SUPPORTING INFORMATION

Cyclometalated Gold(III) Trioxadiborrin Complexes: Studies of the Bonding and Excited States

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Contents

Figure S1. Kohn-Sham orbital energy levels of trioxadiborrin complexes **1**–**8**. For selected orbitals, compositions in terms of fragment electron densities are indicated.

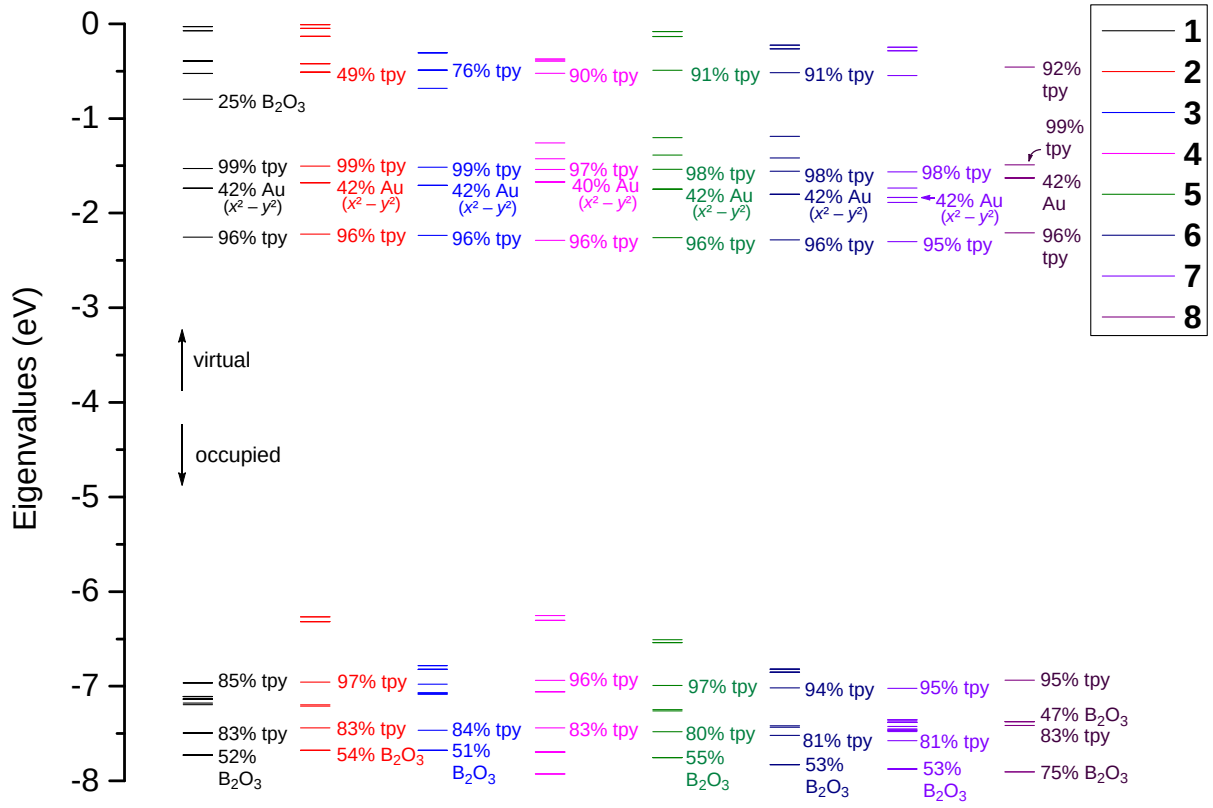
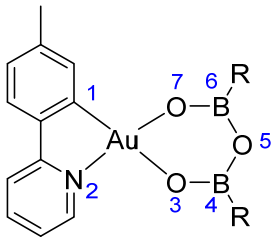


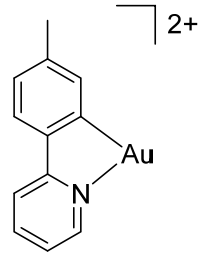
Table S1. Natural atomic charges of selected atoms in **1**–**8** (a.u.). Atom numbering is indicated below.

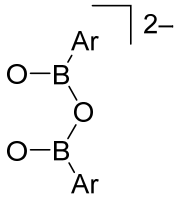


1–**8**

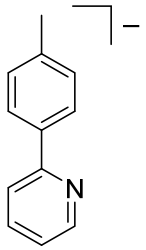
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	Average
Au	1.037	1.035	1.036	1.045	1.038	1.040	1.040	1.025	1.037
C1	-0.120	-0.122	-0.121	-0.121	-0.120	-0.118	-0.116	-0.126	-0.121
N2	-0.411	-0.411	-0.411	-0.416	-0.411	-0.410	-0.410	-0.412	-0.412
O3	-0.956	-0.959	-0.957	-0.972	-0.956	-0.955	-0.953	-0.963	-0.959
B4	1.075	1.073	1.074	1.098	1.073	1.074	1.074	1.095	1.080
O5	-0.889	-0.891	-0.889	-0.905	-0.889	-0.888	-0.887	-0.899	-0.892
B6	1.078	1.078	1.080	1.101	1.076	1.077	1.077	1.100	1.083
O7	-0.876	-0.877	-0.876	-0.893	-0.876	-0.876	-0.875	-0.880	-0.879

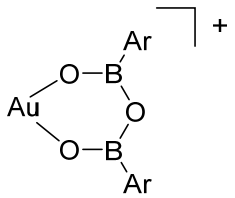
Table S2. Fragment interaction energies, basis set superposition energies, bond snapping and bond dissociation energies for **1**–**8** and propanedionate analogue **1′** (kcal mol^{-1}).





Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**1′**
Fragment interaction energy	-194.7	-198.0	-196.5	-195.3	-193.7	-190.7	-189.1	-203.0	-127.56
Bond snapping enthalpy	190.7	200.7	198.2	192.4	194.7	192.6	184.5	204.6	121.9
Bond dissociation enthalpy	179.9	181.5	181.5	174.4	176.9	175.6	174.0	187.3	82.6
BSSE[a]	4.2	4.0	3.9	3.8	3.7	3.6	3.5	5.0	4.3





Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Fragment interaction energy	-215.25	-210.6	-213.6	-209.3	-214.3	-217.8	-219.5	-207.23
Bond snapping enthalpy	207.5	207.6	206.6	205.6	209.0	210.3	211.8	203.9
Bond dissociation enthalpy	193.8	187.9	191.9	184.3	191.5	195.5	198.0	184.7
BSSE	4.4	4.2	4.4	4.2	4.2	4.3	4.5	4.4

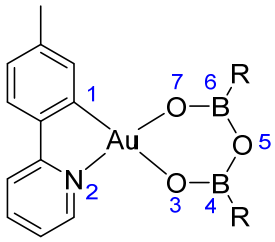
[a] Gas-phase.

Table S3. Contributions of unoccupied fragment Kohn-Sham orbitals (UFOs) to the occupied orbitals of **1**–**8** and charge transfer (a.u.) between fragments.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**1′**
donation (trioxadiborrin^{2-} → (tpy)Au^{2+}) + polarization of (tpy)Au^{2+}									
Contribution UFOs of (tpy)Au^{2+} to all occupied MOs (× 100)	54.7	55.3	54.8	56.0	54.3	53.7	53.3	56.8	44.3
back donation ((tpy)Au^{2+} → trioxadiborrin^{2-}) + polarization of trioxadiborrin^{2-}									
Contribution of UFOs of trioxadiborrin^{2-} to all unoccupied MOs (× 100)	5.7	5.9	5.8	7.0	6.1	6.0	6.0	4.8	5.3
ECDA Net charge transfer									
Trioxadiborrin^{2-} → (tpy)Au^{2+} [a]	1.01	1.02	1.01	1.02	1.01	1.00	0.99	1.06	0.82
NPA charge transfer (Δq^{NPA})									
Trioxadiborrin^{2-} → (tpy)Au^{2+}	0.82	0.83	0.82	0.82	0.81	0.80	0.80	0.85	0.66
donation (tpy^{-} → Au(trioxadiborrin)$^{+}$) + Polarization of (trioxadiborrin)Au^{+}									
Contribution of UFOs of Au(trioxadiborrin)$^{+}$ to all occupied MOs (× 100)	85.1	91.2	84.9	92.9	90.2	87.4	85.9	84.0	104.2
back donation (Au(trioxadiborrin)$^{+}$ → tpy^{-}) + Polarization of tpy^{-}									
Contribution of UFOs of tpy^{-} to all unoccupied MOs (× 100)	11.1	11.1	11.1	11.7	11.1	11.2	11.2	11.1	11.8
ECDA Net charge transfer									
tpy → (trioxadiborrin)Au^{2+} [a]	1.62	1.67	1.65	1.62	1.62	1.68	1.65	1.68	1.78
NPA charge transfer (Δq^{NPA})									
tpy → (trioxadiborrin)Au^{2+} [a]	0.85	0.86	0.86	0.86	0.85	0.84	0.84	0.87	0.71

[a] Net number of electrons transferred

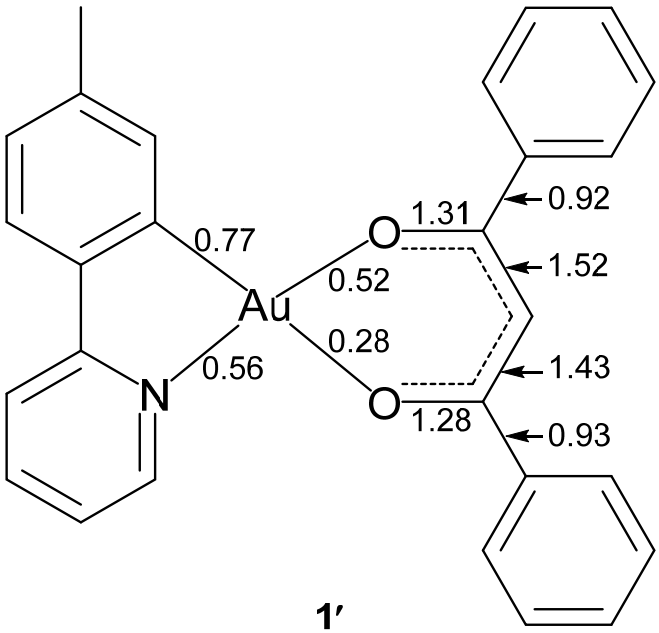
Table S4. Components of Mayer bond orders in C_s-symmetric **1**. Atom numbering is indicated below.



1–8

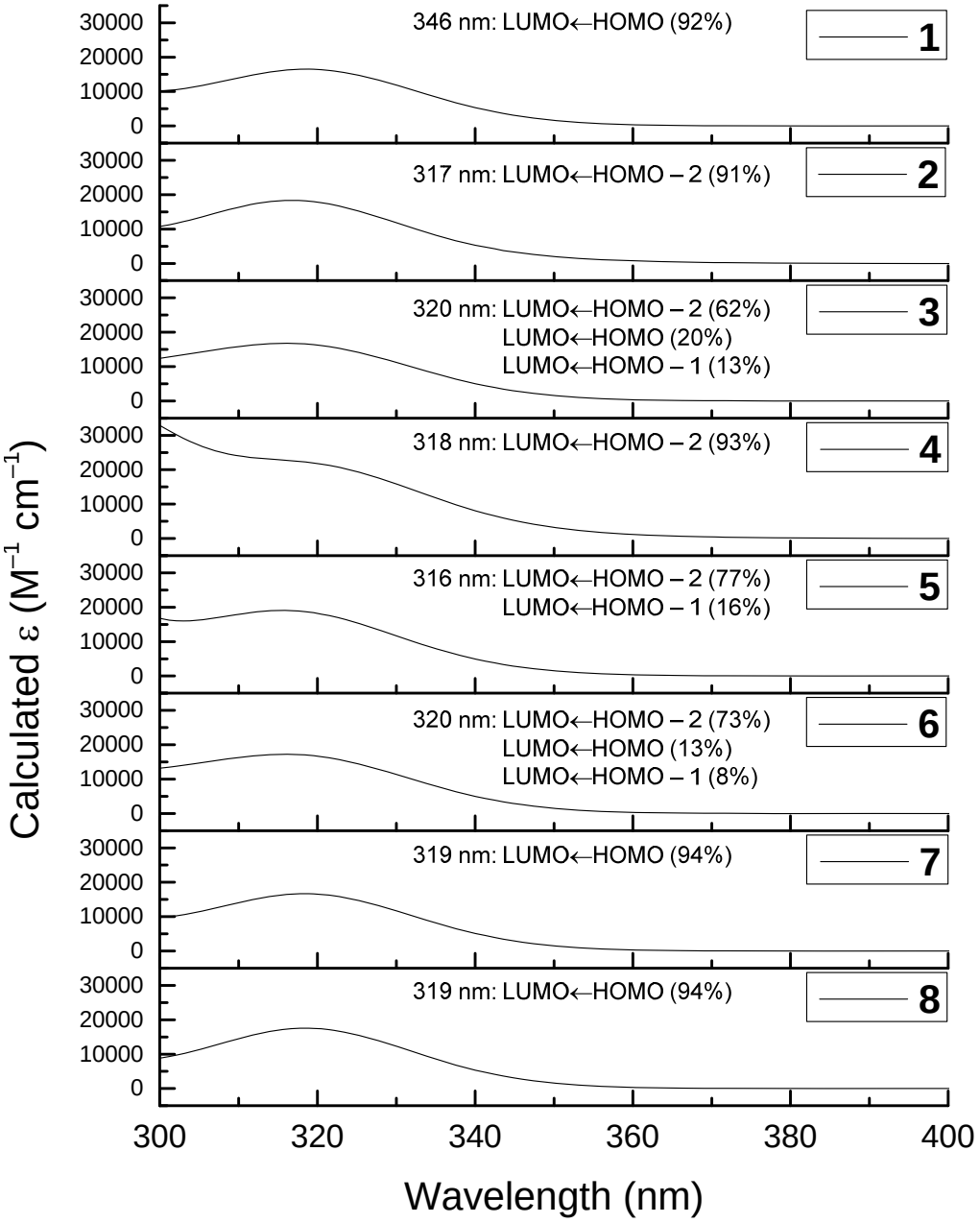
Atom	Atom or Fragment	A′	A″
Au	$B_2O_3Ph_2$	1.02	0.14
Au	tpy	1.40	0.10
Au	C(1)	0.82	0.04
Au	N(2)	0.48	0.02
Au	O(3)	0.34	0.06
Au	O(7)	0.52	0.06

Figure S2. Selected Mayer bond orders calculated for propanedionate complex **1′**.



1′

Figure S3. Simulated absorption spectra of **1**–**8** from TDDFT singlets computations.



***Gaussian09* keyword lines**

Geometry optimizations:

```
# pbe1pbe/gen nosymm pseudo=read scf=(tight,maxcycle=150) pop=minimal
opt freq=noraman scrf(iefpcm,solvent=tetrahydrofuran)
```

Population analyses:

```
#p pbe1pbe/gen nosymm pseudo=read scf=(tight,maxcycle=150)
pop=(full,npa) scrf(iefpcm,solvent=tetrahydrofuran) iop(3/33=1)
```

Time-dependent DFT:

```
# td(singlets,nstates=40) pbe1pbe/gen pseudo=read
scf=(tight,maxcycle=150) pop=minimal symm=veryloose
scrf(iefpcm,solvent=tetrahydrofuran)

# td(triplets,nstates=20) pbe1pbe/gen pseudo=read
scf=(tight,maxcycle=150) pop=minimal symm=veryloose
scrf(iefpcm,solvent=tetrahydrofuran)
```

CIS:

```
# CIS(singlets,nstates=40)/gen pseudo=read
scf=(tight,maxcycle=150) pop=minimal symm=veryloose
scrf(iefpcm,solvent=tetrahydrofuran)

# CIS(triplets,nstates=40)/gen pseudo=read
scf=(tight,maxcycle=150) pop=minimal symm=veryloose
scrf(iefpcm,solvent=tetrahydrofuran)
```

CIS(D):

```
#t CIS(D,singlets,nstates=3)/gen pseudo=read scf=(tight,maxcycle=150)
pop=minimal symm=veryloose
GUESS=CARDS

#t CIS(D,triplets,nstates=3)/gen pseudo=read scf=(tight,maxcycle=150)
pop=minimal symm=veryloose
GUESS=CARDS
```

Summary of calculated electronic transitions (PBE0/TZVP/SDD)

Phenyl **1**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	319.5	31.30	3.881	0.2220	112->113(92.0%)
2	305.6	32.72	4.057	0.0006	112->114(88.9%)
3	290.8	34.38	4.263	0.0917	111->113(46.2%) 107->113(34.6%)
4	282.8	35.36	4.384	0.0323	110->113(82.0%) 107->113(11.1%)
5	281.0	35.59	4.413	0.0087	111->113(49.3%) 107->113(33.6%)
6	280.6	35.64	4.419	0.0001	107->114(51.6%) 111->114(31.0%)
7	278.1	35.96	4.459	0.0001	109->113(88.7%)
8	275.4	36.31	4.502	0.0001	110->114(78.2%)
9	275.3	36.32	4.503	0.0012	108->113(88.5%)
10	270.4	36.98	4.585	0.0004	106->113(95.9%)
11	264.9	37.75	4.680	0.1936	112->115(76.8%) 107->113(11.1%)
12	261.9	38.18	4.734	0.0014	111->114(61.9%) 107->114(31.2%)
13	257.6	38.82	4.813	0.0001	108->114(68.0%) 109->114(27.2%)
14	256.8	38.95	4.829	0.0123	105->114(90.0%)
15	255.7	39.11	4.849	0.0001	109->114(61.0%) 108->114(28.6%)
16	247.2	40.46	5.016	0.0445	111->115(60.6%) 107->115(18.1%) 110->115(11.3%)
17	246.0	40.65	5.040	0.7166	106->114(76.6%)
18	244.7	40.86	5.066	0.0007	105->113(91.7%)
19	243.0	41.16	5.103	0.0015	104->114(75.0%)
20	241.0	41.49	5.144	0.0130	110->115(74.0%) 107->115(17.6%)
21	239.9	41.69	5.169	0.0123	109->115(62.3%) 111->115(11.6%)
22	238.8	41.88	5.193	0.0282	107->115(37.4%) 111->115(19.5%) 109->115(18.7%)
23	236.3	42.31	5.246	0.0090	108->115(37.8%) 108->116(21.2%)
24	235.4	42.48	5.267	0.0003	109->116(36.6%) 111->120(12.6%) 109->115(10.3%)
25	235.1	42.54	5.274	0.0021	108->115(43.3%) 108->116(21.3%)
26	234.6	42.62	5.284	0.3588	104->113(79.6%)
27	230.5	43.38	5.379	0.0013	106->115(96.7%)
28	223.7	44.71	5.543	0.1702	112->117(22.7%) 112->116(22.0%) 102->113(20.4%)
29	222.6	44.92	5.569	0.3344	111->116(45.7%)
30	221.0	45.24	5.609	0.0007	102->114(81.0%)
31	219.4	45.59	5.652	0.1026	112->116(44.9%) 110->116(21.6%) 102->113(11.6%)
32	217.9	45.90	5.691	0.0316	111->116(18.2%) 100->114(14.4%) 96->114(14.2%) 103->114(10.1%)
33	217.5	45.98	5.701	0.0023	103->113(75.5%)
34	216.9	46.09	5.715	0.0221	101->113(46.3%) 110->116(12.2%)
35	215.8	46.34	5.746	0.0174	110->116(36.1%) 112->116(15.0%) 101->113(11.8%)
36	214.9	46.53	5.769	0.0480	102->113(57.6%) 112->117(18.4%)
37	211.8	47.22	5.854	0.0021	106->116(81.2%)
38	211.1	47.37	5.873	0.0004	105->115(89.8%)
39	209.8	47.68	5.911	0.0052	100->113(56.0%) 96->113(21.3%) 103->113(15.1%)
40	207.5	48.19	5.975	0.0442	112->118(27.8%) 110->117(19.3%) 111->117(15.0%) 112->117(10.7%)

Isopropoxy **2**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	346.1	28.89	3.582	0.0078	144->145(84.0%) 143->145(14.5%)
2	340.3	29.38	3.643	0.0042	143->145(83.5%) 144->145(15.3%)
3	317.7	31.47	3.902	0.0034	143->146(85.8%)
4	317.2	31.53	3.909	0.2432	142->145(90.7%)
5	315.1	31.74	3.935	0.0002	144->146(89.9%)
6	298.5	33.50	4.153	0.0002	142->146(80.4%)
7	289.0	34.60	4.290	0.0367	144->147(55.5%) 139->145(22.1%) 143->147(14.7%)
8	287.1	34.83	4.318	0.0631	139->145(55.9%) 144->147(27.9%)
9	282.2	35.43	4.393	0.0109	143->147(82.2%) 144->147(16.0%)
10	276.9	36.12	4.478	0.0000	139->146(74.8%)
11	275.0	36.36	4.508	0.0015	141->145(91.7%)
12	272.6	36.68	4.548	0.0000	140->145(95.3%)
13	271.7	36.80	4.563	0.0002	138->145(91.6%)
14	264.8	37.76	4.682	0.1774	142->147(79.7%)
15	258.3	38.71	4.800	0.0145	137->146(89.7%)
16	255.5	39.14	4.853	0.0007	140->146(71.1%) 136->146(15.7%)
17	251.8	39.71	4.924	0.0056	141->146(84.1%)
18	248.2	40.29	4.995	1.0454	138->146(65.7%)
19	247.5	40.40	5.009	0.0109	137->145(82.8%)
20	246.3	40.59	5.033	0.0020	136->146(55.8%) 140->146(14.4%) 137->145(13.3%)
21	245.8	40.69	5.045	0.1553	144->151(26.9%) 143->150(13.3%) 143->152(11.4%) 144->148(10.8%)
22	245.3	40.77	5.055	0.0657	143->151(30.4%) 144->150(23.0%) 144->152(11.9%)
23	243.4	41.08	5.093	0.0659	139->147(72.8%) 141->147(10.5%)
24	242.2	41.30	5.120	0.4426	144->148(44.1%) 144->149(24.1%)
25	239.0	41.84	5.187	0.3963	136->145(56.5%) 143->148(16.7%) 143->149(10.4%)
26	237.3	42.13	5.224	0.0235	141->147(80.9%)
27	233.9	42.75	5.300	0.0032	140->147(94.9%)
28	233.6	42.81	5.308	0.0130	143->148(60.2%) 136->145(13.7%)
29	232.1	43.09	5.343	0.0015	138->147(86.7%)
30	232.0	43.11	5.345	0.0093	144->149(31.3%) 144->148(26.5%) 143->149(14.4%) 138->147(10.0%)
31	229.2	43.63	5.410	0.0272	143->149(52.4%) 144->149(24.9%)
32	227.8	43.89	5.442	0.0004	135->146(74.1%)
33	226.8	44.09	5.467	0.0367	135->145(64.7%)
34	221.2	45.20	5.604	0.0519	144->150(28.6%) 143->150(18.7%) 144->152(15.6%) 143->152(11.5%)
35	220.5	45.36	5.624	0.0743	144->150(27.7%) 143->150(24.8%) 144->152(10.7%)
36	218.8	45.71	5.667	0.0837	142->148(33.2%) 135->145(16.8%) 142->149(13.3%) 133->145(12.5%)
37	217.5	45.98	5.701	0.0069	128->146(23.0%) 143->150(16.2%)
38	216.9	46.10	5.716	0.0003	133->145(47.4%) 136->147(14.4%)
39	216.6	46.16	5.723	0.0006	134->145(69.4%) 128->145(12.9%)
40	216.1	46.27	5.737	0.0022	144->153(68.8%)

t-butyl **3**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	319.5	31.30	3.881	0.2220	112->113(92.0%)
2	305.6	32.72	4.057	0.0006	112->114(88.9%)
3	290.8	34.38	4.263	0.0917	111->113(46.2%) 107->113(34.6%)
4	282.8	35.36	4.384	0.0323	110->113(82.0%) 107->113(11.1%)
5	281.0	35.59	4.413	0.0087	111->113(49.3%) 107->113(33.6%)
6	280.6	35.64	4.419	0.0001	107->114(51.6%) 111->114(31.0%)
7	278.1	35.96	4.459	0.0001	109->113(88.7%)
8	275.4	36.31	4.502	0.0001	110->114(78.2%)
9	275.3	36.32	4.503	0.0012	108->113(88.5%)
10	270.4	36.98	4.585	0.0004	106->113(95.9%)
11	264.9	37.75	4.680	0.1936	112->115(76.8%) 107->113(11.1%)
12	261.9	38.18	4.734	0.0014	111->114(61.9%) 107->114(31.2%)
13	257.6	38.82	4.813	0.0001	108->114(68.0%) 109->114(27.2%)
14	256.8	38.95	4.829	0.0123	105->114(90.0%)
15	255.7	39.11	4.849	0.0001	109->114(61.0%) 108->114(28.6%)
16	247.2	40.46	5.016	0.0445	111->115(60.6%) 107->115(18.1%) 110->115(11.3%)
17	246.0	40.65	5.040	0.7166	106->114(76.6%)
18	244.7	40.86	5.066	0.0007	105->113(91.7%)
19	243.0	41.16	5.103	0.0015	104->114(75.0%)
20	241.0	41.49	5.144	0.0130	110->115(74.0%) 107->115(17.6%)
21	239.9	41.69	5.169	0.0123	109->115(62.3%) 111->115(11.6%)
22	238.8	41.88	5.193	0.0282	107->115(37.4%) 111->115(19.5%) 109->115(18.7%)
23	236.3	42.31	5.246	0.0090	108->115(37.8%) 108->116(21.2%)
24	235.4	42.48	5.267	0.0003	109->116(36.6%) 111->120(12.6%) 109->115(10.3%)
25	235.1	42.54	5.274	0.0021	108->115(43.3%) 108->116(21.3%)
26	234.6	42.62	5.284	0.3588	104->113(79.6%)
27	230.5	43.38	5.379	0.0013	106->115(96.7%)
28	223.7	44.71	5.543	0.1702	112->117(22.7%) 112->116(22.0%) 102->113(20.4%)
29	222.6	44.92	5.569	0.3344	111->116(45.7%)
30	221.0	45.24	5.609	0.0007	102->114(81.0%)
31	219.4	45.59	5.652	0.1026	112->116(44.9%) 110->116(21.6%) 102->113(11.6%)
32	217.9	45.90	5.691	0.0316	111->116(18.2%) 100->114(14.4%) 96->114(14.2%) 103->114(10.1%)
33	217.5	45.98	5.701	0.0023	103->113(75.5%)
34	216.9	46.09	5.715	0.0221	101->113(46.3%) 110->116(12.2%)
35	215.8	46.34	5.746	0.0174	110->116(36.1%) 112->116(15.0%) 101->113(11.8%)
36	214.9	46.53	5.769	0.0480	102->113(57.6%) 112->117(18.4%)
37	211.8	47.22	5.854	0.0021	106->116(81.2%)
38	211.1	47.37	5.873	0.0004	105->115(89.8%)
39	209.8	47.68	5.911	0.0052	100->113(56.0%) 96->113(21.3%) 103->113(15.1%)
40	207.5	48.19	5.975	0.0442	112->118(27.8%) 110->117(19.3%) 111->117(15.0%) 112->117(10.7%)

Naphthyl **4**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	356.8	28.03	3.475	0.0018	137->139(87.6%) 138->139(11.9%)
2	351.7	28.43	3.525	0.0052	138->139(87.8%) 137->139(11.8%)
3	328.4	30.45	3.775	0.0486	138->140(69.3%) 137->140(27.8%)
4	324.7	30.80	3.819	0.0072	137->140(67.4%) 138->140(29.0%)
5	318.4	31.41	3.894	0.2317	136->139(93.3%)
6	305.2	32.77	4.063	0.0002	136->140(87.1%)
7	296.4	33.74	4.183	0.0094	137->141(85.6%) 138->141(11.7%)
8	291.1	34.35	4.259	0.1774	138->142(49.3%) 138->141(25.5%)
9	290.0	34.48	4.275	0.2054	137->142(38.1%) 138->141(37.4%)
10	289.0	34.60	4.290	0.0191	134->139(79.7%)
11	288.7	34.64	4.295	0.1378	137->142(19.9%) 138->141(19.3%) 138->142(18.1%) 134->139(13.4%) 133->139(11.5%)
12	286.6	34.89	4.326	0.0093	133->139(55.8%) 137->142(17.6%)
13	285.5	35.02	4.342	0.0025	135->139(88.1%)
14	279.9	35.73	4.430	0.0003	133->140(82.3%)
15	275.8	36.25	4.495	0.0038	138->146(25.9%) 135->142(17.0%) 135->140(16.2%) 135->143(14.7%) 138->143(10.1%)
16	275.1	36.35	4.507	0.0067	138->143(40.3%) 137->145(11.7%) 134->142(11.5%) 138->142(10.5%)
17	274.4	36.44	4.518	0.0068	138->143(24.5%) 137->145(23.3%) 134->142(22.0%) 134->143(10.9%)
18	273.7	36.54	4.530	0.0004	132->139(89.2%)
19	272.0	36.76	4.558	0.0126	137->143(78.7%) 137->142(10.0%)
20	265.3	37.69	4.673	0.0989	136->141(47.2%) 134->140(34.2%)
21	264.9	37.75	4.680	0.0120	135->140(63.0%) 134->140(20.7%)
22	264.8	37.77	4.683	0.0875	134->140(41.1%) 136->141(33.7%) 135->140(10.9%)
23	259.3	38.57	4.782	0.0028	129->140(49.9%) 131->140(26.4%) 132->140(11.5%)
24	252.5	39.60	4.910	0.0687	128->140(43.0%) 129->140(13.0%) 132->140(12.7%)
25	248.8	40.19	4.983	0.5050	132->140(56.1%) 131->140(12.9%)
26	247.9	40.34	5.002	0.0033	134->141(93.0%)
27	246.5	40.56	5.029	0.0164	131->139(65.3%) 129->139(23.8%)
28	243.4	41.08	5.093	0.0012	135->141(88.1%)
29	242.7	41.20	5.108	0.0366	133->141(74.9%)
30	237.7	42.08	5.217	0.1106	138->144(32.6%) 129->139(21.8%) 128->139(18.0%)
31	237.2	42.17	5.228	0.0070	136->142(80.9%) 138->144(11.9%)
32	236.8	42.23	5.236	0.0585	138->144(47.0%) 129->139(16.0%) 128->139(12.3%)
33	235.4	42.49	5.268	0.0600	130->139(38.8%) 137->144(13.5%) 129->139(12.7%) 128->139(12.1%)
34	234.9	42.58	5.279	0.0122	135->142(45.9%) 135->143(24.9%)
35	234.4	42.66	5.289	0.0065	137->144(63.2%)
36	233.8	42.78	5.304	0.0001	132->141(85.9%)
37	233.4	42.85	5.313	0.0180	128->140(18.0%) 126->140(15.9%) 131->140(10.9%) 130->140(10.3%)
38	232.7	42.98	5.329	0.0313	134->143(41.8%) 134->142(36.9%)
39	231.3	43.23	5.360	0.0004	132->142(58.5%)
40	230.3	43.42	5.383	0.0096	138->145(65.6%)

Styrenyl **5**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	327.2	30.56	3.789	0.0264	126->127(62.8%) 125->127(24.2%) 124->127(10.9%)
2	321.7	31.08	3.854	0.0116	125->127(58.7%) 126->127(34.4%)
3	315.6	31.69	3.929	0.2270	124->127(77.0%) 125->127(16.5%)
4	308.3	32.44	4.022	0.0002	124->128(50.3%) 125->128(26.4%) 126->128(11.9%)
5	300.4	33.29	4.127	0.0001	125->128(51.6%) 126->128(38.1%)
6	294.3	33.98	4.213	0.0002	126->128(42.8%) 124->128(39.6%) 125->128(16.3%)
7	287.5	34.79	4.313	0.1354	121->127(78.7%)
8	277.6	36.02	4.466	0.0009	121->128(77.9%)
9	275.2	36.33	4.505	0.2270	126->129(53.3%) 126->130(20.3%) 123->127(10.1%)
10	274.2	36.46	4.521	0.1778	123->127(78.2%) 126->130(10.7%)
11	273.3	36.59	4.537	0.5604	126->130(38.7%) 126->129(17.6%) 125->129(15.9%)
12	271.7	36.80	4.563	0.0324	122->127(91.1%)
13	270.1	37.03	4.591	0.6511	125->130(41.6%) 125->129(18.7%) 126->130(11.2%) 126->129(10.8%)
14	269.2	37.15	4.606	0.0052	120->127(95.5%)
15	268.6	37.23	4.616	0.2293	125->129(49.9%) 125->130(27.4%) 126->129(13.0%)
16	264.1	37.87	4.695	0.1750	124->129(76.5%)
17	259.9	38.48	4.771	0.0735	126->131(24.5%) 123->130(20.3%) 123->131(12.9%)
18	258.0	38.75	4.805	0.0048	122->130(44.3%) 122->131(17.7%) 125->134(11.8%)
19	256.6	38.96	4.831	0.0938	119->128(45.3%) 126->131(25.6%)
20	256.1	39.05	4.842	0.0748	126->131(29.2%) 119->128(28.4%) 123->130(13.6%)
21	255.4	39.16	4.855	0.0013	122->128(72.7%) 123->128(10.2%)
22	255.1	39.21	4.861	0.1049	125->131(69.6%) 119->128(10.3%)
23	252.8	39.56	4.905	0.0002	123->128(76.3%) 122->128(18.3%)
24	247.2	40.45	5.015	0.0008	118->128(71.4%)
25	244.1	40.97	5.080	0.1035	120->128(33.6%) 121->129(25.8%) 119->127(19.8%)
26	243.8	41.01	5.085	0.0283	119->127(75.7%)
27	242.3	41.26	5.116	0.1426	121->129(43.2%) 120->128(23.5%)
28	240.1	41.65	5.164	0.0009	124->130(93.9%)
29	236.7	42.26	5.239	0.0026	123->129(86.6%)
30	234.1	42.72	5.297	0.2173	118->127(72.9%) 120->128(13.7%)
31	233.1	42.89	5.318	0.0011	122->129(94.6%)
32	230.8	43.33	5.372	0.0161	124->131(93.8%)
33	230.1	43.46	5.388	0.0002	120->129(95.4%)
34	228.5	43.76	5.426	0.0022	117->128(62.2%) 113->128(18.3%)
35	227.7	43.92	5.445	0.0355	117->127(60.3%)
36	227.0	44.05	5.462	0.0113	123->130(44.9%) 123->131(37.0%)
37	225.9	44.26	5.488	0.0013	120->130(72.9%)
38	225.3	44.38	5.502	0.0052	122->131(49.7%) 122->130(39.7%)
39	222.6	44.92	5.570	0.0048	125->132(58.9%) 126->132(38.4%)
40	222.2	45.00	5.579	0.0010	121->130(81.2%)

Acetylphenyl **6**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	319.5	31.29	3.880	0.2041	122->125(73.1%) 124->125(13.0%)
2	308.1	32.46	4.024	0.0002	122->126(68.3%) 124->126(12.4%)
3	302.4	33.07	4.100	0.0450	124->125(80.3%) 122->125(16.3%)
4	299.0	33.45	4.147	0.0368	123->125(90.7%)
5	286.3	34.93	4.331	0.0937	119->125(72.5%)
6	285.9	34.97	4.336	0.0011	123->126(60.1%) 119->126(13.4%) 124->126(13.2%)
7	284.2	35.18	4.362	0.0003	122->126(30.9%) 124->126(26.3%) 123->126(20.1%) 119->126(17.0%)
8	274.2	36.46	4.521	0.0001	124->126(45.7%) 119->126(45.2%)
9	266.7	37.49	4.648	0.0112	118->125(76.7%) 121->125(11.8%)
10	266.2	37.56	4.657	0.0542	121->125(38.9%) 122->127(26.2%) 118->125(19.0%)
11	264.8	37.77	4.683	0.0480	121->125(34.4%) 122->127(22.6%) 120->125(20.1%) 119->125(10.5%)
12	263.0	38.02	4.714	0.0072	120->125(76.5%)
13	260.0	38.46	4.768	0.9917	124->128(56.2%) 124->127(12.1%)
14	258.2	38.73	4.802	0.8403	123->128(50.1%)
15	256.5	38.98	4.833	0.1646	124->127(58.7%) 124->128(18.7%) 122->127(11.2%)
16	255.2	39.18	4.858	0.0586	115->126(53.5%) 117->126(24.0%)
17	252.7	39.58	4.907	0.0290	123->127(75.1%)
18	251.3	39.79	4.933	0.0604	121->128(36.0%) 121->129(17.0%) 124->132(16.3%)
19	251.2	39.81	4.936	0.0123	120->128(39.6%) 120->129(11.3%) 123->131(11.1%)
20	250.7	39.88	4.945	0.0023	120->126(32.5%) 114->126(27.9%) 121->126(17.1%)
21	247.0	40.49	5.020	0.0001	120->126(53.8%) 121->126(39.1%)
22	244.5	40.90	5.071	0.2825	124->129(35.1%) 118->126(25.1%) 124->128(12.1%) 123->128(10.3%)
23	244.0	40.99	5.082	0.0016	114->126(47.6%) 121->126(32.1%)
24	242.2	41.29	5.119	0.0310	119->127(48.8%) 124->129(17.5%)
25	241.7	41.38	5.130	0.0011	115->125(55.6%) 117->125(38.8%)
26	241.3	41.45	5.139	0.0296	122->128(49.4%) 123->129(28.2%)
27	241.1	41.48	5.143	0.0540	123->129(41.1%) 122->128(36.2%) 119->127(10.9%)
28	240.0	41.67	5.167	0.0901	124->129(28.1%) 118->126(23.0%) 114->125(14.7%)
29	232.0	43.11	5.345	0.1585	114->125(70.1%) 118->126(14.2%)
30	230.7	43.34	5.374	0.0000	117->128(25.3%) 116->128(23.5%) 117->129(17.6%) 116->129(12.1%)
31	230.2	43.44	5.386	0.0014	116->129(18.7%) 117->128(15.6%) 116->128(13.5%) 122->129(11.3%) 118->128(10.8%)
32	230.1	43.46	5.388	0.0089	122->129(64.5%) 121->127(15.3%)
33	229.9	43.51	5.394	0.0033	121->127(63.5%) 122->129(18.7%)
34	228.0	43.85	5.437	0.0004	118->127(81.7%)
35	226.6	44.13	5.472	0.0011	120->127(42.3%) 113->126(20.3%) 118->128(15.8%)
36	226.5	44.14	5.473	0.0011	120->127(46.7%) 113->126(18.6%) 118->128(12.4%)
37	225.1	44.42	5.507	0.0006	118->128(39.3%) 113->126(33.2%)
38	224.4	44.56	5.525	0.0453	113->125(48.0%) 122->130(16.1%)
39	223.5	44.75	5.548	0.0130	119->128(51.5%) 121->128(16.2%)
40	223.3	44.78	5.552	0.0008	116->125(72.4%) 117->125(11.0%)

Carbonyl **7**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	322.2	31.04	3.848	0.0001	129->136(53.7%) 129->138(36.1%)
2	321.5	31.11	3.857	0.0001	130->138(49.7%) 130->136(41.1%)
3	319.0	31.35	3.887	0.2253	134->135(94.0%)
4	308.3	32.43	4.021	0.0013	134->137(89.9%)
5	287.9	34.74	4.307	0.1169	127->135(49.1%) 133->135(26.0%) 131->135(10.2%)
6	281.5	35.53	4.405	0.0005	127->137(49.2%) 133->137(24.9%) 131->137(11.6%)
7	271.4	36.84	4.568	0.0607	132->135(62.9%) 133->135(10.8%)
8	269.9	37.04	4.593	0.0064	133->135(51.1%) 127->135(13.1%) 134->139(10.5%)
9	269.1	37.17	4.608	0.0191	131->136(39.5%) 131->138(28.8%) 131->135(10.1%)
10	268.3	37.28	4.622	0.0170	128->136(21.1%) 132->135(18.1%) 132->136(10.8%)
11	267.7	37.36	4.632	0.0013	132->137(58.1%) 124->137(10.7%)
12	266.3	37.54	4.655	0.0259	131->135(64.0%) 134->139(12.5%)
13	265.7	37.63	4.666	0.0021	126->135(92.1%)
14	264.5	37.81	4.688	0.1039	134->136(73.1%)
15	262.6	38.08	4.721	0.1585	134->139(52.3%) 127->135(17.0%) 134->136(14.2%)
16	261.4	38.26	4.744	0.0589	128->135(86.0%)
17	258.1	38.74	4.803	0.0001	130->135(94.2%)
18	257.7	38.81	4.812	0.6969	133->136(38.1%) 134->138(21.2%)
19	255.9	39.08	4.845	0.6500	125->137(28.1%) 132->136(21.0%) 128->136(13.5%)
20	255.7	39.10	4.848	0.0000	129->135(97.2%)
21	253.7	39.42	4.887	0.1136	133->137(29.8%) 125->137(20.6%) 127->137(19.9%)
22	253.5	39.45	4.891	0.0937	134->138(54.7%) 133->136(15.3%) 133->137(10.6%)
23	253.3	39.47	4.894	0.1596	125->137(30.6%) 133->137(15.0%) 134->138(13.7%) 132->136(10.2%)
24	248.7	40.21	4.986	0.0001	131->137(62.4%) 128->137(20.3%)
25	247.9	40.34	5.001	0.0000	128->137(68.1%) 131->137(15.6%) 132->137(11.7%)
26	244.4	40.92	5.074	0.1206	133->138(54.5%) 133->136(27.1%)
27	243.0	41.15	5.102	0.0039	127->139(38.1%) 133->139(27.4%) 131->139(10.1%)
28	241.7	41.38	5.130	0.0206	132->138(35.3%) 126->136(26.8%) 132->136(11.7%)
29	241.5	41.40	5.133	0.0048	126->136(42.5%) 132->138(13.0%) 131->136(12.6%)
30	241.4	41.42	5.136	0.0353	131->138(31.1%) 131->136(25.8%)
31	240.5	41.58	5.155	0.0031	124->137(46.3%) 125->135(24.8%) 132->137(10.6%)
32	240.3	41.61	5.159	0.0887	126->137(29.3%) 132->138(18.5%) 133->138(12.8%) 124->135(10.8%)
33	239.8	41.70	5.170	0.0007	125->135(71.7%) 124->137(17.8%)
34	238.3	41.96	5.202	0.0069	127->136(33.7%) 128->138(23.8%) 128->136(15.7%) 131->138(11.6%)
35	237.6	42.09	5.218	0.0034	129->137(69.9%) 127->136(11.4%)
36	237.5	42.10	5.220	0.0036	130->137(41.5%) 128->138(29.3%) 127->136(14.9%)
37	237.3	42.13	5.224	0.0132	130->137(42.6%) 129->137(25.5%) 128->138(12.4%)
38	234.6	42.63	5.285	0.0000	130->136(51.5%) 130->138(42.9%)
39	233.5	42.83	5.310	0.0000	129->138(57.5%) 129->136(39.3%)
40	232.7	42.96	5.327	0.0080	133->139(45.2%) 132->139(25.6%) 127->139(19.6%)

Propyl **8**

Summary of calculated electronic transitions:

#	nm	1000 cm-1	eV	f	Assignment (excitations with contrib. greater than 10.0%)
1	318.9	31.36	3.888	0.2392	96->97(94.0%)
2	300.1	33.33	4.132	0.0003	96->98(86.1%) 94->98(10.2%)
3	287.9	34.73	4.306	0.0877	94->97(83.3%)
4	287.0	34.84	4.320	0.0014	95->97(94.8%)
5	274.9	36.38	4.511	0.0001	94->98(81.8%)
6	266.1	37.58	4.659	0.1728	96->99(76.8%)
7	260.3	38.42	4.763	0.0481	93->98(77.3%)
8	253.5	39.45	4.891	0.5572	95->98(80.5%)
9	253.2	39.49	4.896	0.0004	93->97(51.3%) 92->98(30.4%)
10	252.2	39.66	4.917	0.0013	93->97(40.1%) 92->98(37.6%) 90->98(12.2%)
11	243.7	41.04	5.088	0.0156	94->99(84.7%)
12	243.3	41.11	5.097	0.0002	95->99(96.0%)
13	239.6	41.74	5.175	0.2066	92->97(84.4%)
14	235.1	42.54	5.274	0.0008	91->97(89.7%)
15	232.5	43.01	5.333	0.0032	90->98(65.3%) 92->98(18.5%)
16	231.8	43.13	5.348	0.0415	90->97(72.5%)
17	223.3	44.79	5.553	0.1254	91->98(53.6%) 82->98(14.2%)
18	219.9	45.47	5.637	0.1317	96->100(58.4%)
19	217.9	45.89	5.690	0.0001	93->99(92.3%)
20	217.7	45.94	5.696	0.0067	88->97(40.7%) 92->99(21.2%) 89->97(11.9%)
21	216.1	46.27	5.737	0.0046	87->97(62.3%) 82->97(20.1%)
22	210.8	47.45	5.883	0.2644	91->98(25.1%) 82->98(24.3%) 87->98(17.4%)
23	207.4	48.21	5.977	0.0642	92->99(63.0%) 89->97(21.6%)
24	206.4	48.45	6.007	0.0016	95->100(86.7%)
25	206.2	48.49	6.012	0.0232	89->97(52.8%) 88->97(23.3%)
26	205.3	48.71	6.039	0.0007	91->99(84.5%)
27	202.6	49.37	6.121	0.0003	88->98(61.1%) 89->98(18.9%)
28	201.8	49.56	6.145	0.0280	86->97(48.6%) 90->99(44.7%)
29	201.6	49.61	6.151	0.0484	86->97(44.8%) 90->99(38.7%)
30	201.0	49.75	6.168	0.0005	82->97(41.2%) 87->97(16.6%) 96->101(16.1%) 85->97(11.5%)
31	200.6	49.84	6.180	0.0026	96->101(69.3%)
32	199.9	50.02	6.202	0.2379	94->100(58.2%) 96->102(19.2%)
33	197.7	50.59	6.272	0.0114	83->97(45.2%) 88->99(23.0%)
34	197.1	50.73	6.290	0.0102	89->98(42.6%) 88->98(18.8%) 83->98(10.5%)
35	196.7	50.84	6.304	0.0174	87->98(40.4%) 82->98(11.4%) 89->98(11.2%)
36	195.4	51.17	6.344	0.0006	85->97(73.0%) 82->97(13.8%)
37	194.8	51.33	6.364	0.0002	84->97(47.0%) 81->97(29.7%) 80->97(12.8%)
38	191.6	52.19	6.471	0.0001	86->98(35.6%) 84->97(23.0%) 83->98(17.1%)
39	191.2	52.30	6.484	0.0004	86->98(29.5%) 84->97(23.6%) 80->97(12.5%) 81->97(12.0%)
40	190.4	52.53	6.513	0.0011	87->99(45.5%) 81->97(17.6%) 82->99(12.8%)