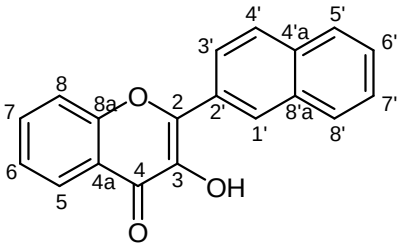
Electronic Supplementary Material for PCCP

Supplementary Material for:

IR spectroscopy applied subsequent to a proton transfer reaction in the excited state of isolated 3-hydroxyflavone and 2-(2-naphthyl)-3-hydroxychromone

by K. Bartl, A. Funk, K. Schwing, H. Fricke, G. Kock, H.-D. Martin, M. Gerhards*

1) NMR-DATA for 2-(2-naphtyl)-3-hydroxychromone



^{1}H-NMR$_{500}$ (DMSO): δ = 7.47-7.52 (m, 1H, 6-H), 7.59-7.64 (m, 2H, 7'-H, 6'-H), 7.84 (d, 2H, 7-H, 8-H), 7.99 (m, 1H, 8'-H), 8.06-8.09 (m, 2H, 5'-H, 4'-H), 8.15 (d, 1H, 5-H), 8.33 (dd, 1H, 3'-H), 8.82 (bs, 1H, 1'H), 9.79 (bs, 1H, -OH) ppm; ^{13}C-NMR$_{500}$ (DMSO): 118.4 (C-8), 121.3 (C-4a), 124.3 (C-3', 4'a), 124.5 (C-6), 124.8 (C-5), 126.7 (C-6'), 127.5 (C-7', C-8'), 127.8 (C-1'), 127.9 (C-4'), 128.8 (C-5), 132.4 (C-2'), 133.1 (C-8'a), 133.7 (C-7), 139.4 (C-3), 145.1 (C-2), 154.6 (C-8'a), 172.9 (C-4) ppm;

2) Geometries, dipole moments, polarizabilities and frequencies of 3Hydroxyflavon (3-HF)

a) Geometries (in Å)

S_0	x	y	z
C	1.562083	0.906418	0.000086
C	2.249550	-0.311765	0.000072
C	3.654371	-0.300134	-0.000071
C	4.339494	0.896619	-0.000208
C	3.631364	2.109199	-0.000198
C	2.249894	2.123104	-0.000045
C	1.477003	-1.544001	0.000071
C	0.026134	-1.387049	0.000077
C	-0.576949	-0.162440	0.000084
O	0.205643	0.966173	0.000098
C	-2.009764	0.152701	0.000033
C	-2.429565	1.494788	0.000333
C	-3.778724	1.817028	0.000264
C	-2.992031	-0.853055	-0.000342
C	-4.340194	-0.518781	-0.000431
C	-4.742590	0.812714	-0.000126
O	-0.652363	-2.557620	0.000198
O	1.949777	-2.686631	0.000062
H	0.054225	-3.237709	0.000246
H	4.170097	-1.251861	-0.000073
H	5.422057	0.905145	-0.000325
H	4.172173	3.047804	-0.000323
H	1.688959	3.048639	-0.000040
H	-2.699645	-1.890753	-0.000600
H	-5.080944	-1.309441	-0.000750
H	-1.692445	2.284230	0.000630
H	-5.795940	1.065856	-0.000197
H	-4.078146	2.858241	0.000519

S_0'	x	y	z
C	-4.749221	0.772571	-0.000281
C	-3.806915	1.800541	0.000015
C	-2.453063	1.509417	0.000222
C	-2.006271	0.172319	0.000137
C	-2.966635	-0.858939	-0.000137
C	-4.320604	-0.550995	-0.000352
C	-0.589039	-0.137766	0.000238
C	-0.007424	-1.428145	0.000106
C	1.432392	-1.467986	0.000072
C	2.235404	-0.315022	0.000074
C	1.553417	0.919359	0.000208
O	0.209335	0.967527	0.000331
C	3.653126	-0.305364	-0.000210
C	4.330649	0.888312	-0.000374
C	3.626376	2.111630	-0.000224
C	2.248566	2.133414	0.000081
O	1.924878	-2.689553	0.000065
O	-0.591912	-2.555998	0.000026
H	1.086361	-3.240417	0.000080
H	4.178384	-1.251199	-0.000286
H	5.413254	0.896229	-0.000627
H	4.174994	3.045221	-0.000343
H	1.690728	3.060763	0.000231
H	-2.628249	-1.884642	-0.000185
H	-5.046279	-1.355535	-0.000583
H	-1.732402	2.314898	0.000466
H	-5.807570	1.004446	-0.000459
H	-4.131610	2.834221	0.000081

S_{0t}	x	y	z
C	-4.729642	0.035840	-0.763495
C	-3.841655	-0.680710	-1.562383
C	-2.484601	-0.688252	-1.270287
C	-1.991808	0.021382	-0.166884
C	-2.890767	0.753858	0.621637
C	-4.249372	0.756566	0.324635
C	-0.548905	0.005416	0.136063
C	0.004827	-0.129694	1.371167
C	1.463456	-0.115793	1.567801
C	2.234236	0.001050	0.316459
C	1.576551	0.083623	-0.912458
O	0.216183	0.086740	-0.998282
C	3.637796	0.009968	0.326867
C	4.347537	0.102226	-0.853342
C	3.664971	0.185867	-2.075855
C	2.283353	0.177661	-2.113522
O	1.980958	-0.204886	2.670867
O	-0.715205	-0.292176	2.513382
H	-1.638810	-0.476258	2.297099
H	4.133808	-0.058379	1.286639
H	5.430115	0.110937	-0.838572
H	4.222569	0.259060	-3.001677
H	1.736776	0.244872	-3.045367
H	-2.522429	1.357923	1.442519
H	-4.929806	1.334592	0.938031
H	-1.797131	-1.245645	-1.893023
H	-5.787970	0.039222	-0.993851
H	-4.209215	-1.237941	-2.415639

S_1	x	y	z
C	1.722627	0.670593	-0.000059
C	2.411591	-0.565319	0.000031
C	3.830565	-0.531486	0.000140
C	4.501406	0.686606	0.000157
C	3.799334	1.885845	0.000065
C	2.384849	1.877527	-0.000045
C	1.651215	-1.763569	-0.000093
C	0.165413	-1.603063	-0.000099
C	-0.476815	-0.366275	-0.000080
O	0.329282	0.735707	-0.000145
C	-1.881981	-0.076979	-0.000032
C	-2.321221	1.274714	-0.000269
C	-3.668251	1.578216	-0.000218
C	-2.869827	-1.098704	0.000263
C	-4.212448	-0.774520	0.000310
C	-4.626306	0.560680	0.000069
O	-0.448219	-2.771390	-0.000187
O	2.046649	-2.954586	-0.000168
H	0.342388	-3.401956	-0.000211
H	4.364007	-1.472060	0.000196
H	5.584772	0.698180	0.000236
H	4.325356	2.831560	0.000069
H	1.816207	2.797867	-0.000137
H	-2.571200	-2.135504	0.000465
H	-4.949795	-1.568127	0.000538
H	-1.586444	2.066192	-0.000490
H	-5.681493	0.804682	0.000104
H	-3.981661	2.615170	-0.000409

S_1'	x	y	z
C	-4.770161	0.779752	0.000298
C	-3.811403	1.791491	-0.000582
C	-2.461837	1.484028	-0.000794
C	-2.022665	0.135140	-0.000122
C	-3.011132	-0.881122	0.000758
C	-4.354852	-0.553807	0.000942
C	-0.616017	-0.156687	-0.000220
C	0.031041	-1.415363	-0.000310
C	1.459405	-1.479591	-0.000058
C	2.246649	-0.308910	0.000010
C	1.550228	0.921018	-0.000001
O	0.179503	0.967053	-0.000065
C	3.657569	-0.280343	0.000188
C	4.331140	0.934827	0.000317
C	3.622798	2.133656	0.000284
C	2.221887	2.130575	0.000123
O	2.033040	-2.688613	-0.000094
O	-0.591322	-2.548766	-0.000580
H	1.289888	-3.326185	-0.000210
H	4.196259	-1.218057	0.000215
H	5.413844	0.947759	0.000459
H	4.151332	3.078619	0.000399
H	1.653833	3.051535	0.000113
H	-2.703665	-1.915131	0.001293
H	-5.091444	-1.348661	0.001645
H	-1.731769	2.280128	-0.001494
H	-5.825307	1.024846	0.000496
H	-4.119793	2.830390	-0.001113

b) Dipole Moments

S_0	a.u.	Debye
μ_x	-0.0368	-0.0935
μ_y	1.2935	3.2878
μ_z	-0.0001	-0.0003
$\|\mu\|$	1.2940	3.2891

S_o'	a.u.	Debye
μ_x	0.7792	1.9806
μ_y	1.5169	3.8557
μ_z	-0.0001	-0.0003
$\|\mu\|$	1.7053	4.3346

S_{0t}	a.u.	Debye
μ_x	-1.1687	-2.9706
μ_y	0.0468	0.1190
μ_z	-1.7887	-4.5465
$\|\mu\|$	2.1372	5.4323

S_1	a.u.	Debye
μ_x	-1.4599	-3.7108
μ_y	0.8123	2.0647
μ_z	0.0000	0.0000
$\|\mu\|$	1.6707	4.2465

S_1'	a.u.	Debye
μ_x	0.4225	1.0739
μ_y	0.7873	2.0012
μ_z	0.0003	0.0008
$\|\mu\|$	0.8935	2.2711

Polarizabilities / Å³ [1]

S_0	x	y	z
x	44.072	1.280	0.000
y		30.300	0.001
z			12.679
$\|\alpha\|$	25.678		

S_0'	x	y	z
x	54.514	0.191	0.000
y		30.618	0.000
z			12.707
$\|\alpha\|$	27.680		

c) Unscaled Frequencies

S_0			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
61	phenyl torsion	1014	CC str
79	phenyl bend oop	1021	CC bend ip
95	CC bend oop	1054	CH bend ip
131	phenyl bend ip	1061	CH bend ip
144	CC bend oop	1112	CH bend ip
189	CC bend oop	1139	CH bend ip
268	CC bend ip	1157	CH bend ip
276	CC bend oop	1184	CH bend ip
299	CC bend ip	1194	CH bend ip
333	CO/CC bend ip	1213	CH bend ip
371	CO/CC bend oop	1227	Ch bend ip
375	CO bend ip	1256	CH bend ip
418	CC bend oop	1266	CH bend ip/CC str
427	all bend oop	1325	CH/OH bend ip
442	CC bend ip	1340	CH bend ip/CC str
456	all bend oop	1357	OH bend ip
518	CC bend ip	1373	CH/OH bend ip
519	CC bend oop	1381	CC str/OH bend ip
573	CC bend oop	1441	CC str/OH bend ip
593	phenyl str	1486	CH bend ip
611	CC bend oop	1505	CH bend ip
638	CC bend ip	1511	CH bend ip
653	OH bend oop	1532	Ch bend ip
675	all bend ip	1606	CC str
689	all bend ip	1614	CC str
694	CC bend oop	1643	CC str
699	CO/OH bend oop	1652	CC str
716	CC bend ip	1659	C=O str
769	CH bend oop	1682	CH str
784	CH bend oop	3170	CH str
854	CC str	3178	CH str
862	CH bend oop	3183	CH str
866	CH bend oop	3191	CH str
914	CC bend ip	3195	CH str
931	CH bend oop	3205	CH str
971	CH bend oop	3211	CH str
981	CH bend oop	3224	CH str
987	CH bend oop	3252	CH str
1000	CH bend oop	3537	OH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

S_0'			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
63	phenyl bend oop	1012	CC str
71	phenyl torsion	1022	CC bend ip
103	CC bend oop	1049	CH bend ip
127	phenyl bend ip	1058	CH bend ip
142	CC bend oop	1110	CH bend ip
183	CC bend oop	1142	CH bend ip
261	CC bend ip	1178	CH bend ip
276	CC bend oop	1185	CH bend ip
288	CC/CO bend ip	1191	CH bend ip
330	CC/CO bend ip	1213	CH bend ip
358	CO bend ip	1243	OH/OH bend ip
359	CC bend oop	1259	CC str
413	CC bend oop	1265	CO str
420	CC bend oop	1325	OH/CH bend ip
458	CC bend ip	1341	CC str
461	CC bend oop	1368	CH bend ip
496	CC bend oop	1388	CC str
506	CC bend ip	1418	CC str/OH bend
551	CC bend oop	1448	OH/OH bend ip
577	CC bend oop	1477	CH bend ip
589	CC bend ip	1483	CH bend ip
637	CC bend ip	1520	CH bend ip
637	CC bend oop	1527	CH bend ip
675	CC bend ip	1559	CC str
679	CC bend oop	1585	CC str
685	CC bend ip	1607	CC str/OH bend
722	CC bend ip	1617	CC str/OH bend
755	CH bend oop	1639	CC str
773	CH bend oop	1652	CC str
852	CH bend oop	3168	CH str
857	CH bend oop	3178	OH/CH str
863	CH bend oop	3180	OH/CH str
898	OH bend oop	3184	OH/CH str
919	CC bend ip	3192	CH str
925	CH bend oop	3194	CH str
964	CH bend oop	3207	CH str
978	CH bend oop	3211	CH str
983	CH bend oop	3214	CH str
1006	CH bend oop	3225	CH str

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S_{0t}			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
71	phenyl torsion	1000	CH bend oop
76	phenyl bend oop	1019	CC bend ip
93	phenyl bend ip	1052	CH bend ip
105	CC bend oop	1056	CH bend ip
151	CC bend oop	1107	CH bend ip
209	CC bend oop	1132	CH bend ip
248	CC bend ip	1150	CH/OH bend ip
277	CC bend ip	1182	CH bend ip
299	CC bend ip	1193	CH bend ip
316	OH bend oop	1199	CO str
356	CO bend ip	1210	CH bend ip
387	CC bend oop	1246	CC str
409	CC/OH bend oop	1253	CC str
433	CC bend ip	1307	OH bend ip
439	OH/CC/CH bend oop	1323	CH bend
460	CC bend oop	1328	CC str
494	CC bend oop	1362	CH bend ip
517	CC bend ip	1373	CC str
536	CC bend oop	1438	CC str/OH bend ip
590	CC bend ip	1481	CH bend ip
627	CC bend ip	1499	CH bend ip
644	CC bend ip	1507	CH bend ip
664	CC bend ip	1529	CH bend ip
672	CC bend oop	1608	CC str
689	phenyl bend ip	1618	CH bend ip
710	CC bend ip	1644	CC str
717	CH bend oop	1648	CC str
772	CH bend oop	1652	CC str
790	CH bend oop	1719	C=O str
808	CH bend oop	3172	CH str
850	CC bend ip	3173	CH str
869	CH bend oop	3178	CH str
873	CH bend oop	3187	CH str
901	CC bend ip	3190	CH str
947	CH bend oop	3196	CH str
967	CH bend oop	3202	CH str
977	CH bend oop	3204	CH str
991	CH bend oop	3209	CH str
1000	CH bend oop	3768	OH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

S_1			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
75	phenyl bend oop	994	CH bend oop
87	CC bend oop	1007	CC bend ip
109	phenyl torsion	1041	CC bend ip
121	phenyl bend ip	1043	CC str
144	CC bend oop	1092	CC str
180	CC bend oop	1101	CC bend ip
240	CC bend oop	1111	CC bend ip
263	CC bend ip	1167	CH bend ip
291	CC bend ip	1186	Ch bend ip
323	CC bend oop	1192	Ch bend ip
329	CO/CC bend ip	1204	Ch bend ip
362	CO/CO bend ip	1217	Ch bend ip
363	CC bend oop	1253	Ch bend ip
411	CC bend oop	1299	CH bend ip
430	CC bend oop	1334	CC str
435	CC bend ip	1368	CC str
471	CC bend oop	1372	OH/CH bend ip
500	CC bend ip	1374	OH/CH bend ip
519	CC bend oop	1407	OH bend ip
540	CC bend oop	1472	CH bend ip
572	CC bend ip	1477	CH bend ip
578	CC bend oop	1479	CH bend ip
626	CC bend ip	1515	CH bend ip
663	CC bend oop	1552	CC str
665	CC bend ip	1556	CC str
675	CC bend ip	1568	CC str
689	CC bend ip	1611	CC str
754	CH bend oop	1628	CC str
773	CH bend oop	1653	C=O/CC str
823	CH bend oop	3050	OH str
826	CC bend ip	3175	CH str
854	CH bend oop	3176	CH str
862	CH bend oop	3183	CH str
891	CC bend ip	3193	CH str
934	CH bend oop	3197	CH str
936	OH bend oop	3206	CH str
960	CH bend oop	3213	CH str
980	CC str	3226	CH str
991	CH bend oop	3242	CH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

S_1'			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
53	phenyl torsion	999	CC str
67	phenyl bend oop	1013	CC bend ip
80	CC bend oop	1048	CC str
128	phenyl bend ip	1054	CC str
134	CC bend oop	1103	CC str
179	CC bend oop	1118	CC str
238	CC bend oop	1126	CC str
262	CC bend ip	1149	CH bend ip
292	CC bend ip	1188	CH bend ip
331	CC bend oop	1191	CH bend ip
333	phenyl/CO bend ip	1207	CH bend ip
337	CC bend oop	1216	OH bend ip
361	CO bend ip	1236	CH bend ip
408	CC bend oop	1259	CH bend ip
435	CC bend oop	1299	OH/CH bend ip
450	CC bend ip	1341	CC str
469	CC bend oop	1360	CC str
489	CC bend oop	1372	CH bend ip
494	CC bend ip	1392	OH/CH bend ip
519	CC bend oop	1416	CC str
549	CC bend oop	1473	CH bend ip
584	CC bend ip	1482	CH bend ip
634	CC bend ip	1509	CH bend ip
643	CC bend oop	1525	CH bend ip
661	CC bend ip	1554	CC str/OH bend ip
678	CC bend ip	1586	CC str/CH bend ip
684	OH bend oop	1599	CC str
702	CC bend ip	1626	CC str
736	CH bend oop	1636	CC str
752	CH bend oop	3167	CH str
826	CH bend oop	3178	CH str
843	CH bend oop	3181	CH str
845	CH bend oop	3192	CH str
892	CH bend oop	3194	CH str
895	CC bend ip	3208	CH str
907	CH bend oop	3215	CH str
950	CH bend oop	3218	CH str
963	CH bend oop	3241	CH str
975	CH bend oop	3573	OH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

3) Geometries, dipole moments, polarizabilities and frequencies of 2-(2-naphthyl)-3-hydroxychromone (2-NHC)

a) Geometries (in Å)

S_0	x	y	z
C	-3.626455	-1.012128	0.000215
C	-2.591474	-1.980946	0.000578
C	-1.274566	-1.614378	0.000638
C	-0.893047	-0.238778	0.000334
C	-1.889968	0.724020	-0.000010
C	-3.257785	0.367061	-0.000080
C	0.528754	0.114945	0.000308
C	1.097678	1.356605	0.000356
C	2.541937	1.555832	0.000130
C	3.349285	0.345977	0.000043
C	2.697579	-0.891721	0.000009
O	1.343065	-0.991140	0.000209
C	4.753770	0.374792	-0.000239
C	5.473472	-0.801566	-0.000519
C	4.800893	-2.034119	-0.000545
C	3.420318	-2.087924	-0.000280
O	2.981914	2.711952	0.000018
O	0.383647	2.506144	0.000493
H	1.069710	3.207081	0.000409
H	5.241695	1.341126	-0.000239
H	6.555820	-0.778459	-0.000743
H	5.368585	-2.956660	-0.000791
H	2.886322	-3.029276	-0.000302
H	-1.632612	1.771892	-0.000239
H	-0.507016	-2.373885	0.000910
H	-2.857967	-3.032071	0.000808
C	-4.282502	1.349171	-0.000549
C	-4.999345	-1.357050	0.000023
C	-5.966742	-0.382711	-0.000436
C	-5.604527	0.983183	-0.000725
H	-5.276338	-2.405378	0.000235
H	-7.014612	-0.657853	-0.000608
H	-6.378237	1.741523	-0.001116
H	-4.001866	2.396356	-0.000785

S_0'	x	y	z
C	-2.088418	-3.431809	-0.000191
C	-0.900948	-2.692927	0.000017
C	0.357844	-3.328313	-0.000098
C	0.399847	-4.745321	-0.000443
C	-0.768279	-5.466569	-0.000667
C	-2.016508	-4.808228	-0.000539
O	-0.998647	-1.350602	0.000278
C	0.077790	-0.513902	0.000418
C	1.390148	-1.049604	0.000389
C	1.481975	-2.484690	0.000117
C	-0.278839	0.888520	0.000451
C	-1.651901	1.289622	0.000721
C	-1.996073	2.610404	0.000594
C	-1.008269	3.631313	0.000190
C	0.366262	3.242423	-0.000055
C	0.704910	1.871278	0.000093
O	2.492497	-0.418413	0.000575
O	2.720468	-2.938802	0.000094
H	3.246728	-2.087572	0.000298
H	1.364294	-5.235758	-0.000522
H	-0.735875	-6.548758	-0.000944
H	-2.929336	-5.390632	-0.000711
H	-3.035392	-2.907958	-0.000073
H	1.743817	1.572267	-0.000073
H	-2.423599	0.533292	0.001025
H	-3.042203	2.896110	0.000798
C	-1.332828	5.007348	-0.000079
C	1.363104	4.252739	-0.000560
C	-0.343650	5.961507	-0.000568
C	1.016352	5.580497	-0.000811
H	-2.376861	5.300407	0.000100
H	-0.604545	7.013094	-0.000787
H	1.785803	6.343166	-0.001205
H	2.405341	3.954951	-0.000752

S_{0t}	x	y	z
C	-2.082238	-0.418575	3.383359
C	-0.902028	-0.183139	2.674281
C	0.324898	-0.043344	3.326196
C	0.354459	-0.140282	4.726226
C	-0.805094	-0.371951	5.438220
C	-2.025835	-0.510927	4.761331
O	-1.004958	-0.106428	1.317160
C	0.109481	0.116859	0.550762
C	1.338113	0.311232	1.101998
C	1.553291	0.221406	2.555078
C	-0.209974	0.180438	-0.886048
C	-1.378530	0.869674	-1.314552
C	-1.691329	0.952363	-2.643604
C	-0.869385	0.352968	-3.632480
C	0.297464	-0.355134	-3.212056
C	0.597778	-0.424518	-1.829995
O	2.453395	0.609305	0.384208
O	2.652319	0.365075	3.069002
H	2.208602	0.817186	-0.527743
H	1.312326	-0.026408	5.217773
H	-0.775436	-0.447139	6.517944
H	-2.935440	-0.693750	5.320446
H	-3.012712	-0.526251	2.841028
H	1.458578	-1.006792	-1.519405
H	-2.016191	1.331568	-0.572573
H	-2.580971	1.486324	-2.958344
C	-1.167569	0.422946	-5.014937
C	1.115318	-0.973580	-4.191680
C	-0.352866	-0.181999	-5.939373
C	0.797923	-0.887978	-5.523638
H	-2.052437	0.962568	-5.333183
H	-0.590801	-0.122001	-6.994529
H	1.997989	-1.515851	-3.871603
H	1.430328	-1.363000	-6.263785

S_1	x	y	z
C	-3.645908	-1.011166	0.000254
C	-2.608743	-1.986997	0.000585
C	-1.286825	-1.631418	0.000490
C	-0.889107	-0.262792	0.000076
C	-1.911125	0.719619	-0.000354
C	-3.265488	0.369984	-0.000236
C	0.504614	0.077503	-0.000024
C	1.090286	1.331088	0.000242
C	2.555229	1.544166	0.000138
C	3.360726	0.369084	0.000070
C	2.722807	-0.893104	-0.000147
O	1.344654	-1.017382	-0.000169
C	4.777106	0.396808	0.000044
C	5.502266	-0.785898	-0.000160
C	4.850161	-2.016871	-0.000363
C	3.444876	-2.070794	-0.000372
O	2.926027	2.745539	0.000192
O	0.421541	2.481316	0.000503
H	1.176349	3.142738	0.000491
H	5.266174	1.361625	0.000177
H	6.585149	-0.750590	-0.000179
H	5.418397	-2.938209	-0.000535
H	2.917298	-3.015690	-0.000565
H	-1.642324	1.765797	-0.000797
H	-0.522095	-2.393522	0.000711
H	-2.881703	-3.036419	0.000940
C	-4.293499	1.356662	-0.000631
C	-5.007471	-1.347668	0.000333
C	-5.987902	-0.361790	-0.000041
C	-5.624067	0.993971	-0.000531
H	-5.292424	-2.393751	0.000688
H	-7.034170	-0.640570	0.000026
H	-6.392222	1.757407	-0.000854
H	-4.011581	2.403351	-0.001005

S_1'	x	y	z
C	-5.418389	1.166014	0.160831
C	-4.094720	1.524012	0.183179
C	-3.070833	0.541287	0.062798
C	-3.454381	-0.832802	-0.076485
C	-4.824162	-1.165803	-0.094916
C	-5.789665	-0.189849	0.020201
C	-1.710948	0.886954	0.088491
C	-0.704823	-0.082764	-0.038784
C	-1.106358	-1.455999	-0.165588
C	-2.423518	-1.806401	-0.185761
C	0.685655	0.251881	-0.038676
C	1.282580	1.541050	-0.095824
C	2.707061	1.656107	-0.025705
C	3.537167	0.516503	0.004544
C	2.889414	-0.739527	0.035880
O	1.521929	-0.838253	0.034302
C	3.607563	-1.921931	0.067771
C	5.006814	-1.870226	0.086572
C	5.668407	-0.644366	0.063011
C	4.948808	0.542532	0.023270
O	0.621504	2.639049	-0.203573
O	3.232739	2.885420	-0.070783
H	2.462895	3.489673	-0.118867
H	5.450870	1.500260	0.003240
H	6.750738	-0.615114	0.077380
H	5.571741	-2.793398	0.116846
H	3.075401	-2.863942	0.086774
H	-1.433776	1.924745	0.202940
H	-0.345485	-2.217583	-0.255550
H	-2.701396	-2.849645	-0.289978
H	-5.109511	-2.206748	-0.200930
H	-6.838820	-0.459360	0.003571
H	-6.187144	1.924283	0.250852
H	-3.807358	2.563941	0.288965

b) Dipole Moments

S_0	a.u.	Debye
μ_x	-0.1335	-0.3393
μ_y	-1.2452	-3.1650
μ_z	-0.0002	-0.0005
$\|\mu\|$	1.2523	3.1832

S_0'	a.u.	Debye
μ_x	-1.4049	-3.5710
μ_y	-0.6426	-1.6334
μ_z	-0.0005	-0.0013
$\|\mu\|$	1.5449	3.9268

S_{0t}	a.u.	Debye
μ_x	-1.7581	-4.4687
μ_y	-0.1598	-0.4062
μ_z	-1.3342	-3.3913
$\|\mu\|$	2.2128	5.6245

S_1	a.u.	Debye
μ_x	-2.8594	-7.2680
μ_y	-1.0815	-2.7490
μ_z	-0.0001	-0.0003
$\|\mu\|$	3.0571	7.7705

S_1'	a.u.	Debye
μ_x	0.2953	0.7506
μ_y	-0.7843	-1.9935
μ_z	0.0776	0.1972
$\|\mu\|$	0.8416	2.1393

Polarizabilities / Å³ [1]

S_0	x	y	z
x	53.976	-0.372	0.001
y		34.052	0.001
z			15.590
$\|\alpha\|$	30.600		

S_0'	x	y	z
x	70.242	0.421	-0.001
y		33.944	-0.001
z			15.636
$\|\alpha\|$	33.406		

c) Unscaled Frequencies

S_0			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
23	naphthyl torsion	984	CH bend oop
49	naphthyl bend oop	986	CH bend oop
84	CC bend oop	1021	CC str
92	naphthyl bend ip	1044	CC str
107	CC bend oop	1054	CC str
146	CC bend oop	1135	CC str
186	CC bend oop	1144	CH bend ip
207	CC bend ip	1167	CH bend ip
227	CC bend oop	1182	CH bend ip
266	CC bend ip	1183	CH bend ip
288	CC bend oop	1193	CH bend ip
299	CC bend ip	1204	CO str/CH bend ip
359	CO/CO bend ip	1233	CC str/CH bend ip
361	CC bend oop	1246	CC str/CH bend ip
399	CC bend oop	1262	CC str/CH bend ip
430	CC bend ip	1282	CC str/CH bend ip
437	CC bend oop	1304	CC str/CH bend ip
445	CC bend ip	1330	CC str/CH bend ip
457	CC bend oop	1352	OH bend ip
485	CC bend ip	1371	CC str/OH bend ip
506	CC bend ip	1385	CC str/CH bend ip
512	CC bend oop	1400	CC str/CH bend ip
530	CC bend ip	1411	CC str/CH bend ip
550	CC/OH bend oop	1438	CC str/OH bend ip
563	CC bend ip	1475	CH bend ip
600	CC bend oop	1502	CH bend ip
627	CC bend ip	1505	CH bend ip
635	CH/OH bend oop	1511	CC str/CH bend ip
644	CH/OH bend oop	1540	CC str/CH bend ip
655	CC bend ip	1602	CC str/CH bend ip
678	CC bend ip	1605	CC str/CH bend ip
691	C=O/OH bend oop	1637	CC str/CH bend ip
714	CC str	1647	CC str/CH bend ip
735	CC bend oop	1651	CC str/CH bend ip
759	CH bend oop	1666	CC str/CH bend ip
776	CH bend oop	1678	C=O/CC str/OH bend ip
786	CC str	3162	CH str
803	CC bend ip	3168	CH str
823	CH bend oop	3170	CH str
860	CH bend oop	3179	CH str

Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
866	CH bend oop	3181	CH str
901	CC bend ip	3190	CH str
916	CC bend ip	3194	CH str
920	CH bend oop	3203	CH str
958	CH bend oop	3207	CH str
965	CH bend oop	3224	CH str
967	CC bend ip	3239	CH str
971	CH bend oop	3533	OH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

S_0'			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
37	naphthyl bend oop	980	CH bend oop
46	naphthyl torsion	986	CH bend oop
85	CC bend oop	1024	CC str
89	naphthyl bend ip	1043	CC str
103	CC bend oop	1050	CC str
147	CC bend oop	1137	CC str
187	CC bend oop	1151	CH bend ip
207	CC bend dip	1177	CH bend ip
221	CC bend oop	1179	CH bend ip
265	CC bend ip	1184	CH bend ip
279	CC bend ip	1189	CH bend ip
288	CC bend oop	1225	pyranic CO str/CH bend ip
350	CC bend ip	1241	pyranic CO str/CH bend ip
354	CC bend oop	1246	CC str/CH bend
400	CC bend oop	1262	pyranic CO/CC str/CH bend ip
416	CC bend oop	1286	CH bend ip
427	CC bend ip	1297	CH bend ip
455	CC bend oop	1324	CH/OH bend ip
457	CC bend ip	1378	CC str
484	CC bend oop	1387	CH bend ip
497	CC bend ip	1393	CC str/CH bend ip
504	CC bend oop	1408	CC str/OH bend ip
528	CC bend ip	1424	CC str/OH bend ip
539	CC bend oop	1441	CH/OH bend ip
556	CC bend ip	1471	CH bend ip
568	CC bend oop	1476	CH bend ip
621	CC bend oop	1505	CH bend ip
626	CC bend oop	1518	CH bend ip
627	CC bend ip	1537	CH bend ip
653	CC bend ip	1556	CO str
675	CC bend ip	1579	CC str/CH/OH bend ip
720	CC bend ip	1597	CC str/CH/OH bend ip
727	CC bend oop	1611	CC str/CH/OH bend ip
755	CH bend oop	1638	CC str/CH bend ip
765	CH bend oop	1650	CC str/CH bend ip
783	CC str	1659	CC str/CH bend ip
802	CC str	3162	CH str
816	CH bend oop	3167	CH str
850	CH bend oop	3171	CH str
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
865	CH bend oop	3182	CH str

876	OH bend oop	3182	CH str
904	CC bend ip	3193	CH str
917	CC bend ip	3193	CH str
930	CH bend oop	3205	CH str
956	CH bend oop	3210	CH str
957	CH bend oop	3210	CH str
967	CC bend ip	3215	CH str
971	CH bend oop	3216	OH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

S_{0t}			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
40	naphthyl bend oop	988	CH bend oop
59	naphthyl torsion	988	CH bend oop
66	naphthyl bend ip	1007	CC str
93	CC bend oop	1045	CC str
130	CC bend oop	1053	CC str
151	CC bend oop	1128	CH/OH bend ip
187	CC bend oop	1140	CC str/CH bend ip
193	CC bend ip	1167	CH bend ip
215	CC bend oop	1179	CH bend ip
275	CC bend oop	1182	CH bend ip
290	CC bend oop	1186	CH bend ip
319	CC bend oop	1195	pyranic CO str/CH/OH bend ip
349	OH bend oop	1224	CH bend ip
369	CC bend oop	1241	CC str/CH bend ip
400	CC bend oop	1250	CC str/CH bend ip
413	CC bend ip/OH bend oop	1269	CH/OH bend ip
430	CC bend ip/OH bend oop	1296	CH bend ip
435	CC bend ip/OH bend oop	1312	OH bend ip
458	CC bend oop	1322	CH bend ip
494	CC bend oop	1366	CC str
501	CC bend ip	1379	CC str/CH bend ip
512	CC bend oop	1398	CC str
526	CC bend ip	1408	CC str/CH bend ip
533	CC bend oop	1436	CC str
560	CC bend ip	1473	CH bend
602	CC bend oop	1498	CH bend
627	CC bend ip	1505	CH bend
645	CC bend ip	1507	CH bend
664	CC bend oop	1539	CH bend
673	CC bend oop	1606	CC str
685	CC bend oop	1607	CC str
711	CC bend ip	1640	CC str
741	CC bend oop	1644	CC str/CH bend ip
763	CC bend oop	1649	CC str/CH bend ip
771	CC bend oop	1668	CC str/CH bend ip
783	CC str	1715	C=O str
798	CC bend ip	3165	CH str
803	CH bend oop	3167	CH str
Frequency / cm^{-1}	Assignment	Frequency	Assignment

		/ cm^{-1}	
837	CH bend oop	3171	CH str
870	CH bend oop	3172	CH str
872	CH bend oop	3177	CH str
895	CH bend oop	3186	CH str
902	CH bend oop	3190	CH str
920	CH bend oop	3197	CH str
960	CH bend oop	3202	CH str
965	CC str	3202	CH str
966	CH bend oop	3205	CH str
982	CH bend oop	3754	OH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

S_1			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
38	naphthyl bend oop	968	CH bend oop
47	naphthyl torsion	973	CH bend oop
77	CC bend oop	1000	CC str
88	naphthyl bend ip	1045	CC str
94	CC bend oop	1049	CC str
137	CC bend oop	1094	CC str/CH bend ip
190	CC bend oop	1112	CH bend ip
205	CC bend ip	1123	CC/CO str/CH bend ip
223	CC bend oop	1151	CH bend ip
243	CC bend oop	1175	CH bend ip
261	CC bend ip	1182	CH bend ip
295	CC bend ip	1194	CH bend ip
329	CC bend oop	1200	CH bend ip
354	CC bend oop	1226	CH bend ip
355	CC bend oop	1253	CC str/CH bend ip
398	CC bend oop	1259	CC str/CH bend ip
423	CC bend ip	1283	CC str/CH bend ip
432	CC bend oop	1301	CC str/CH bend ip
441	CC bend ip	1330	CC str/CH bend ip
449	CC bend oop	1359	CC str/CH/OH bend ip
477	CC bend ip	1365	CC str/CH/OH bend ip
484	CC bend oop	1375	CH/OH bend ip
502	CC bend oop	1402	CH/OH bend ip
522	CC bend ip	1424	CH bend ip
530	CC bend oop	1470	CH/OH bend ip
542	CC bend ip	1477	CH bend ip
581	CC bend oop	1482	CH bend ip
594	CC bend oop	1494	CH bend ip
617	CC bend ip	1514	CH/OH bend ip
620	CC bend oop	1534	CH/OH bend ip
646	CC bend ip	1557	CH bend ip
669	CC bend ip	1572	CC str/CH bend ip
688	CC bend ip	1604	CC str/CH bend ip
734	CH bend oop	1605	C=O/CC str/CH/OH bend ip
752	CH bend oop	1621	CC str/OH bend
772	CC str	1636	C=O/CC str
783	CC bend ip	3157	OH str
811	CH bend oop	3169	CH str
820	CH bend oop	3173	CH str
853	CH bend oop	3173	CH str
Frequency /	Assignment	Frequency /	Assignment

cm^{-1}		cm^{-1}	
855	CH bend oop	3176	CH str
869	CH bend oop	3186	CH str
880	CH bend ip	3190	CH str
888	CH bend oop	3198	CH str
908	CC/CO bend ip	3202	CH str
945	CH bend oop	3209	CH str
946	CH bend oop	3227	CH str
955	CC str	3230	CH str

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S_1'			
Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
41	naphthyl bend oop	972	CH bend oop
60	naphthyl torsion	979	CH bend oop
79	naphthyl bend ip	1006	CC str
88	CC bend oop	1042	CC str
105	CC bend ip	1054	CC str
146	CC bend oop	1116	CC bend ip
193	CC bend oop	1121	CC str
206	CC bend ip	1135	pyranic CO str
232	CC bend oop	1161	CH bend ip
247	CC bend oop	1179	CH bend ip
269	CC bend ip	1183	CH bend ip
282	CO bend ip	1193	CH bend ip
336	CC bend oop	1207	CH bend ip
350	CO/CO bend ip	1222	CH bend ip
370	CC bend oop	1240	CC str/CH bend ip
411	CC bend oop	1259	CC str/CH bend ip
425	CC bend ip	1277	CC str/CH bend ip
448	CC bend ip	1300	CH/OH bend ip
470	CC bend oop	1304	CH/OH bend ip
487	CC bend oop	1357	CC str/CH bend ip
489	CC bend ip	1376	CH bend ip
505	CC bend oop	1390	CO str/CH/OH bend ip
513	CC bend oop	1395	CC str/CH bend ip
525	CC bend ip	1407	CC str/CH bend ip
550	CC bend ip	1425	CC str/CH bend ip
556	CC bend oop	1470	CH bend ip
614	CC bend oop	1472	CH bend ip
624	CC bend ip	1502	CH bend ip
651	CC bend ip	1507	CH bend ip
664	CC bend ip	1531	CH bend ip
667	CC bend oop	1552	CC str/CH/OH bend ip
689	OH bend oop	1576	CC str/CH bend ip
699	CC bend oop	1595	CC str/CH bend ip
701	CC bend ip	1625	CC str/CH bend ip
750	CC bend oop	1633	CC str/CH bend ip
759	CC bend oop	1651	CC str/CH bend ip
777	CC str	3163	CH str
794	CC bend ip	3166	CH str
824	CH bend oop	3170	CH str
833	CH bend oop	3180	CH str
864	CH bend oop	3181	CH str

Frequency / cm^{-1}	Assignment	Frequency / cm^{-1}	Assignment
889	CH bend ip	3193	CH str
895	CH bend oop	3194	CH str
904	CH bend oop	3205	CH str
907	CH bend oop	3211	CH str
950	CH bend oop	3218	CH str
951	CH bend oop	3220	CH str
957	CC str	3558	OH str

str = stretching vibration bend = bending vibration ip = in plane oop = out of plane

[1] The polarizabilities are calculated using the Gaussian 03 program:
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