264,-2.7288186179,0.4983146545
C,0,0.9632552296,-3.6774774133,0.1140032404
C,0,0.6796412597,-5.0577900633,0.2530192644
C,0,1.6083550634,-6.0102850482,-0.1067830175
C,0,2.8580018469,-5.6083280034,-0.6202779654
C,0,3.1549361418,-4.2370488518,-0.7645403778
C,0,2.2251273777,-3.2871693879,-0.4042484763
C,0,3.8215562481,-6.585701055,-0.9937538783
N,0,4.6123886787,-7.3870395742,-1.3002946001
H,0,-4.934542012,3.6786857752,2.3764482926
H,0,-5.0987244739,1.1924598124,2.4866190432
H,0,-3.2531407698,-0.2123460318,1.7629938367
H,0,1.2037782645,0.7325962622,-0.0606168478
H,0,1.3064759454,3.2216166789,-0.1458445534
H,0,-2.4285387237,7.5085282453,0.334263424
H,0,-0.657272977,7.4214978051,0.5767479164
H,0,-1.7608509634,7.5373714701,1.9811859382
H,0,-1.6750725479,-1.1282183707,1.1388522503
H,0,-0.9780698154,-3.1110281162,0.8909771599
H,0,-0.2869410756,-5.3656238321,0.6501531212
H,0,1.3851942156,-7.0694701185,0.0021403224
H,0,4.1225123427,-3.9369149787,-1.1619360809
H,0,2.4504684484,-2.228667478,-0.5140365594

4-NO₂

Ground state S₀

C,0,-3.4313024195,3.3271518111,2.1898810278
C,0,-3.5620720484,1.9348489528,2.2758917317
C,0,-2.5334152176,1.1160565474,1.8602379406
C,0,-1.3315856723,1.6491976863,1.3415630279
C,0,-1.2027092338,3.0643922712,1.2557763709
C,0,-2.2716152632,3.8850956231,1.6884098207
C,0,-0.2305787382,0.8409452978,0.895172411
C,0,0.9200383384,1.4440148509,0.396437253
C,0,1.0144188943,2.8317221169,0.3257455226
C,0,-0.0221033012,3.652109803,0.7447263497
C,0,0.1185690049,5.104142767,0.6531120221
N,0,-0.9715238373,5.8708606937,1.0959521033
C,0,-2.156232392,5.3507857608,1.6072928448
C,0,-0.8843995448,7.3262322702,1.0269365638
O,0,1.125150747,5.6527063523,0.2162684783
O,0,-3.0503941759,6.1085916598,1.9677844639
N,0,-0.3338017746,-0.5275465066,0.9691804939
N,0,0.6602134654,-1.3343293286,0.5676217042
C,0,0.4606139903,-2.599766487,0.6802657206
C,0,1.4646945616,-3.5719116679,0.2780813804
C,0,1.1698155125,-4.9346717199,0.4333479069
C,0,2.0880092155,-5.9050709269,0.0673866811
C,0,3.3098914156,-5.4964681348,-0.4579549162
C,0,3.6331019175,-4.1489360787,-0.624856198
C,0,2.7078089565,-3.1908780178,-0.2555899032
N,0,4.283271905,-6.5078244322,-0.8463709121
O,0,5.3559862349,-6.1332127926,-1.3081909581
O,0,3.9862044668,-7.6879427002,-0.6940675458
H,0,-4.2357088203,3.9837975139,2.5145817958
H,0,-4.4760553444,1.498266697,2.6710110787
H,0,-2.6831130208,0.0417272838,1.9471693573
H,0,1.7439653527,0.820312981,0.0628279825
H,0,1.9204165646,3.2890681021,-0.0665955915
H,0,-1.6842625593,7.7178781908,0.3907992945
H,0,0.0873413385,7.5898995139,0.6108782381
H,0,-0.9929819098,7.7541581236,2.0283998779
H,0,-1.1809316101,-0.9569381497,1.3363995019
H,0,-0.4817888951,-2.9942366441,1.0870529554
H,0,0.207406176,-5.2327758509,0.8465678877
H,0,1.8690906491,-6.9623716414,0.1836751819
H,0,4.5978795137,-3.8701328483,-1.0386655189
H,0,2.9368425577,-2.1344629429,-0.3761384272

4-NO₂

Excited state S₁

C,0,-3.4439070062,3.307016264,2.1960317191
C,0,-3.5617291404,1.9203947538,2.2766094205
C,0,-2.5222247655,1.0998038511,1.8563030508
C,0,-1.3364160475,1.6414059094,1.3439437541
C,0,-1.2151032333,3.056900241,1.2612420493
C,0,-2.282157568,3.8736874309,1.6932611717
C,0,-0.2125922255,0.8480515974,0.8874587402
C,0,0.9541151322,1.4795625303,0.3811426874
C,0,1.0279560004,2.8519989273,0.3194239132
C,0,-0.0379827644,3.6520204222,0.7513455134
C,0,0.09344434779,5.1135419136,0.6633506928
N,0,-0.9926942708,5.8709928405,1.1047451294
C,0,-2.1746390475,5.3413025275,1.6152262888
C,0,-0.9117866807,7.3282469546,1.0381628272
O,0,1.1052126414,5.647443719,0.2245790524
O,0,-3.0742983737,6.0875003095,1.9782021099
N,0,-0.2671601583,-0.4897569686,0.9402893587
N,0,0.7528227484,-1.2751794701,0.5273170249
C,0,0.5218043569,-2.5578517558,0.6533215327
C,0,1.4773342196,-3.5466059712,0.2720685937
C,0,1.156824658,-4.914102829,0.43773493
C,0,2.0493451424,-5.9020030809,0.0830388957
C,0,3.2995789751,-5.5373244468,-0.4526887527
C,0,3.6406092429,-4.1805142969,-0.6267727642
C,0,2.7417230426,-3.2028878859,-0.269165323
N,0,4.2234389519,-6.5400642478,-0.8202730708
O,0,5.3352353627,-6.2002708693,-1.2969905226
O,0,3.9073733624,-7.7452648727,-0.6601242796
H,0,-4.2517172065,3.9576808073,2.5223670491
H,0,-4.4709907379,1.4737081482,2.6701759258
H,0,-2.6681790821,0.0249749369,1.9418072937
H,0,1.7780856517,0.8576872448,0.0473527459
H,0,1.9201673319,3.3373753989,-0.0678218314
H,0,-1.7136251241,7.714840099,0.4020981667
H,0,0.0585756759,7.5974223359,0.6227264726
H,0,-1.0220627666,7.7513307891,2.0410673111
H,0,-1.1074317205,-0.9452322569,1.3049482119
H,0,-0.4334393547,-2.9150371626,1.0643698402
H,0,0.1868804518,-5.1869246469,0.8531343394
H,0,1.8061610697,-6.9525658941,0.2090235498
H,0,4.6111202864,-3.9257993106,-1.0420061297
H,0,2.9964844921,-2.1530179649,-0.4000216882