Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First Principles Investigation of the Spectral Properties of Neutral, Zwitterionic, and *bis*-Cationic Azaacenes

Supporting Information

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Contents

S.1 Ground-state Cartesian coordinates

Atomic coordinates of Isodiphenylfluorindone **1** at PBE0/6-31+G(d) level of theory

C	0.000010	0.848466	-3.519873
C	0.000001	0.791763	-1.214108
C	-0.000015	-0.639700	-1.198991
C	-0.000010	-0.612046	-3.608052
C	0.000007	1.477065	-0.000000
C	-0.000024	-1.347114	0.000000
C	-0.000015	-0.639700	1.198991
C	0.000001	0.791763	1.214108
C	0.000010	0.848466	3.519873
C	-0.000010	-0.612046	3.608052
H	0.000019	2.562598	-0.000000
H	-0.000035	-2.434516	0.000000
C	-0.000009	-1.257381	4.813412
C	0.000010	1.590929	4.758222
H	0.000019	2.674671	4.680045
C	-0.000001	-0.515305	6.050345
C	-0.000009	-1.257381	-4.813412
C	-0.000001	-0.515305	-6.050345
C	0.000010	1.590929	-4.758222
H	-0.000011	-2.342976	4.872074
H	0.000019	2.674671	-4.680045
H	-0.000011	-2.342976	-4.872074
C	0.000007	0.955316	5.948717
C	0.000007	0.955316	-5.948717
O	0.000019	-1.069134	-7.163860
O	0.000019	-1.069134	7.163860
N	-0.000023	-1.271024	2.405987
N	0.000006	1.495840	2.385020
N	-0.000023	-1.271024	-2.405987
N	0.000006	1.495840	-2.385020
H	0.000025	1.506059	-6.885485
H	0.000025	1.506059	6.885485
H	-0.000045	-2.284539	-2.420228
H	-0.000045	-2.284539	2.420228

Atomic coordinates of Isodiphenylfluorindinone **2** at PBE0/6-31+G(d) level of theory

C	-1.45341727	-0.33411287	0.00000000
C	-0.75041791	-1.51379553	0.00000000
C	-0.79037206	0.91966709	0.00000000
C	0.68582679	-1.48119900	0.00000000
N	-1.36344057	-2.75326101	0.00000000
C	0.63387256	0.93037367	0.00000000
N	-1.50444825	2.06227286	0.00000000
C	1.35739388	-0.26731659	0.00000000
N	1.35668696	-2.67040225	0.00000000
C	-0.67323526	-3.95515182	0.00000000
N	1.24739032	2.14400158	0.00000000
C	-0.87227438	3.22621395	0.00000000
H	2.44447459	-0.25052703	0.00000000
C	0.73307867	-3.91788514	0.00000000
C	-1.32373604	-5.18760509	0.00000000
C	0.57183905	3.33755287	0.00000000
C	-1.62077425	4.44792723	0.00000000
C	1.46334798	-5.10183117	0.00000000
H	-2.41078389	-5.21628142	0.00000000
C	-0.58681292	-6.37299884	0.00000000
C	1.21176931	4.55808940	0.00000000
H	-2.70493142	4.36633537	0.00000000
C	-0.99411642	5.65221184	0.00000000
C	0.80481678	-6.33295155	0.00000000
H	2.55021356	-5.05861551	0.00000000
H	-1.10932043	-7.32534805	0.00000000
C	0.46681267	5.78188634	0.00000000
H	2.29783943	4.61596206	0.00000000
H	-1.56376862	6.57824941	0.00000000
H	1.38392120	-7.25161405	0.00000000
H	-2.53995601	-0.33487208	0.00000000
O	1.00775599	6.91517648	0.00000000
H	-2.37333756	-2.78107555	0.00000000
H	2.36760196	-2.64841790	0.00000000
H	2.26107306	2.17206590	0.00000000

Atomic coordinates of 3-Benzoyloxyisodiphenylfluorindine **3** at PBE0/6-31+G(d) level of theory

C	-3.13260600	1.61003104	-0.00280199
C	-4.22682501	0.73476705	0.01041801
C	-1.80407401	1.17534702	-0.09321200
C	-3.93974503	-0.69594596	-0.07677100
N	-5.48304201	1.18832406	0.09861003
C	-1.57658002	-0.26635998	-0.17621201
N	-0.78407700	2.04216001	-0.10228700
C	-2.63309403	-1.17020297	-0.16545401
N	-4.99328303	-1.53157195	-0.06514000
C	-6.50863702	0.29688407	0.11054603
N	-0.29777003	-0.68058099	-0.26698403
C	0.48574699	1.56671100	-0.18796901
H	-2.43966904	-2.23904197	-0.22251802
C	-6.30395203	-1.10487393	0.03009901
C	-7.84445201	0.74801108	0.20678804
C	0.78098398	0.18148100	-0.27416603
C	1.57964700	2.46028499	-0.19921802
C	-7.36892804	-2.00917092	0.04601101
H	-8.01259500	1.81985208	0.26924505
C	-8.89987102	-0.14635191	0.22141104
C	2.09173498	-0.29175601	-0.36249204
H	1.36650101	3.52346599	-0.13767901
C	2.88148100	2.00356998	-0.28893903
C	-8.66724303	-1.53023591	0.14144403
H	-7.17176605	-3.07740793	-0.01484400
H	-9.91877401	0.22440410	0.29613405
C	3.12385098	0.62823898	-0.36575404
H	2.30320596	-1.35594901	-0.42672005
H	3.71702501	2.69716797	-0.30138803
H	-9.49992604	-2.22745490	0.15450003
H	-3.32385899	2.67657104	0.06128702
O	4.42751298	0.16996697	-0.53156705
C	5.20006199	0.03827795	0.57643094
C	6.57702198	-0.39873706	0.24503493
C	7.47450698	-0.59161908	1.30153792
C	6.99376497	-0.61357905	-1.07417708
C	8.77871198	-0.99775609	1.04147190
H	7.13742499	-0.41907608	2.31933392

C	8.30034296	-1.01961807	-1.32968209
H	6.29809796	-0.46133204	-1.89295507
C	9.19250997	-1.21196808	-0.27435110
H	9.47362698	-1.14658310	1.86336990
H	8.62349395	-1.18507106	-2.35380510
H	10.21232996	-1.52846309	-0.47749711
O	4.79178900	0.25547294	1.69629294
H	-4.82113804	-2.52917295	-0.12991301
H	-0.11734104	-1.67632099	-0.33371104

Atomic coordinates of 3,9-Dibenzoyloxyisodiphenylfluorindine **4** at PBE0/6-31+G(d) level of theory

C	0.00327493	-2.61736601	0.18815805
C	-1.22480207	-1.95883402	0.04367102
C	1.23905093	-1.97254301	0.04688004
C	-1.18559808	-0.53191103	-0.27061002
N	-2.38722107	-2.60703802	0.18754504
C	1.21673392	-0.54553802	-0.26871701
N	2.39359193	-2.63350699	0.19484506
C	0.01960892	0.14708997	-0.42078503
N	-2.36769908	0.09673996	-0.41014105
C	-3.54966007	-1.92060304	0.03821501
N	2.40615992	0.06946199	-0.40718002
C	3.56426193	-1.96039799	0.04817005
H	0.02586391	1.20976397	-0.65480507
C	-3.58622308	-0.53571405	-0.26877203
C	-4.79039507	-2.58069704	0.18329102
C	3.61743992	-0.57633800	-0.26169199
C	4.79661893	-2.63371598	0.20006508
C	-4.78793908	0.15806994	-0.42334606
H	-4.77697706	-3.64163303	0.41574305
C	-5.98664707	-1.90413005	0.03272399
C	4.82683392	0.10368100	-0.41453700
H	4.77080794	-3.69387397	0.43499711
C	6.00091293	-1.96954298	0.05510607
C	-5.97202008	-0.53764406	-0.26650005
H	-4.79922209	1.21875294	-0.66116909
H	-6.93692107	-2.41832805	0.14187700
C	6.00279292	-0.60439598	-0.24842998
H	4.84914391	1.16341800	-0.65576004
H	6.94589493	-2.49185797	0.17167509
H	-0.00281706	-3.67711600	0.42324008
O	7.22037692	0.03371702	-0.46362399
C	7.77072091	0.71968805	0.57043099
C	9.06875491	1.33268405	0.20152198
C	9.62379591	1.19085501	-1.07598901
C	9.74466990	2.07220608	1.17885496
C	10.84693091	1.78694401	-1.36908202
H	9.09990892	0.61628499	-1.83290700
C	10.96624989	2.66613908	0.88132395

H	9.30238389	2.17279011	2.16555796
C	11.51818390	2.52392205	-0.39288504
H	11.27745292	1.67597098	-2.36051501
H	11.48905789	3.23949811	1.64190894
H	12.47331790	2.98785204	-0.62513805
O	7.24586690	0.80776308	1.65880799
O	-7.17399608	0.12630693	-0.49213907
C	-7.82712209	0.63733995	0.58244091
C	-9.10031909	1.29217993	0.19929388
C	-9.86778810	1.87493796	1.21432386
C	-9.54435109	1.33982089	-1.12763713
C	-11.06987311	2.50179794	0.90518883
H	-9.51102311	1.82933899	2.23899186
C	-10.74851909	1.96793387	-1.43219415
H	-8.94953708	0.88651487	-1.91392411
C	-11.51102110	2.54873590	-0.41831717
H	-11.66381411	2.95344796	1.69500181
H	-11.09294308	2.00393684	-2.46209315
H	-12.45093510	3.03838389	-0.65973119
O	-7.39982410	0.55874099	1.71335591
H	-2.36512409	1.08726595	-0.62647808
H	2.41492691	1.05983998	-0.62415805

Atomic coordinates of 3-Hydroxy-12,14-diphenyl-7,14-dihydroquinoxalino[2,3-b]phenazine-5,12-diium bis perchlorate **5** at PBE0/6-31+G(d) level of theory

C	-0.41700405	1.48747305	0.00000000
C	0.80815796	0.82605806	0.00000000
C	-1.59310004	0.75304803	0.00000000
C	0.85642198	-0.62319794	0.00000000
N	1.98165395	1.47996008	0.00000000
C	-1.54454202	-0.69872597	0.00000000
N	-2.81018605	1.33218802	0.00000000
C	-0.32057301	-1.35906195	0.00000000
N	2.07179398	-1.20564392	0.00000000
C	3.21862196	0.88019609	0.00000000
N	-2.71543901	-1.35802798	0.00000000
C	-4.00854304	0.64775800	0.00000000
H	-0.28627900	-2.44477195	0.00000000
C	3.27078597	-0.52805891	0.00000000
C	4.40817695	1.62023911	0.00000000
C	-3.95952402	-0.75870600	0.00000000
C	-5.24091205	1.30711499	0.00000000
C	4.49413298	-1.19803689	0.00000000
H	4.37307793	2.70577410	0.00000000
C	5.61700696	0.96245212	0.00000000
C	-5.13979601	-1.50655601	0.00000000
H	-5.27754506	2.39323199	0.00000000
C	-6.40590104	0.55776797	0.00000000
C	5.66547597	-0.44932288	0.00000000
H	4.52315600	-2.28501589	0.00000000
H	6.54976795	1.51648913	0.00000000
C	-6.35616002	-0.84494303	0.00000000
H	-5.09411500	-2.59194501	0.00000000
H	-7.36577004	1.06421896	0.00000000
H	-7.27672601	-1.41963404	0.00000000
H	-0.45073706	2.57317705	0.00000000
O	6.89044198	-0.99823986	0.00000000
H	6.84477099	-1.96662886	0.00000000
H	-2.85100906	2.34642302	0.00000000
H	1.95721994	2.49534007	0.00000000
H	-2.68785800	-2.37279498	0.00000000
H	2.10739800	-2.22026492	0.00000000

Atomic coordinates of 13-Methoxyisodiphenylfluorindone **6** at PBE0/6-31+G(d) level of theory

C	-1.24615097	-0.90601487	0.00000000
C	-0.05736198	-1.62832688	0.00000000
C	1.13623703	-0.92111189	0.00000000
C	1.18905304	0.51424911	0.00000000
C	-0.03285395	1.23595012	0.00000000
C	-1.26450796	0.51934513	0.00000000
C	3.50355604	0.49892409	0.00000000
C	3.55440502	-0.95709092	0.00000000
C	4.74095502	-1.63711193	0.00000000
H	4.76835701	-2.72397793	0.00000000
C	5.99693403	-0.92775494	0.00000000
C	5.93236104	0.54397606	0.00000000
C	4.75753504	1.21073907	0.00000000
H	-0.06289399	-2.71506888	0.00000000
H	6.88256504	1.07125105	0.00000000
H	4.70976106	2.29634907	0.00000000
C	-3.65976397	-0.88251085	0.00000000
C	-3.57028096	0.57282215	0.00000000
C	-4.86415698	-1.53158884	0.00000000
C	-6.10092697	-0.79047983	0.00000000
C	-4.80565495	1.31509816	0.00000000
C	-5.99759396	0.67839817	0.00000000
H	-4.72905294	2.39911016	0.00000000
H	-6.93382695	1.23027418	0.00000000
H	-4.92010899	-2.61742884	0.00000000
N	-2.45419098	-1.53523386	0.00000000
N	-2.42933996	1.21456714	0.00000000
N	2.38010704	1.16750110	0.00000000
N	2.33227802	-1.57595290	0.00000000
O	-0.17628894	2.55178112	0.00000000
O	-7.21596798	-1.34544582	0.00000000
O	7.09655702	-1.51116395	0.00000000
C	0.88849807	3.50450811	0.00000000
H	0.37882608	4.46900011	0.00000000
H	1.50768706	3.39945112	0.89204707
H	1.50768706	3.39945112	-0.89204707
H	2.31640601	-2.58932490	0.00000000
H	-2.46349599	-2.54873686	0.00000000

Atomic coordinates of 7,14-dihydro-5*α*-benzo[b]quinoxalino[2,3-i]phenazine **7** at PBE0/6-31+G(d) level of theory

C	-1.19470423	-1.42952712	0.00000000
C	-2.42614373	-0.76352491	0.00000000
C	0.03826999	-0.76184961	0.00000000
C	-2.40009854	0.69850236	0.00000000
N	-3.58490129	-1.43516652	0.00000000
C	0.00244327	0.70261183	0.00000000
N	1.19373826	-1.43123866	0.00000000
C	-1.19821613	1.40252221	0.00000000
N	-3.58609851	1.33035936	0.00000000
C	-4.75146791	-0.74371674	0.00000000
N	1.18645860	1.34250942	0.00000000
C	2.36763596	-0.74031558	0.00000000
H	-1.19975705	2.49072115	0.00000000
C	-4.79930773	0.67558819	0.00000000
C	-5.98795716	-1.43123615	0.00000000
C	2.41016587	0.69486020	0.00000000
C	3.58781774	-1.41398269	0.00000000
C	-6.01082631	1.37460434	0.00000000
H	-5.96234074	-2.51760880	0.00000000
C	-7.18479236	-0.74076412	0.00000000
C	3.59687553	1.39437579	0.00000000
H	3.57100147	-2.50134179	0.00000000
C	4.81799986	-0.73051438	0.00000000
C	-7.20178846	0.66661649	0.00000000
H	-6.00877407	2.46284278	0.00000000
C	4.82923114	0.70511025	0.00000000
H	3.59009135	2.48337296	0.00000000
H	-1.19437349	-2.51518784	0.00000000
H	-3.59181222	2.34472036	0.00000000
H	1.18717240	2.35614407	0.00000000
C	6.07453981	1.38612095	0.00000000
C	6.06418199	-1.41850199	0.00000000
C	7.25268682	-0.72900571	0.00000000
C	7.25981418	0.68852908	0.00000000
H	8.20660148	1.22242996	0.00000000
H	6.07633486	2.47430829	0.00000000
H	8.19532028	-1.27057388	0.00000000
H	6.05821964	-2.50648083	0.00000000

H	-8.14708266	1.20135987	0.00000000
H	-8.12313834	-1.28896745	0.00000000

Atomic coordinates of 6,17-dihydro-8α-benzo[b]benzo[6,7]quinoxalino[2,3-i]phenazine **8** at PBE0/6-31+G(d) level of theory

C	0.00000000	0.00000000	1.42494695
C	0.00000000	1.23205600	0.75842995
C	0.00000000	-1.23205600	0.75842995
C	0.00000000	1.20088400	-0.70679505
N	0.00000000	2.38792000	1.42813395
C	0.00000000	-1.20088400	-0.70679505
N	0.00000000	-2.38792000	1.42813395
C	0.00000000	0.00000000	-1.40888205
N	0.00000000	2.38409900	-1.34363905
C	0.00000000	3.56052600	0.73981394
N	0.00000000	-2.38409900	-1.34363905
C	0.00000000	-3.56052600	0.73981394
H	0.00000000	0.00000000	-2.49705405
C	0.00000000	3.60540100	-0.69530105
C	0.00000000	4.78046000	1.41727595
C	0.00000000	-3.60540100	-0.69530105
C	0.00000000	-4.78046000	1.41727595
C	0.00000000	4.79446700	-1.39335005
H	0.00000000	4.76079200	2.50448194
C	0.00000000	6.00938200	0.73586595
C	0.00000000	-4.79446700	-1.39335005
H	0.00000000	-4.76079200	2.50448194
C	0.00000000	-6.00938200	0.73586595
C	0.00000000	6.02297500	-0.70103105
H	0.00000000	4.79009900	-2.48227906
C	0.00000000	-6.02297500	-0.70103105
H	0.00000000	-4.79009900	-2.48227906
H	0.00000000	0.00000000	2.51056294
H	0.00000000	2.38616700	-2.35769906
H	0.00000000	-2.38616700	-2.35769906
C	0.00000000	7.27073400	-1.37965805
C	0.00000000	7.25518900	1.42668495
C	0.00000000	-7.27073400	-1.37965805
C	0.00000000	-7.25518900	1.42668495
C	0.00000000	8.44365100	0.73931994
C	0.00000000	8.45320100	-0.67938606
C	0.00000000	-8.44365100	0.73931994
C	0.00000000	-8.45320100	-0.67938606

H	0.00000000	7.24692300	2.51453594
H	0.00000000	9.38562600	1.28186395
H	0.00000000	9.40130300	-1.21082505
H	0.00000000	7.27490500	-2.46770806
H	0.00000000	-9.40130300	-1.21082505
H	0.00000000	-7.27490500	-2.46770806
H	0.00000000	-9.38562600	1.28186395
H	0.00000000	-7.24692300	2.51453594

Atomic coordinates of 5,14-dihydro-12*α*-quinoxalino[2,3-b]phenazine-2-carbonitrile **9** at PBE0/6-31+G(d) level of theory

C	-0.67076096	1.51471305	0.00000000
C	-1.86773797	0.77678606	0.00000000
C	0.58829303	0.91794705	0.00000000
C	-1.75810297	-0.67983494	0.00000000
N	-3.05435296	1.38545506	0.00000000
C	0.64058403	-0.54389995	0.00000000
N	1.71169904	1.65875505	0.00000000
C	-0.51776897	-1.31289895	0.00000000
N	-2.90897997	-1.37577694	0.00000000
C	-4.18544597	0.63240806	0.00000000
N	1.86163803	-1.11152996	0.00000000
C	2.90778403	1.03448304	0.00000000
H	-0.45496998	-2.39877295	0.00000000
C	-4.15498697	-0.78614894	0.00000000
C	-5.45333497	1.25623407	0.00000000
C	3.03889003	-0.38409996	0.00000000
C	4.10527304	1.79139004	0.00000000
C	-5.32851697	-1.54717893	0.00000000
H	-5.48291096	2.34227107	0.00000000
C	-6.61291597	0.50451807	0.00000000
C	4.27788703	-1.00891596	0.00000000
H	4.01859104	2.87401204	0.00000000
C	5.34128903	1.18306803	0.00000000
C	-6.55412497	-0.90117693	0.00000000
H	-5.27088598	-2.63342593	0.00000000
H	-7.57884797	1.00211407	0.00000000
H	4.34923503	-2.09341096	0.00000000
H	6.24674004	1.78222903	0.00000000
H	-7.46978797	-1.48521193	0.00000000
H	-0.73303696	2.59825505	0.00000000
H	-2.86142298	-2.38924094	0.00000000
H	1.92383303	-2.12374096	0.00000000
C	6.71579503	-0.85521097	0.00000000
N	7.76233503	-1.36699197	0.00000000
C	5.43908303	-0.22625797	0.00000000

Atomic coordinates of 5,14-dihydro-7*α*-quinoxalino[2,3-b]phenazine-2-carbonitrile **10** at PBE0/6-31+G(d) level of theory

C	1.33218080	-0.50947501	0.00000000
C	0.59545534	0.67870832	0.00000000
C	0.73624641	-1.77974070	0.00000000
C	-0.86306086	0.56143412	0.00000000
N	1.19842751	1.87583714	0.00000000
C	-0.72322204	-1.83568771	0.00000000
N	1.47285204	-2.89536902	0.00000000
C	-1.49475407	-0.67396435	0.00000000
N	-1.56958624	1.71160005	0.00000000
C	0.43287314	2.99651485	0.00000000
N	-1.28775428	-3.05419867	0.00000000
C	0.84846909	-4.10121751	0.00000000
H	-2.58090789	-0.73741889	0.00000000
C	-0.98747222	2.96091672	0.00000000
C	1.04210731	4.26589430	0.00000000
C	-0.56500347	-4.22909587	0.00000000
C	1.60559457	-5.29502509	0.00000000
C	-1.75982971	4.12486222	0.00000000
H	2.12642728	4.31688708	0.00000000
C	0.26915141	5.42534422	0.00000000
C	-1.19432091	-5.47781979	0.00000000
H	2.68858683	-5.20728174	0.00000000
C	0.98431912	-6.52969256	0.00000000
C	-1.13960101	5.36216679	0.00000000
H	-2.84535670	4.05608726	0.00000000
C	-0.41927421	-6.62649538	0.00000000
H	-2.28080182	-5.53786247	0.00000000
H	1.58510512	-7.43519367	0.00000000
H	-1.72774891	6.27362262	0.00000000
H	2.41584337	-0.44767276	0.00000000
H	-2.58191172	1.65621557	0.00000000
H	-2.30025938	-3.11694179	0.00000000
H	-0.89948908	-7.60060115	0.00000000
C	0.91361210	6.70147120	0.00000000
N	1.43173072	7.74292582	0.00000000

Atomic coordinates of 5,14-dihydro-12α-quinoxalino[2,3-b]phenazine-2-amine **11** at PBE0/6-31+G(d) level of theory

C	0.43189387	1.49604798	0.00001919
C	-0.82686311	0.86842494	0.00254315
C	1.63940989	0.79140401	0.00057717
C	-0.84717407	-0.58893706	0.00671607
N	-1.96127213	1.57510091	0.00258118
C	1.55694794	-0.66746699	0.00268409
N	2.82503088	1.42321005	-0.00242579
C	0.33130795	-1.32905602	0.00683504
N	-2.05604605	-1.18727009	0.00710103
C	-3.15096311	0.91905188	0.00429513
N	2.71929695	-1.34628196	0.00252406
C	3.96580790	0.68468608	-0.00296882
H	0.29622098	-2.41679902	0.00951098
C	-3.24902807	-0.49576612	0.00463905
C	-4.36864613	1.63561185	0.00234716
C	3.96152794	-0.73486092	0.00005610
C	5.22903788	1.31830111	-0.00619578
C	-4.47605905	-1.16092516	0.00007601
H	-4.31936016	2.72126885	0.00056222
C	-5.58571211	0.98814981	0.00139711
C	5.14210096	-1.47931989	-0.00038993
H	5.24865085	2.40498612	-0.00836972
C	6.40189090	0.58132015	-0.00660281
C	-5.66144607	-0.42570919	-0.00131396
H	-4.50439902	-2.24929916	0.00178995
H	-6.50663813	1.56685679	0.00467414
H	5.09509799	-2.56672889	0.00184401
H	7.35956289	1.09575817	-0.00915177
H	0.46528484	2.58136898	-0.00220875
H	-2.09047502	-2.20058009	0.01048397
H	2.68681398	-2.35933196	0.00430701
C	6.36610494	-0.82212185	-0.00370988
N	-6.89619305	-1.05477423	0.06119299
H	-7.67488207	-0.51598723	-0.29554598
H	-6.92062902	-2.00828421	-0.27669306
H	7.28820496	-1.39612883	-0.00404190

Atomic coordinates of 5,14-dihydro-7*α*-quinoxalino[2,3-b]phenazine-2-amine **12** at PBE0/6-31+G(d) level of theory

C	0.32670393	-1.35805707	-0.00366202
C	-0.88176005	-0.64856804	-0.00472903
C	1.58335395	-0.73644411	-0.00073104
C	-0.79814501	0.81036596	-0.00139805
N	-2.06264607	-1.28085200	-0.00650300
C	1.60592299	0.72647089	-0.00111807
N	2.71434592	-1.45117415	0.00022596
C	0.43241101	1.46900092	-0.00051308
N	-1.95896499	1.48426899	-0.00049006
C	-3.20740305	-0.54759697	-0.00536201
N	2.81816401	1.31727385	-0.00019809
C	3.90953494	-0.80015118	0.00096894
H	0.47072804	2.55659592	0.00043590
C	-3.19679901	0.87182503	-0.00251104
C	-4.45971107	-1.19322893	-0.00381699
C	4.00907299	0.61519482	0.00112691
C	5.11808492	-1.53072722	0.00229694
C	-4.38698598	1.60199607	0.00244696
H	-4.46861410	-2.28051393	-0.00738197
C	-5.65060405	-0.47297290	-0.00197999
C	5.24457901	1.26682178	0.00228889
H	5.05278189	-2.61569521	0.00233997
C	6.34374794	-0.88622925	0.00352592
C	-5.60258500	0.94166810	0.00097298
H	-4.35711895	2.68973807	0.00728494
C	6.41280798	0.51625274	0.00349189
H	5.28364904	2.35452178	0.00232187
H	7.25983992	-1.47117628	0.00451393
H	-6.52787499	1.51222513	-0.00190102
H	0.28845890	-2.44310507	-0.00500400
H	-1.92927896	2.49785699	0.00135192
H	2.86074704	2.33010085	-0.00054211
H	7.37618300	1.01801772	0.00440188
N	-6.87993207	-1.11856086	-0.06856697
H	-6.88014509	-2.07740085	0.25544305
H	-7.65948205	-0.60157983	0.31767203

Atomic coordinates of **13** at PBE0/6-31+G(d) level of theory

C	0.00000802	1.65755605	0.00000000
C	0.00001499	0.98810907	-1.22805299
C	0.00001499	0.98810907	1.22805299
C	0.00002997	-0.47412393	-1.19972002
N	0.00001098	1.66396809	-2.38479198
C	0.00002997	-0.47412393	1.19972002
N	0.00001098	1.66396809	2.38479198
C	0.00003998	-1.17738595	0.00000000
N	0.00002994	-1.10607291	-2.38702203
C	0.00000596	0.97633211	-3.54788999
N	0.00002994	-1.10607291	2.38702203
C	0.00000596	0.97633211	3.54788999
H	0.00004896	-2.26518195	0.00000000
C	0.00001194	-0.44557489	-3.59882102
C	-0.00000805	1.67032313	-4.78169198
C	0.00001194	-0.44557489	3.59882102
C	-0.00000805	1.67032313	4.78169198
C	-0.00000309	-1.13895387	-4.80356503
H	-0.00001004	2.75582813	-4.75217996
C	-0.00001908	0.99539615	-5.98189799
C	-0.00000309	-1.13895387	4.80356503
H	-0.00001004	2.75582813	4.75217996
C	-0.00001908	0.99539615	5.98189799
C	-0.00001910	-0.41823885	-6.00061702
H	-0.00000611	-2.22579987	-4.81519705
H	-0.00002908	1.54268017	-6.91933498
H	-0.00000611	-2.22579987	4.81519705
H	-0.00002908	1.54268017	6.91933498
H	-0.00000397	2.74279605	0.00000000
H	0.00005193	-2.12013191	-2.39443505
H	0.00005193	-2.12013191	2.39443505
C	-0.00003092	-1.11514208	7.24376897
N	-0.00004291	-1.68084410	8.26122196
C	-0.00001910	-0.41823885	6.00061702
C	-0.00003092	-1.11514208	-7.24376897
N	-0.00004291	-1.68084410	-8.26122196

Atomic coordinates of **14** at PBE0/6-31+G(d) level of theory

C	0.00000000	0.00000000	-1.18716389
C	0.00000000	1.22985500	-0.51870789
C	0.00000000	-1.22985500	-0.51870789
C	0.00000000	1.19942800	0.94328011
N	0.00000000	2.38802300	-1.18921389
C	0.00000000	-1.19942800	0.94328011
N	0.00000000	-2.38802300	-1.18921389
C	0.00000000	0.00000000	1.64672511
N	0.00000000	2.38592700	1.58043811
C	0.00000000	3.55114900	-0.49172489
N	0.00000000	-2.38592700	1.58043811
C	0.00000000	-3.55114900	-0.49172489
H	0.00000000	0.00000000	2.73468811
C	0.00000000	3.59819500	0.92782111
C	0.00000000	4.78185700	-1.17733089
C	0.00000000	-3.59819500	0.92782111
C	0.00000000	-4.78185700	-1.17733089
C	0.00000000	4.80643200	1.63113911
H	0.00000000	4.76749900	-2.26263889
C	0.00000000	5.98270600	-0.47420489
C	0.00000000	-4.80643200	1.63113911
H	0.00000000	-4.76749900	-2.26263889
C	0.00000000	-5.98270600	-0.47420489
C	0.00000000	6.00213400	0.93745811
H	0.00000000	4.80294900	2.71860611
C	0.00000000	-6.00213400	0.93745811
H	0.00000000	-4.80294900	2.71860611
H	0.00000000	6.94719100	1.46984411
H	0.00000000	0.00000000	-2.27247489
H	0.00000000	2.38916700	2.59466611
H	0.00000000	-2.38916700	2.59466611
H	0.00000000	-6.94719100	1.46984411
C	0.00000000	7.21967600	-1.19187289
N	0.00000000	8.22918700	-1.76913989
C	0.00000000	-7.21967600	-1.19187289
N	0.00000000	-8.22918700	-1.76913989

Atomic coordinates of **15** at PBE0/6-31+G(d) level of theory

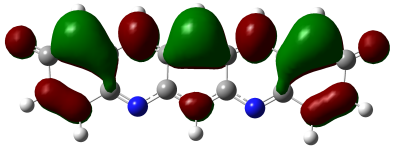
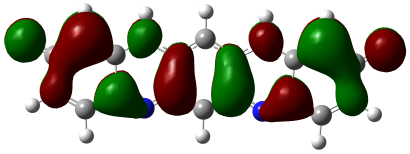
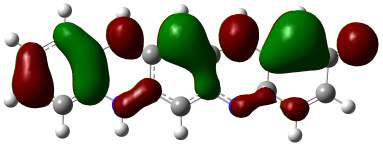
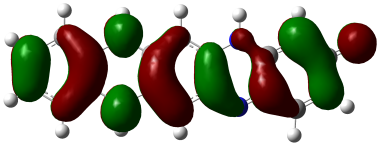
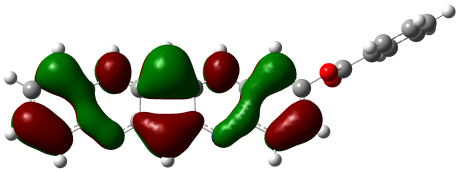
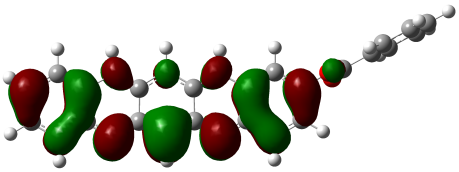
C	0.00580584	1.58636602	0.00000000
C	0.00252389	0.91982304	-1.23498497
C	0.00252389	0.91982304	1.23498497
C	-0.00221301	-0.53771196	-1.20308200
N	0.00332285	1.58674707	-2.39760496
C	-0.00221301	-0.53771196	1.20308200
N	0.00332285	1.58674707	2.39760496
C	-0.00463796	-1.23866098	0.00000000
N	-0.00343297	-1.18055593	-2.38880301
C	-0.00040810	0.88480909	-3.56239897
N	-0.00343297	-1.18055593	2.38880301
C	-0.00040810	0.88480909	3.56239897
H	-0.00839989	-2.32720398	0.00000000
C	-0.00278101	-0.53210491	-3.60843200
C	0.00036185	1.55054612	-4.80790196
C	-0.00278101	-0.53210491	3.60843200
C	0.00036185	1.55054612	4.80790196
C	-0.00190196	-1.24420588	-4.80837101
H	0.00386378	2.63741012	-4.80290093
C	-0.00262610	0.85559514	-6.00114697
C	-0.00190196	-1.24420588	4.80837101
H	0.00386378	2.63741012	4.80290093
C	-0.00262610	0.85559514	6.00114697
C	-0.00256500	-0.55765086	-6.02291700
H	-0.00536188	-2.33302188	-4.79251804
H	-0.00752314	1.40012116	-6.94293196
H	-0.00536188	-2.33302188	4.79251804
H	-0.00752314	1.40012116	6.94293196
H	0.00893577	2.67242002	0.00000000
H	-0.00802390	-2.19406993	-2.38633803
H	-0.00802390	-2.19406993	2.38633803
C	-0.00256500	-0.55765086	6.02291700
N	-0.07231296	-1.23990684	-7.23375201
H	0.30054501	-0.73512580	-8.02801600
H	0.27738211	-2.18962382	-7.21298603
N	-0.07231296	-1.23990684	7.23375201
H	0.27738211	-2.18962382	7.21298603
H	0.30054501	-0.73512580	8.02801600

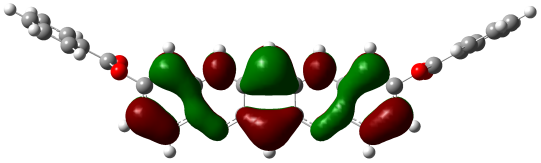
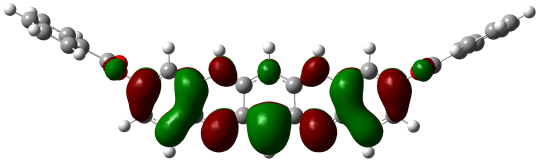
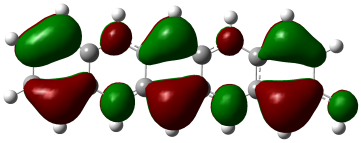
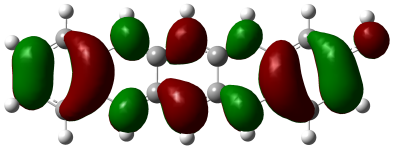
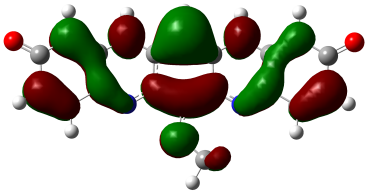
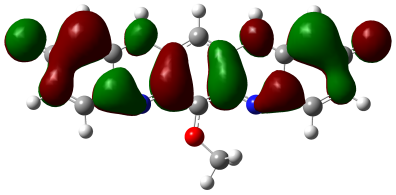
Atomic coordinates of **16** at PBE0/6-31+G(d) level of theory

C	-0.00724398	-1.26801593	0.00000000
C	-0.00508701	-0.60228890	-1.23388496
C	-0.00508701	-0.60228890	1.23388496
C	-0.00141208	0.85972810	-1.20330992
N	-0.00642896	-1.27812187	-2.38965198
C	-0.00141208	0.85972810	1.20330992
N	-0.00642896	-1.27812187	2.38965198
C	0.00074787	1.56044607	0.00000000
N	0.00026990	1.49070513	-2.39103191
C	-0.00483698	-0.58769084	-3.56231496
N	0.00026990	1.49070513	2.39103191
C	-0.00483698	-0.58769084	3.56231496
H	0.00338082	2.64884807	0.00000000
C	-0.00145406	0.83065816	-3.60543092
C	-0.00290994	-1.28062381	-4.78881098
C	-0.00145406	0.83065816	3.60543092
C	-0.00290994	-1.28062381	4.78881098
C	0.00400892	1.51359519	-4.82256591
H	-0.00669988	-2.36774181	-4.75638401
C	-0.00043296	-0.60697478	-6.00722096
C	0.00400892	1.51359519	4.82256591
H	-0.00669988	-2.36774181	4.75638401
C	-0.00043296	-0.60697478	6.00722096
C	0.00267097	0.80704222	-6.01346892
H	0.00909487	2.60190419	-4.83502088
C	0.00267097	0.80704222	6.01346892
H	0.00909487	2.60190419	4.83502088
H	-0.00020605	1.34261324	-6.95947191
H	-0.01063493	-2.35390693	0.00000000
H	0.00202985	2.50433713	-2.39897788
H	0.00202985	2.50433713	2.39897788
H	-0.00020605	1.34261324	6.95947191
N	-0.06717091	-1.30251975	-7.21112798
H	0.32716907	-0.81806371	-8.00757296
H	0.26174813	-2.25892874	-7.16938700
N	-0.06717091	-1.30251975	7.21112798
H	0.26174813	-2.25892874	7.16938700
H	0.32716907	-0.81806371	8.00757296

S.2 Molecular Orbitals

We show below the frontier molecular orbitals for all dyes represented with a contour threshold of 0.02 au. We also give the energies of all orbitals in eV. All calculations have been made at the PBE0/6-31+G(d) level of theory.

Molecule	**HOMO-1**	**HOMO**
1		
	E = -6.76	E= -6.11
2		
	E= -6.30	E= -5.08
3		
	E= -6.40	E= -4.88

4		
	E= -6.46	E= -4.89
5		
	E= -7.92	E= -6.93
6		
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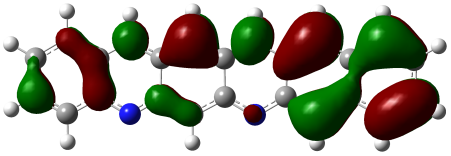
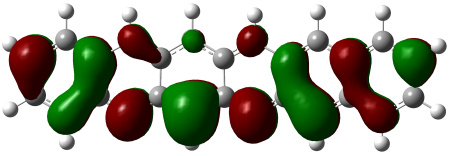
7		
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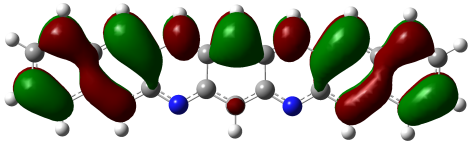
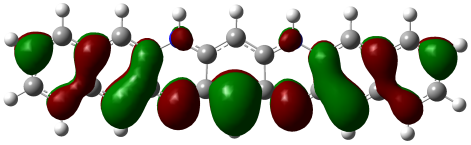
8		
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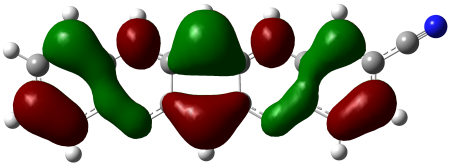
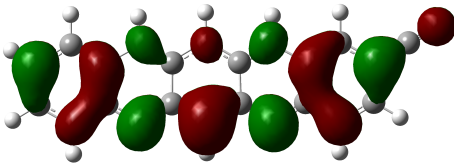
9		
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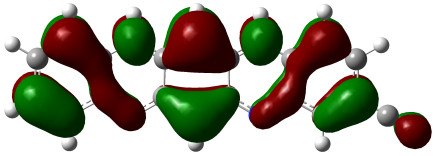
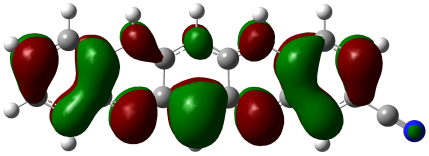
10		
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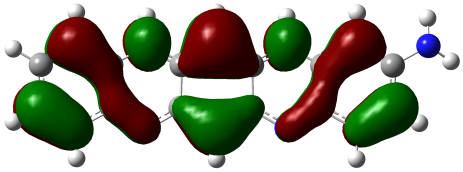
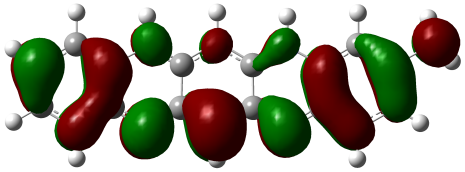
11		
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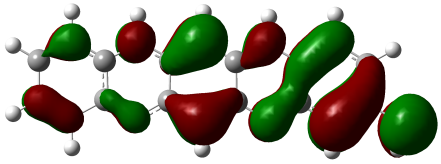
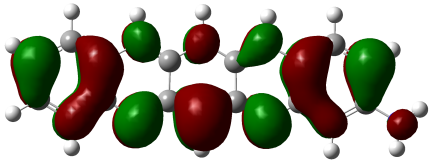
12		
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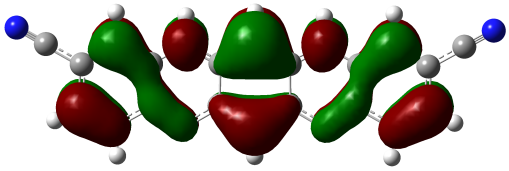
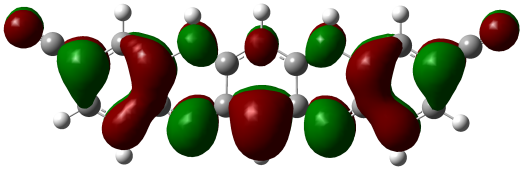
13		
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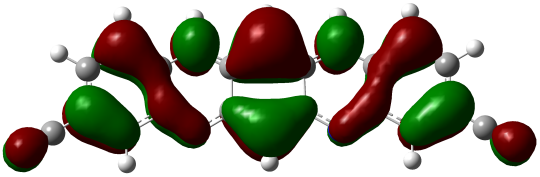
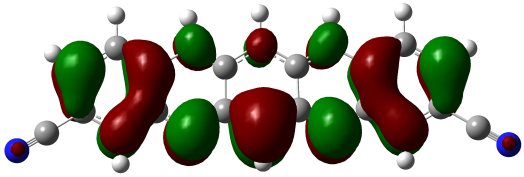
14		
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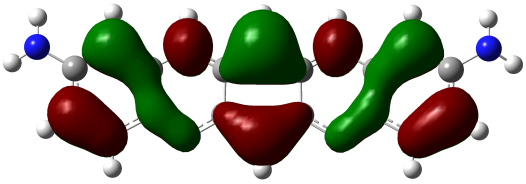
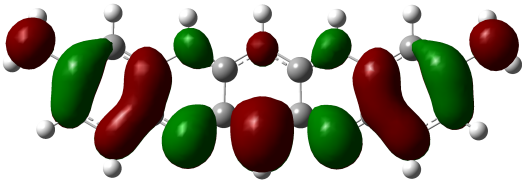
15		
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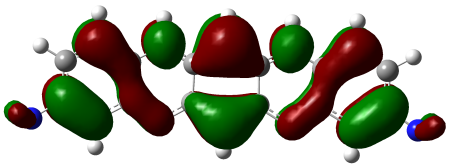
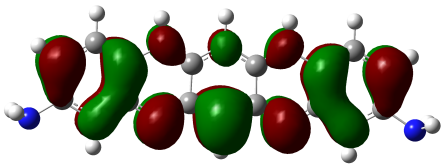
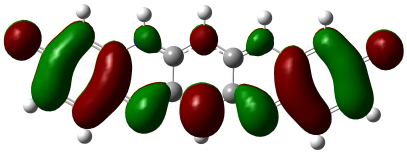
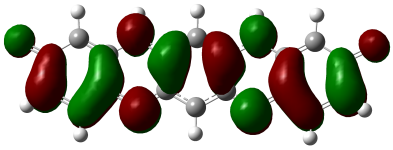
		
16		
	E= -5.68	E= -4.67

Molecule	**LUMO**	**LUMO + 1**
1		
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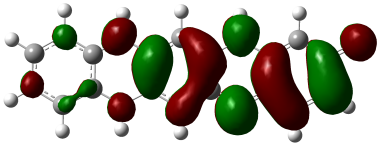
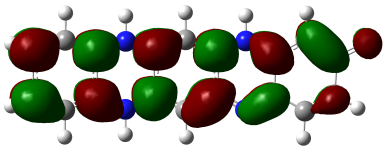
2		
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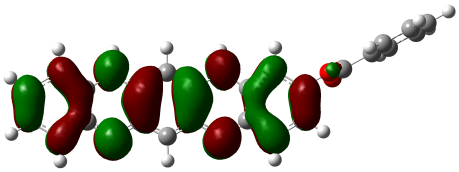
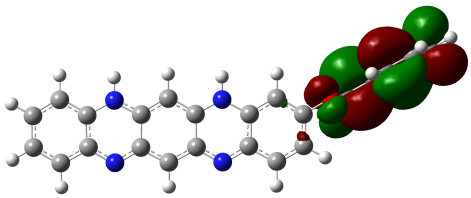
3		
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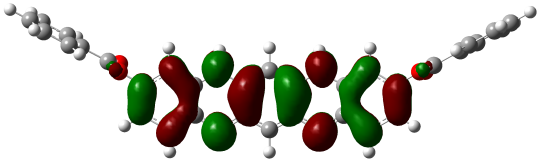
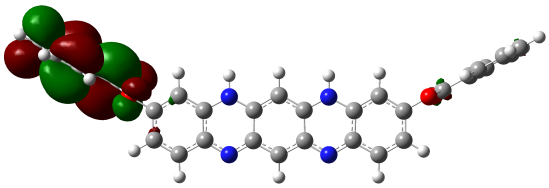
4		
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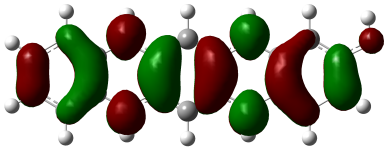
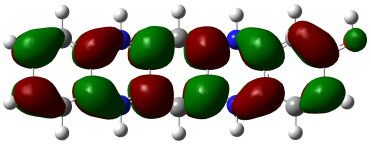
5		
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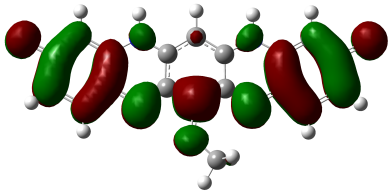
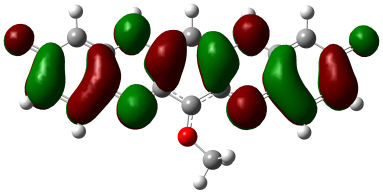
6		
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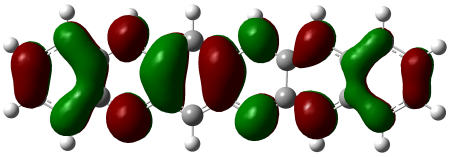
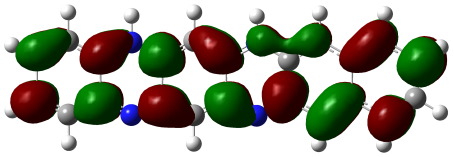
7		
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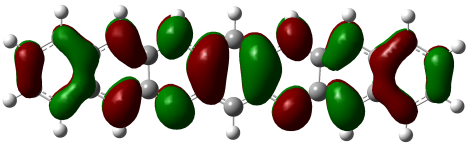
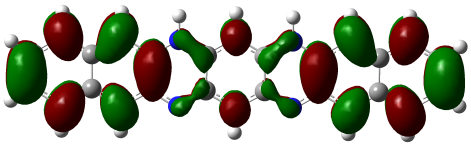
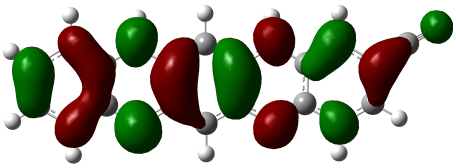
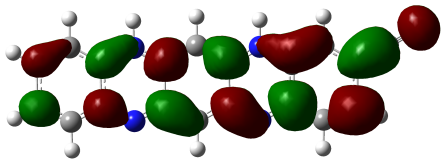
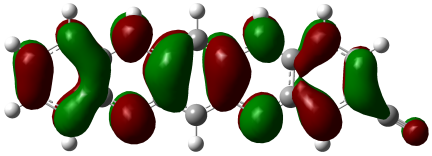
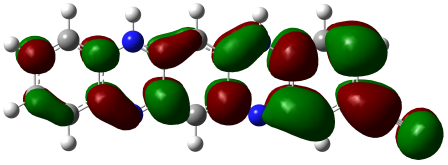
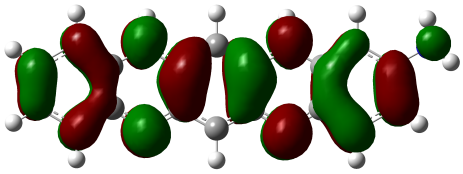
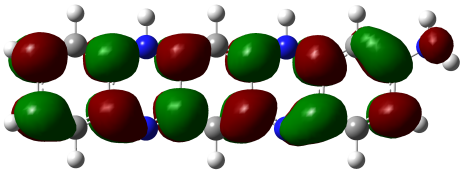
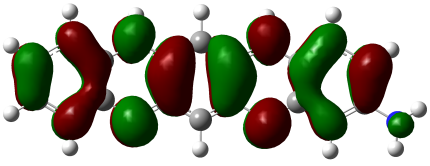
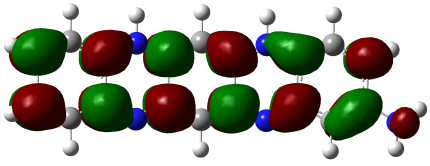
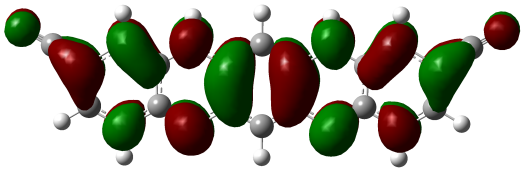
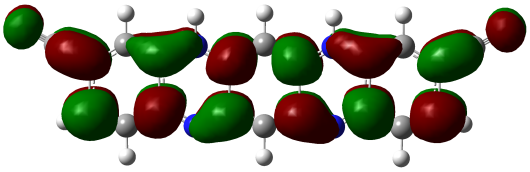
8		
	E= -2.98	E= -1.17

9		
	E= -2.89	E=
10		
	E= -2.98	E= -1.47
11		
	E= -2.50	E= -0.81
12		
	E= -2.53	E= -0.84

13		
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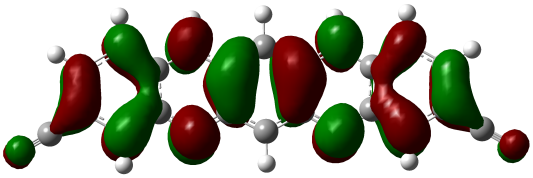
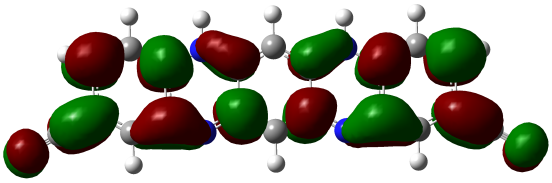
14		
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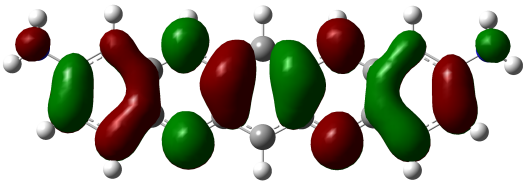
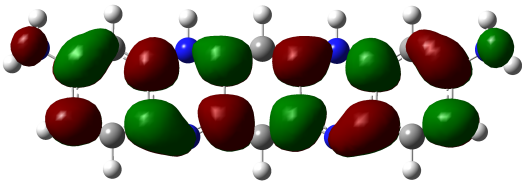
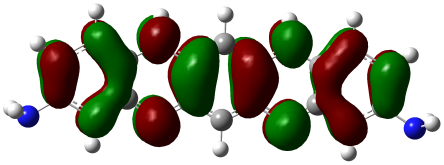
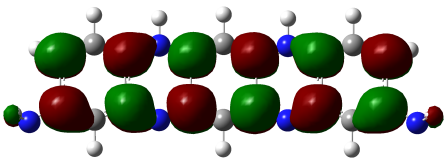
15		
	E= -2.39	E= -0.66
16		
	E= -2.44	E= -0.71

S.3 List of vertical transitions

List of the transition energies to the ten lowest singlet excited states computed by TD-DFT using the PBE0 functional and the *aug*-cc-pVTZ basis set for compounds **1**–**6**. We report the computed vertical absorption wavelength (in nm), oscillator strength and dominant molecular orbital composition (H = HOMO, L = LUMO).

Molecule	State	Vertical transition wavelength (nm)	f	MO Composition
1	1	544	1.27	H → L (97 %)
	2	483	0.00	H - 1 → L (97 %)
	3	437	0.00	H - 2 → L (85 %)
	4	436	0.00	H - 3 → L (85 %)
	5	434	0.00	H → L + 1 (96 %)
	6	360	0.69	H - 1 → L + 1 (87 %)
	7	349	0.03	H - 4 → L (90 %)
	8	333	0.00	H - 6 → L (85 %)
	9	332	0.00	H - 5 → L (85 %)
	10	331	0.00	H - 7 → L (85 %)
2	1	608	0.75	H → L (98 %)
	2	422	0.09	H - 1 → L (90 %)
	3	403	0.00	H - 3 → L (96 %)
	4	382	0.01	H → L + 1 (52 %); H - 2 → L (41 %)
	5	363	0.58	H - 2 → L + 1 (54 %); H → L + 1 (39 %)
	6	327	0.09	H → L + 2 (74 %)
	7	320	0.03	H → L + 3 (74 %)
	8	314	0.00	H - 6 → L (98 %)
	9	301	0.00	H - 4 → L (74 %)
	10	297	0.00	H → L + 4 (97 %)

Molecule	State	Vertical transition wavelength (nm)	f	MO Composition
3	1	680	0.62	H → L (97 %)
	2	455	0.01	H → L + 1 (97 %)
	3	438	0.00	H - 1 → L (46 %); H → L + 2 (48 %)
	4	390	1.19	H - 1 → L (47 %); H → L + 2 (44 %)
	5	335	0.01	H → L + 4 (74 %)
	6	329	0.00	H - 4 → L (97 %)
	7	326	0.00	H - 5 → L (97 %)
	8	323	0.02	H - 2 → L (70 %)
	9	320	0.00	H → L + 3 (74 %)
	10	319	0.01	H → L + 5 (55 %)
4	1	690	0.66	H → L (96 %)
	2	453	0.01	H → L + 1 (92 %)
	3	452	0.00	H → L + 2 (96 %)
	4	437	0.01	H - 1 → L (43 %); H → L + 3 (51 %)
	5	389	1.35	H - 1 → L (51 %); H → L + 2 (41 %)
	6	338	0.00	H → L + 5 (80 %)
	7	328	0.00	H - 4 → L (95 %)
	8	327	0.00	H - 5 → L (95 %)
	9	324	0.03	H → L + 6 (95 %)
	10	322	0.02	H - 2 → L (77 %)
5	1	621	1.05	H → L (98 %)
	2	515	0.10	H - 1 → L (96 %)
	3	416	0.01	H - 2 → L (94 %)
	4	367	0.02	H → L +1 (97 %)
	5	355	0.00	H - 3 → L (82 %)

Molecule	State	Vertical transition wavelength (nm)	f	MO Composition
	6	331	0.00	H - 4 → L (86 %)
	7	295	0.00	H → L + 2 (96 %)
	8	278	0.33	H → L + 3 (35 %); H - 1 → L + 1 (31 %)
	9	272	0.29	H - 5 → L (69 %); H → L + 1 (22 %)
	10	272	0.35	H → L + 4 (30 %); H → L + 3 (37 %)
6	1	526	1.05	H → L (93 %)
	2	493	0.03	H - 1 → L (93 %)
	3	431	0.02	H → L + 1 (96 %)
	4	425	0.00	H - 3 → L (80 %)
	5	424	0.00	H - 4 → L (81 %)
	6	396	0.06	H - 2 → L (87 %)
	7	390	0.84	H → L + 1 (84 %)
	8	350	0.12	H - 2 → L + 1 (78 %)
	9	340	0.00	H - 6 → L (85 %)
	10	330	0.00	H - 7 → L (76 %)

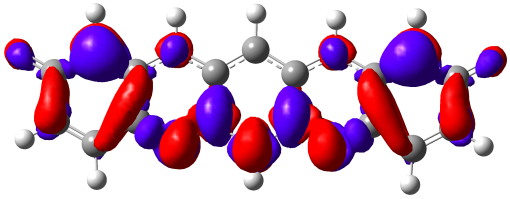
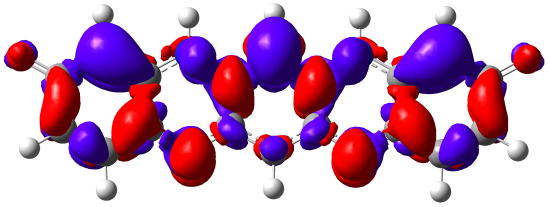
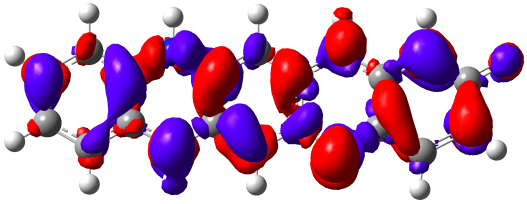
List of the transition energies to the three or four lowest singlet excited states computed by TD-DFT using the PBE0 functional and the *aug*-cc-pVTZ basis set for compounds **7**–**16**. We report the computed vertical absorption wavelength (in nm), oscillator strength and dominant molecular orbital composition (H = HOMO, L = LUMO).

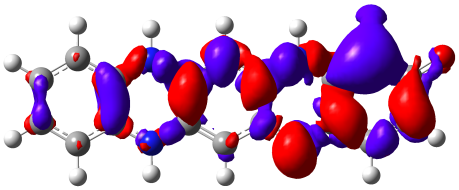
Molecule	State	Vertical transition wavelength (nm)	f	MO Composition
7	1	723	0.64	H → L (96 %)
	2	479	0.24	H - 1 → L (86 %)
	3	404	0.46	H → L + 1 (51 %); H - 2 → L (30 %)
8	1	795	0.66	H → L (97 %)
	2	505	0.53	H - 1 → L (91 %)
	3	467	0.03	H - 2 → L (98 %)
	4	394	1.42	H → L + 2 (87 %)
9	1	659	0.76	H → L (95 %)
	2	453	0.07	H → L + 1 (62 %); H - 1 → L (33 %)
	3	410	0.92	H - 1 → L (62 %); H → L + 1 (31 %)
10	1	689	0.56	H → L (95 %)
	2	459	0.04	H - 1 → L (31 %); H → L + 1 (64 %)
	3	401	0.94	H - 1 → L (64 %); H → L + 1 (29 %)
11	1	724	0.59	H → L (96 %)
	2	440	0.04	H → L + 1 (61 %); H - 1 → L (36 %)
	3	390	1.16	H - 1 → L (57 %); H → L + 1 (32 %)
12	1	653	0.72	H → L (95 %)
	2	470	0.12	H - 1 → L (88 %)
	3	407	0.57	H → L + 1 (85 %)
13	1	658	0.95	H → L (95 %)

Molecule	State	Vertical transition wavelength (nm)	f	MO Composition
	2	446	0.09	H → L + 1 (69 %); H - 1 → L (28 %)
	3	421	0.83	H - 1 → L (67 %); H → L + 1 (26 %)
14	1	709	0.54	H → L (95 %)
	2	467	0.04	H → L + 1 (66 %); H - 1 → L (31 %)
	3	401	1.27	H - 1 → L (65 %); H → L + 1 (28 %)
15	1	784	0.57	H → L (92 %)
	2	4442	0.12	H → L + 1 (71 %); H - 1 → L (27 %)
	3	387	0.00	H - 2 → L (88 %)
	4	387	1.30	H - 1 → L (68 %); H → L + 1 (24 %)
16	1	641	0.87	H → L (95 %)
	2	489	0.15	H - 1 → L (93 %)
	3	405	0.43	H → L + 1 (93 %)

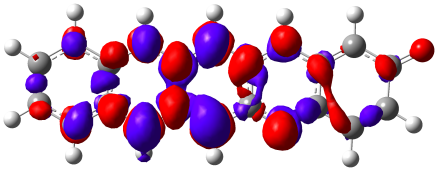
S.4 Electronic Density Difference plots

We show below the density difference plots for the most important electronic excited states. All calculations are performed at the PCM-PBE0/6-31+G(d) level. We use a contour threshold of 8×10^{-4} au. Blue and red colors indicate density depletion and accumulation, respectively.

Molecule and transition	**EDD**
1	
$S_0 \rightarrow S_1$	
$S_0 \rightarrow S_6$	
2	
$S_0 \rightarrow S_1$	

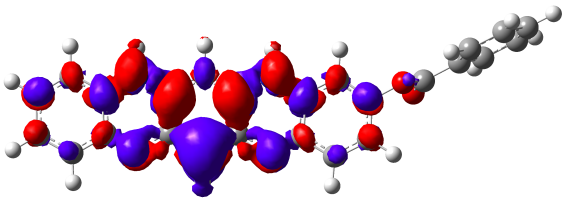


$S_0 \rightarrow S_2$

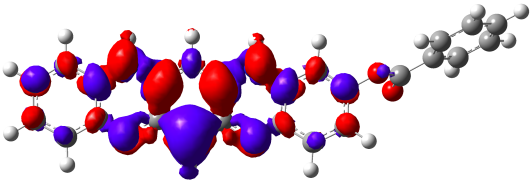


$S_0 \rightarrow S_5$

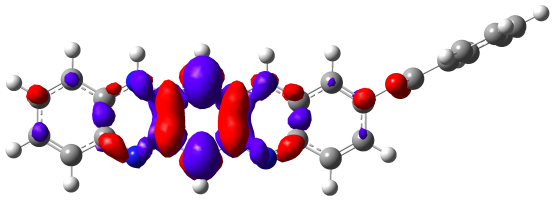
3



$S_0 \rightarrow S_1$

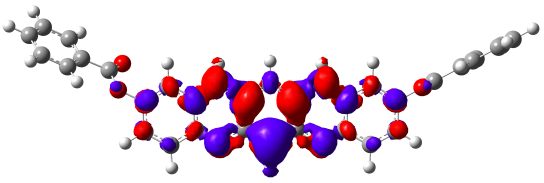


$S_0 \rightarrow S_2$

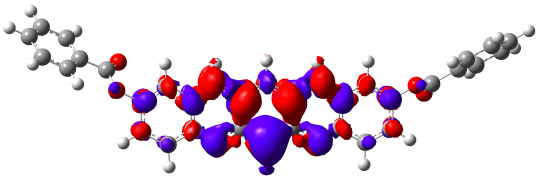


$S_0 \rightarrow S_4$

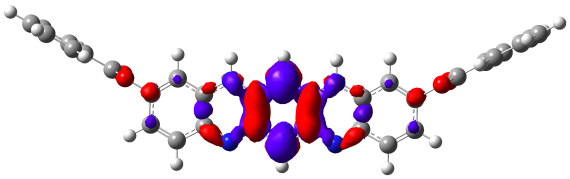
4



$S_0 \rightarrow S_1$

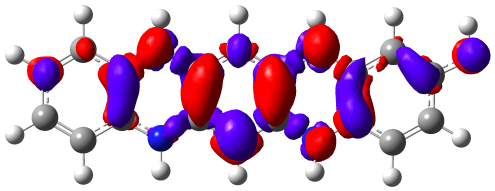


$S_0 \rightarrow S_2$

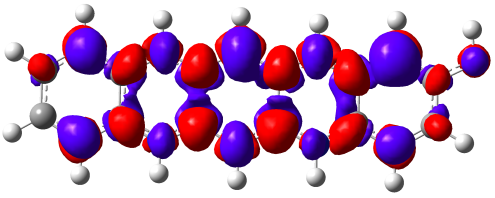


$S_0 \rightarrow S_5$

5

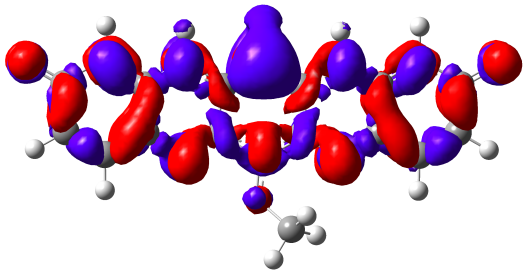


$S_0 \rightarrow S_1$

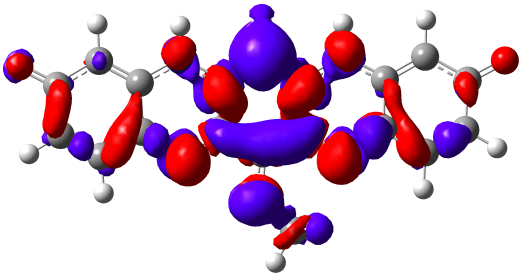


$S_0 \rightarrow S_8$

6

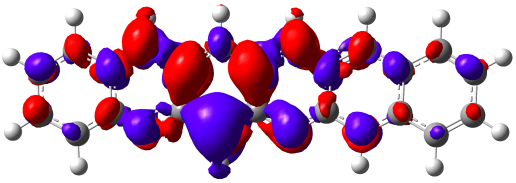


$S_0 \rightarrow S_1$

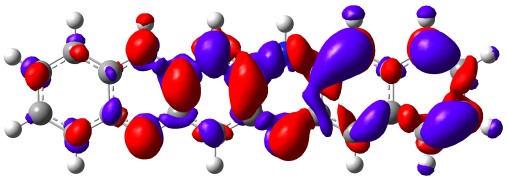


$S_0 \rightarrow S_7$

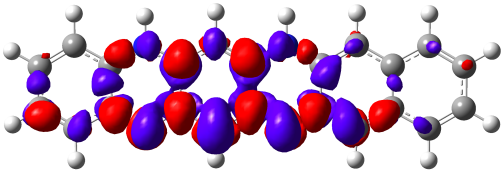
7



$S_0 \rightarrow S_1$

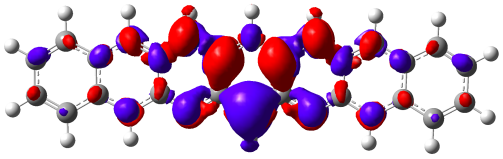


$S_0 \rightarrow S_2$

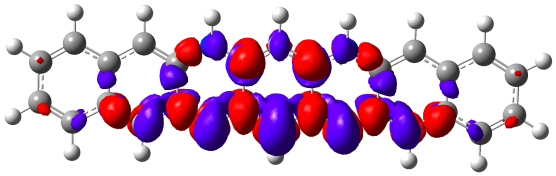


$S_0 \rightarrow S_3$

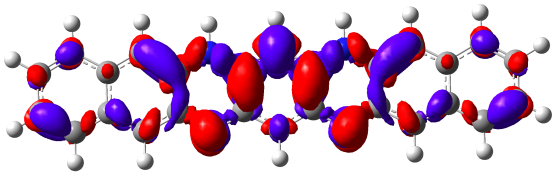
8



$S_0 \rightarrow S_1$

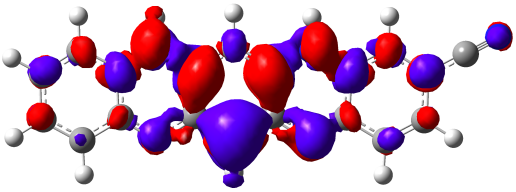


$S_0 \rightarrow S_2$

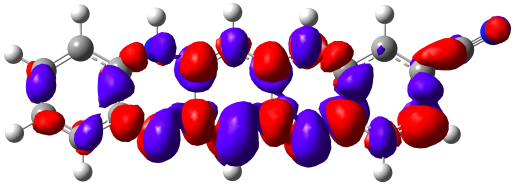


$S_0 \rightarrow S_4$

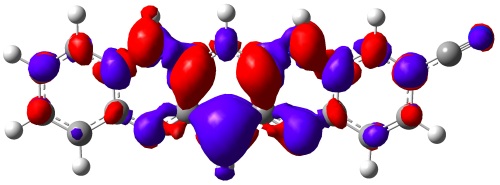
9



$S_0 \rightarrow S_1$

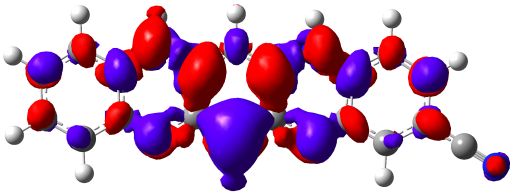


$S_0 \rightarrow S_2$

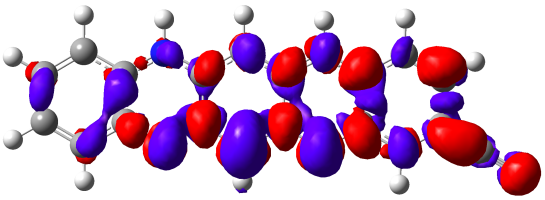


$S_0 \rightarrow S_3$

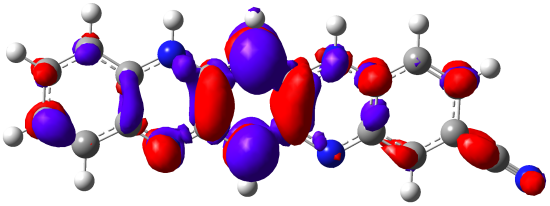
10



$S_0 \rightarrow S_1$

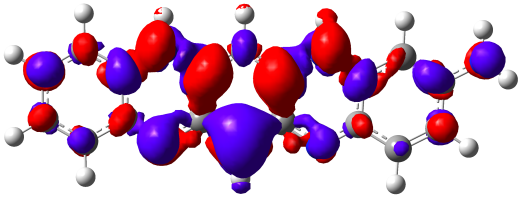


$S_0 \rightarrow S_2$

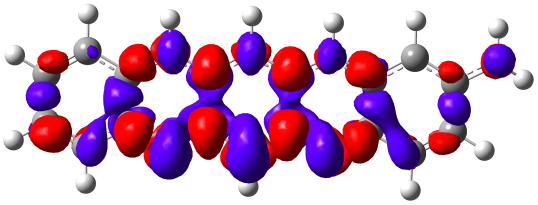


$S_0 \rightarrow S_3$

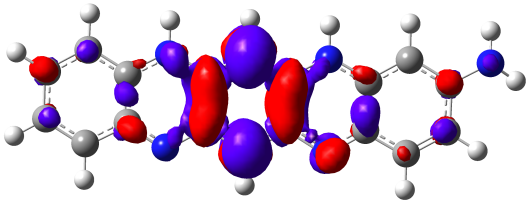
11



$S_0 \rightarrow S_1$

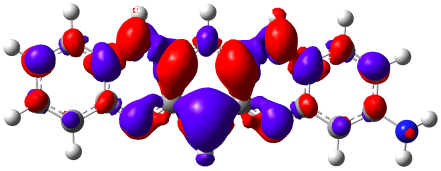


$S_0 \rightarrow S_2$

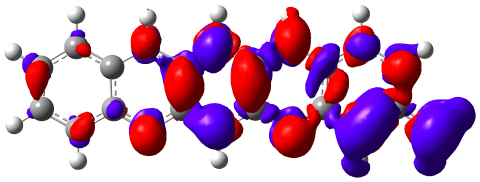


$S_0 \rightarrow S_3$

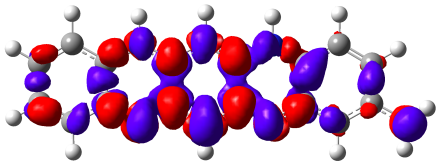
12



$S_0 \rightarrow S_1$

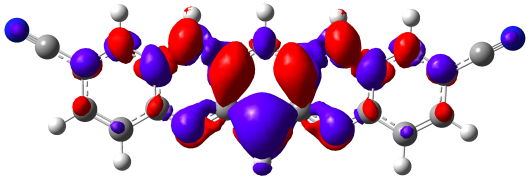


$S_0 \rightarrow S_2$

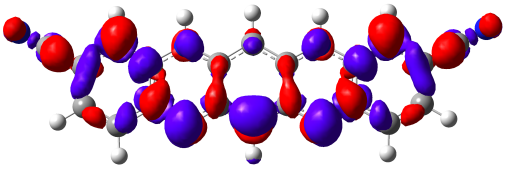


$S_0 \rightarrow S_3$

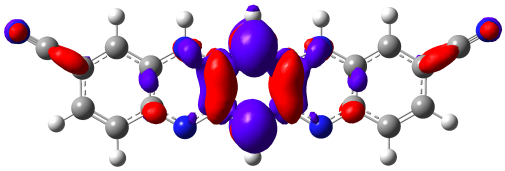
13



$S_0 \rightarrow S_1$

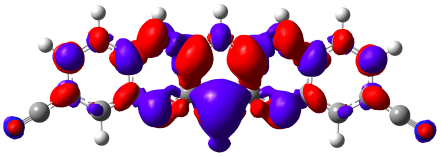


$S_0 \rightarrow S_2$

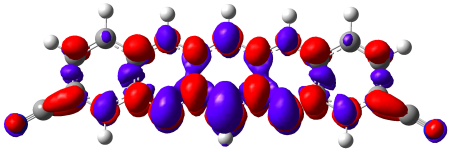


$S_0 \rightarrow S_3$

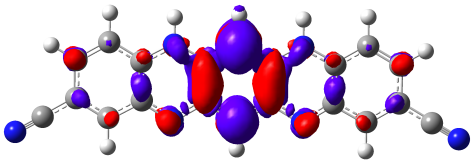
14



$S_0 \rightarrow S_1$

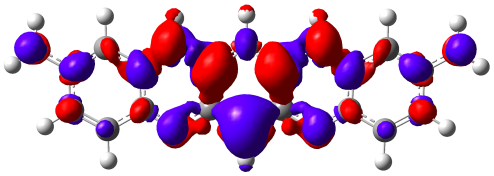


$S_0 \rightarrow S_2$

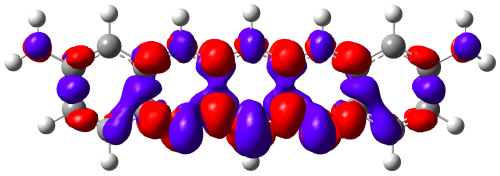


$S_0 \rightarrow S_3$

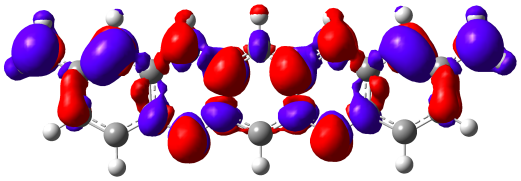
15



$S_0 \rightarrow S_1$

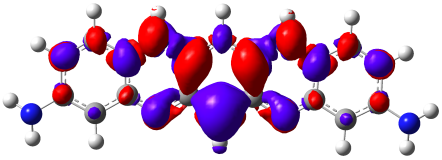


$S_0 \rightarrow S_2$

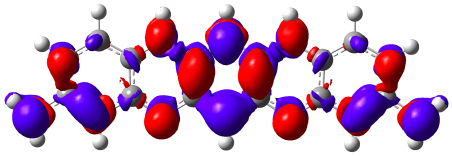


$S_0 \rightarrow S_4$

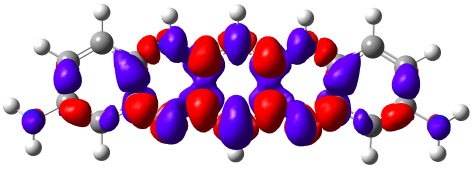
16



$S_0 \rightarrow S_1$



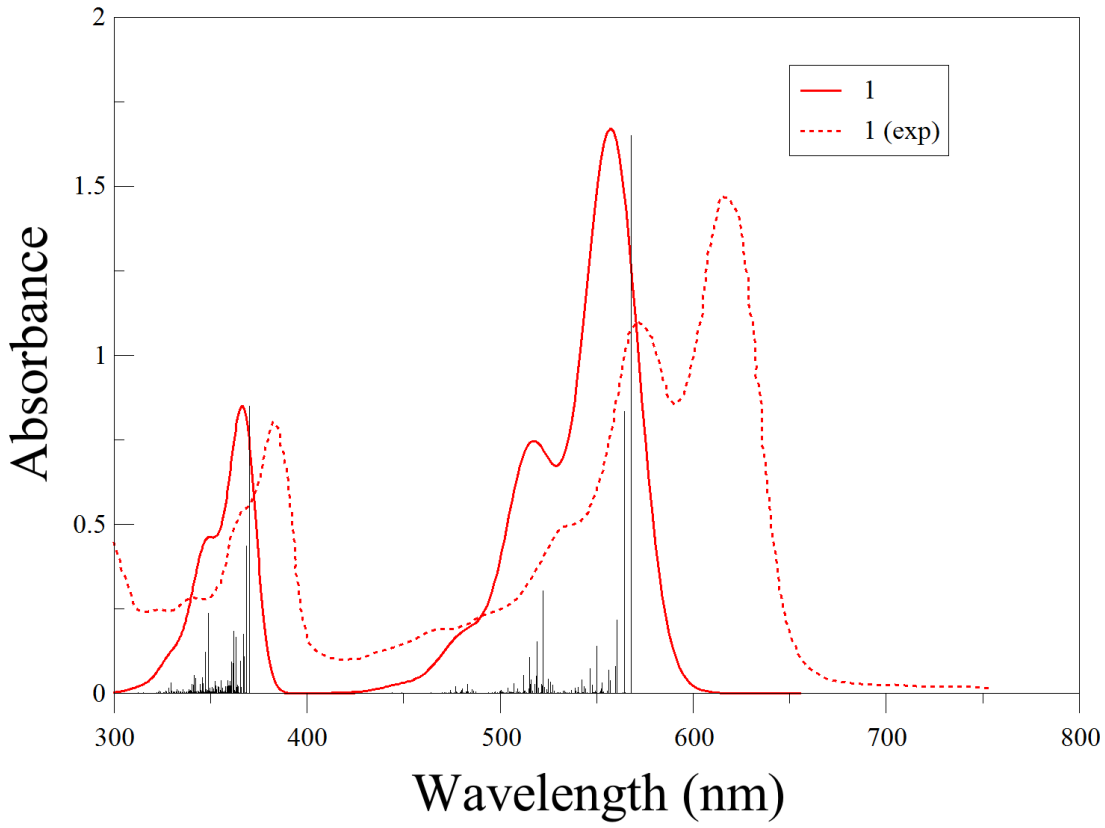
$S_0 \rightarrow S_2$

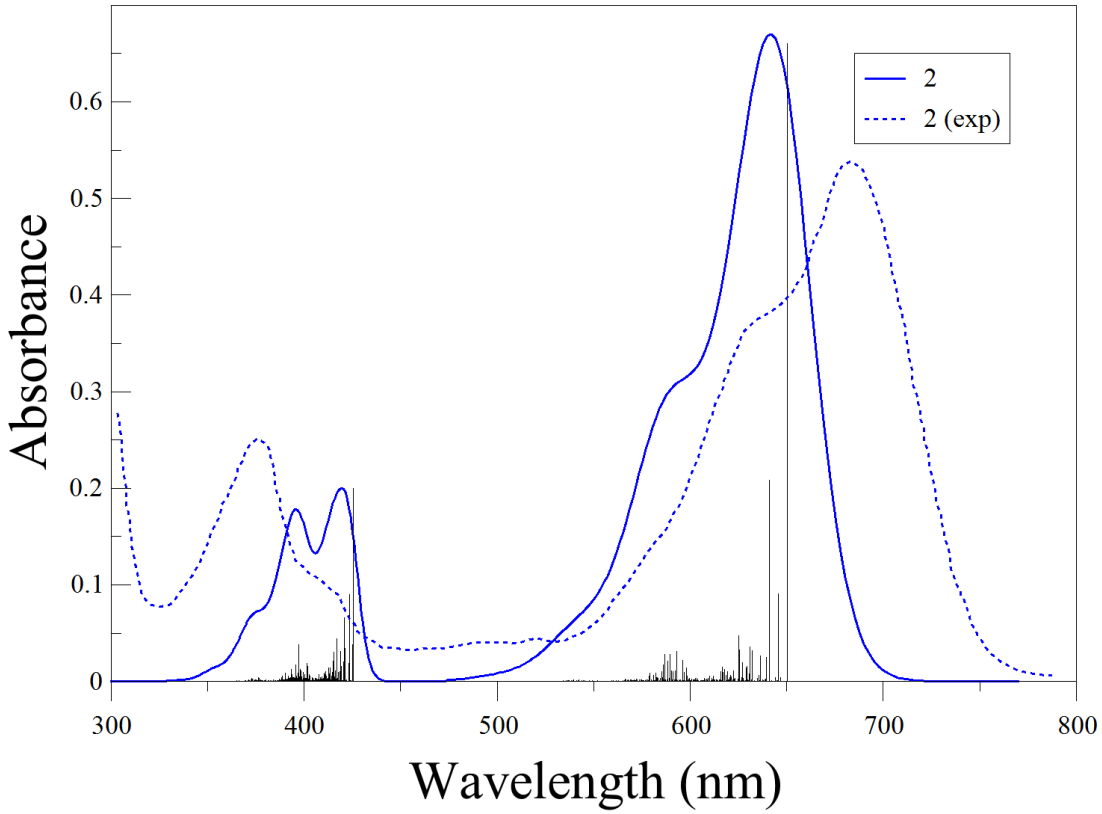


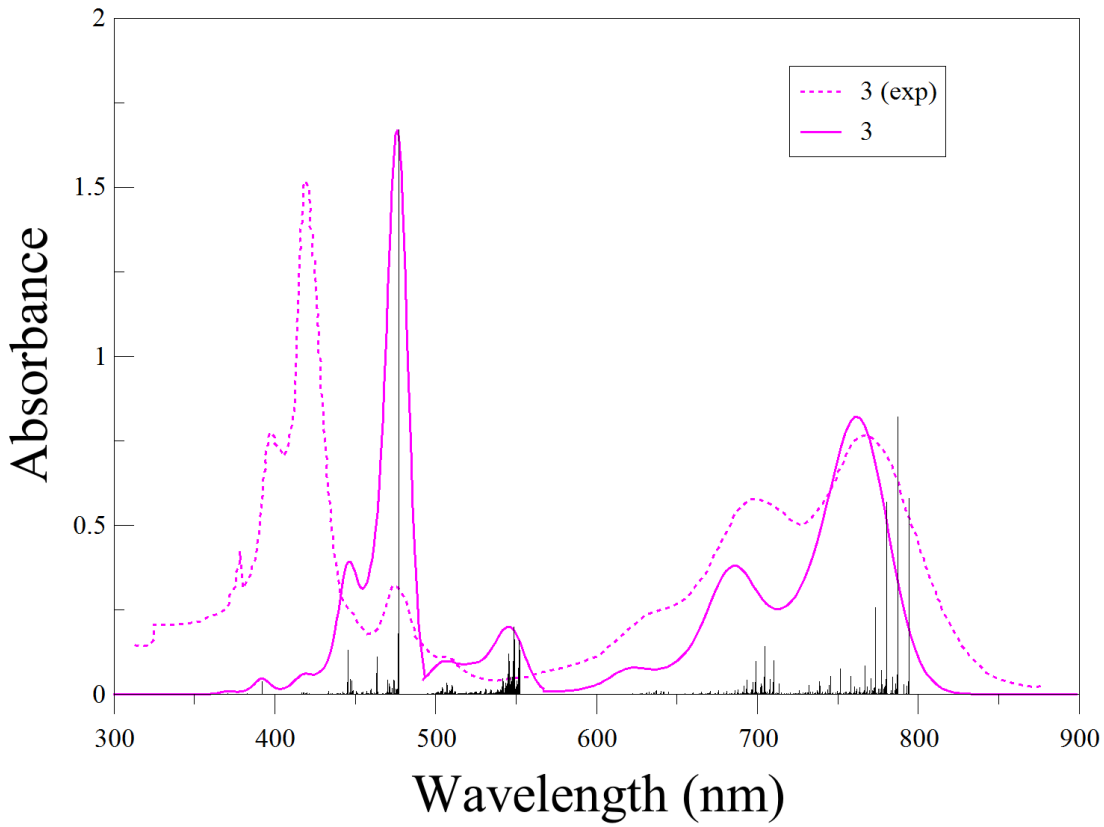
$S_0 \rightarrow S_3$

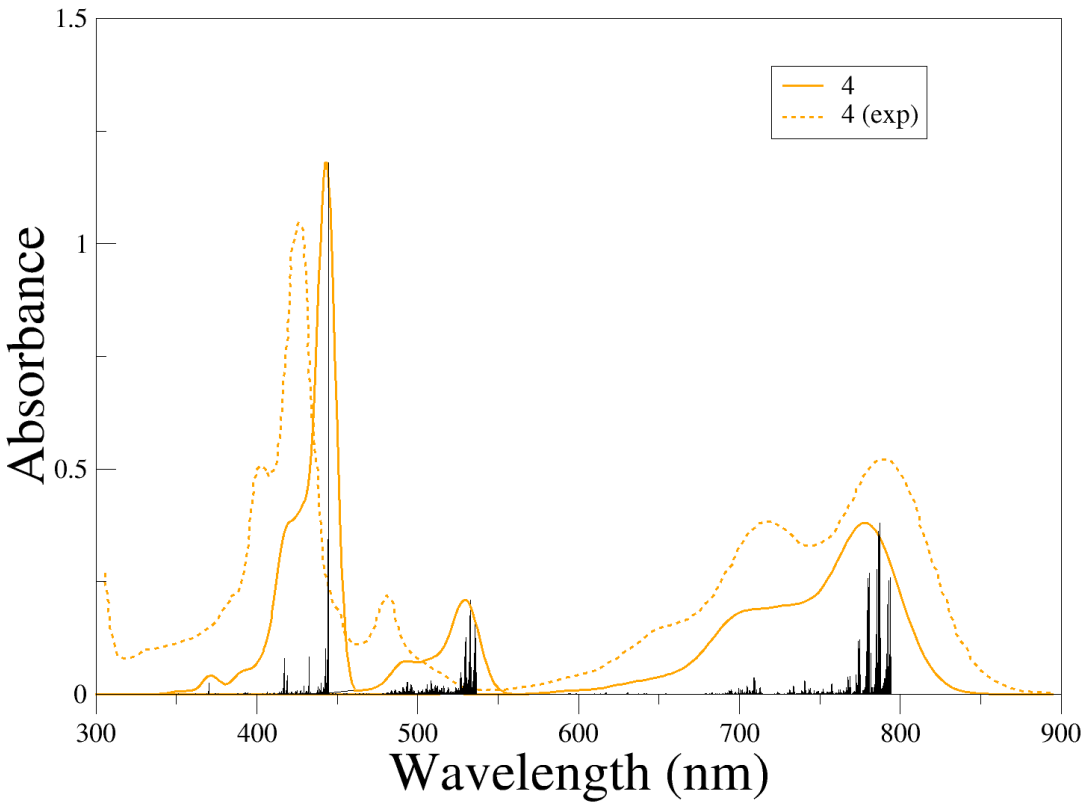
S.5 Vibrationally resolved spectra

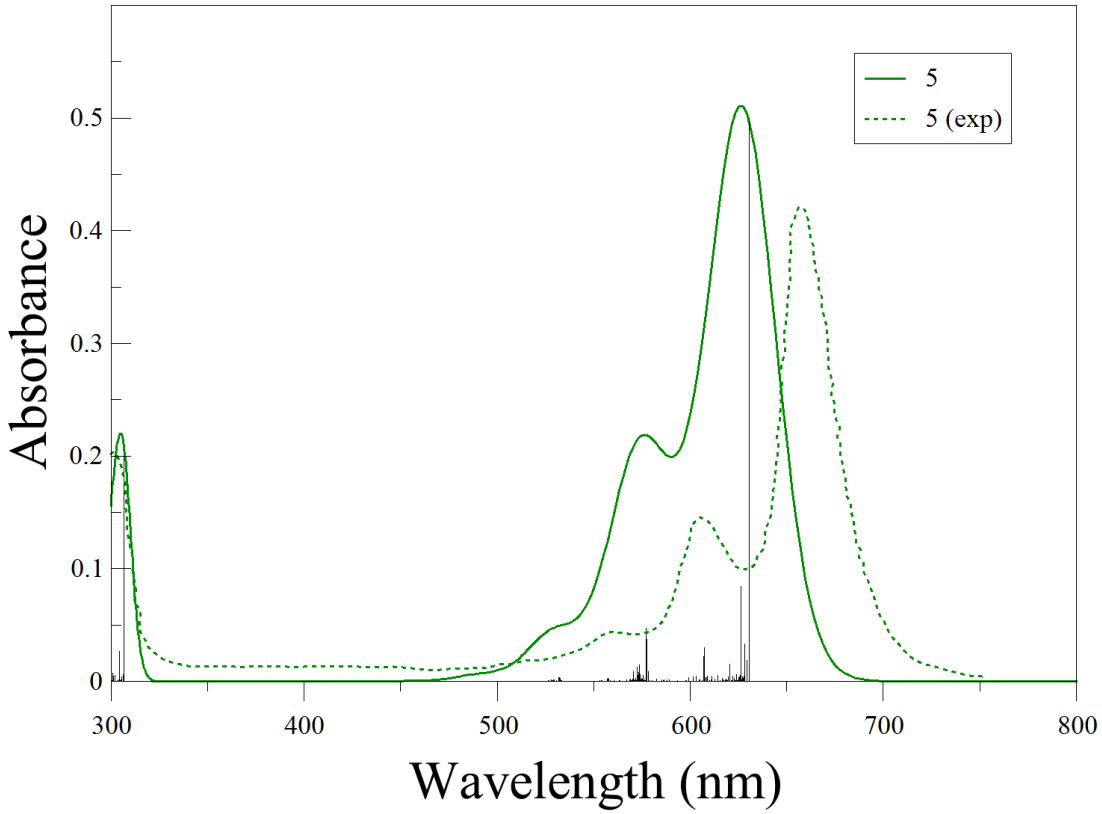
Below we show all the vibronic spectra we obtained (considering the electronic states with large f) in the simulations and compare them to experiment[1] for compounds **1–6**. Theoretical lines are shown in full line together with the original stick spectrum giving the individual vibronic contributions. The experimental graph is displayed in dashed lines. **1–6** that have experimental counterparts are presented in absorbance, whereas, for the other compounds we normalized the intensity to 1.

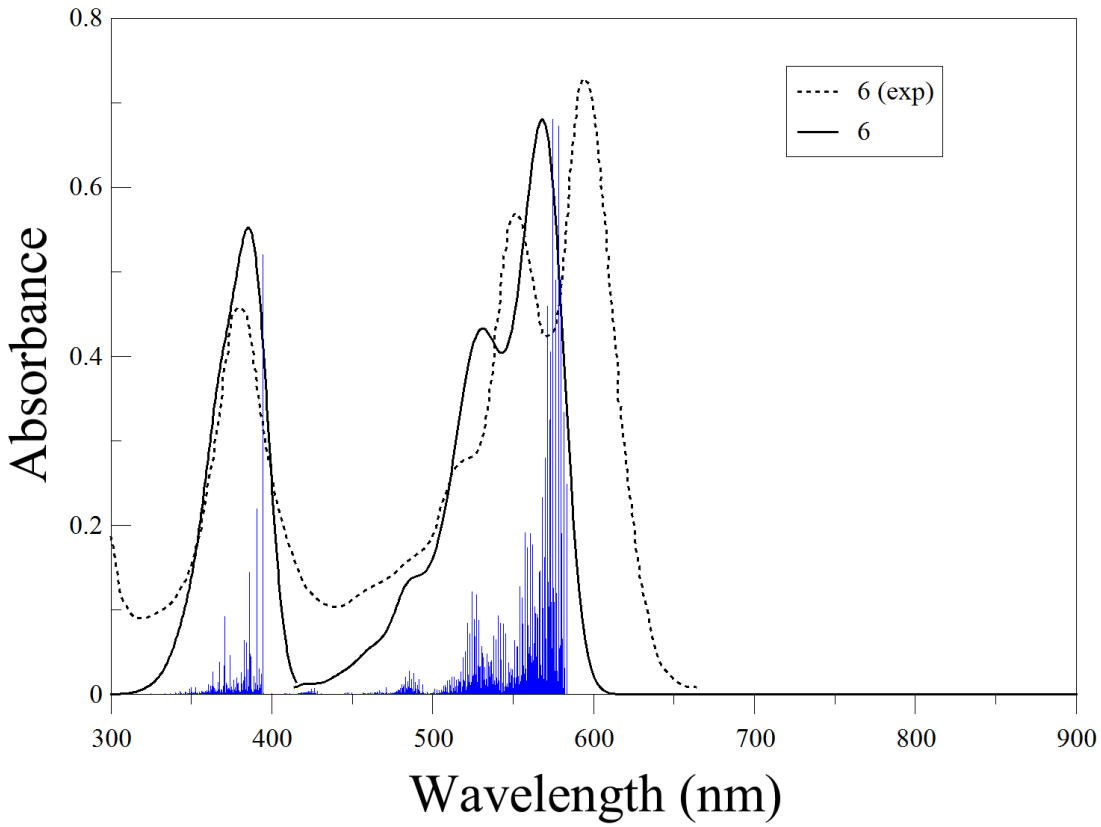


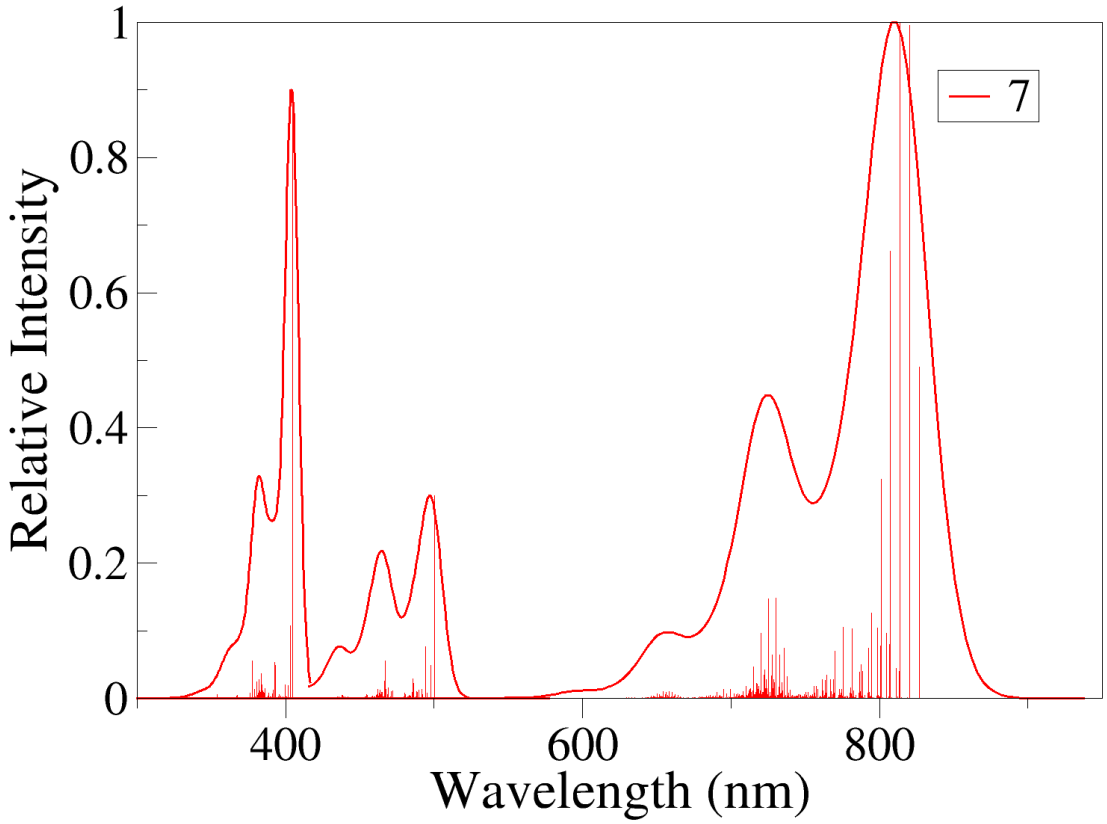

2
2 (exp)
Absorbance
0
0.1
0.2
0.3
0.4
0.5
0.6
300
400
500
600
700
800
Wavelength (nm)

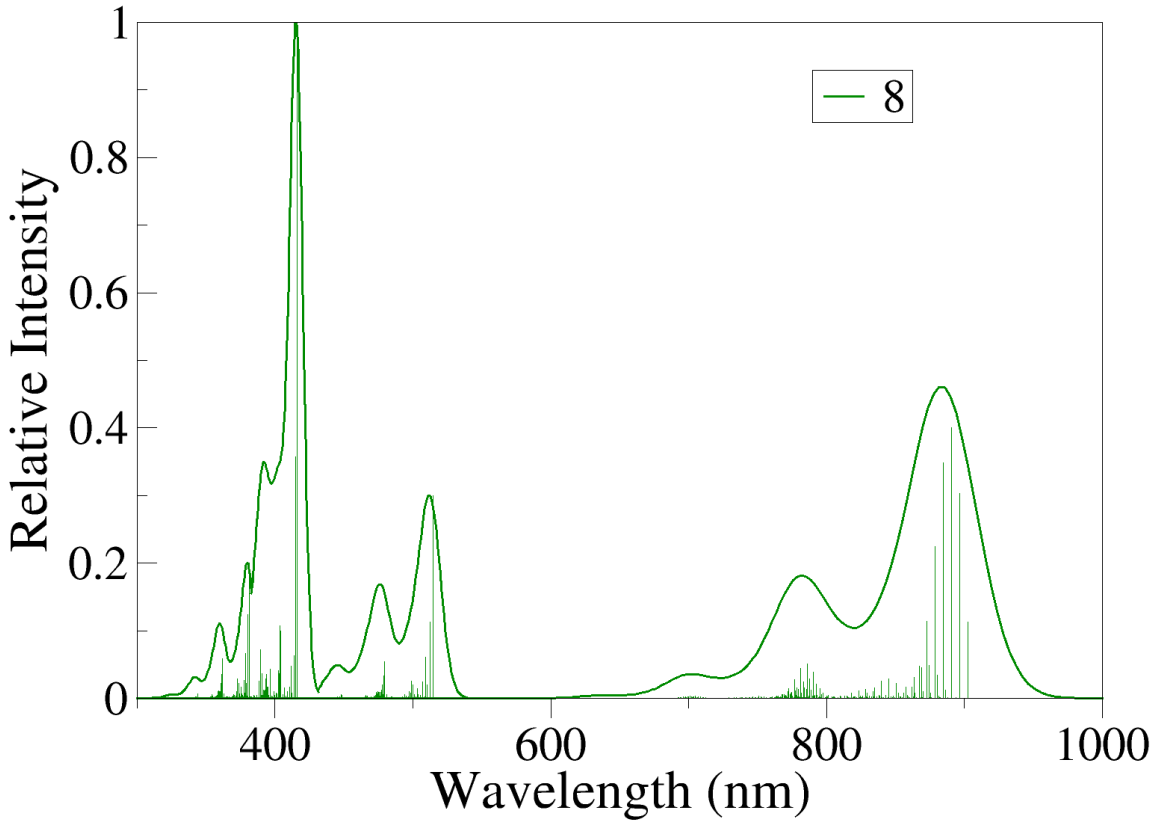

3 (exp)
3
Absorbance
Wavelength (nm)
0
0.5
1
1.5
2
300
400
500
600
700
800
900

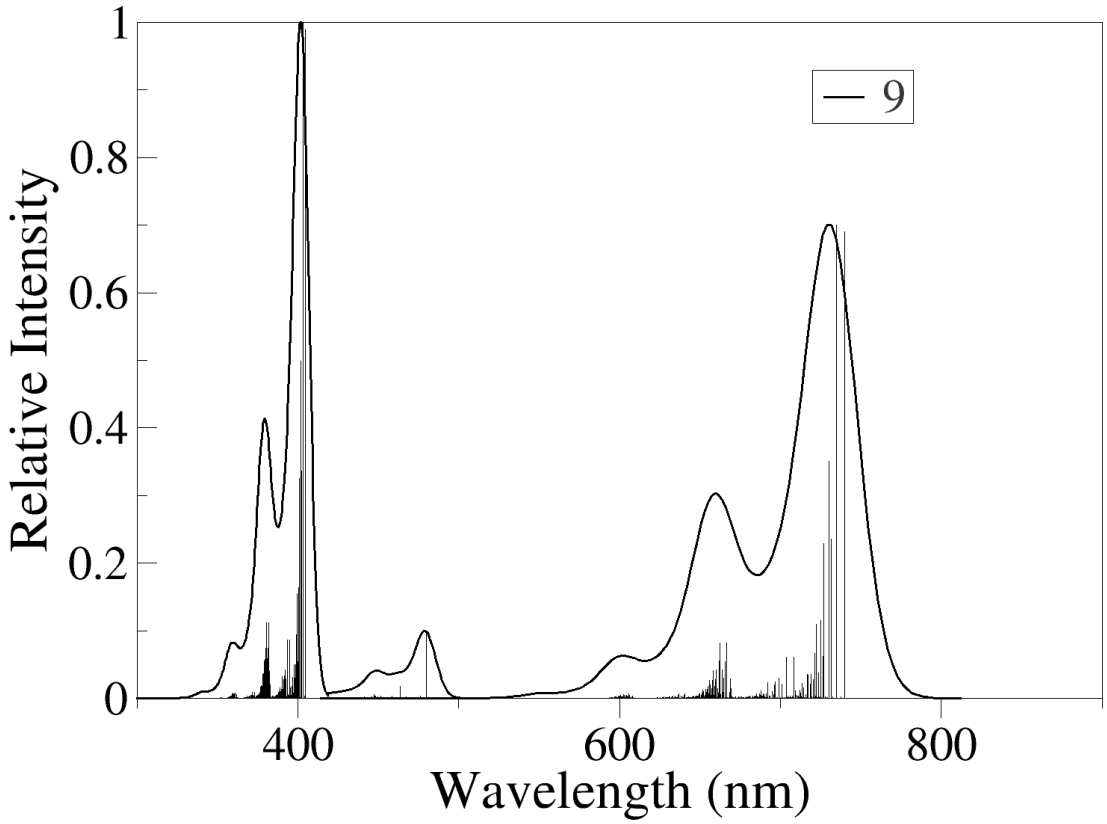

1.5
1
0.5
0
Absorbance
300
400
500
600
700
800
900
Wavelength (nm)
4
4 (exp)

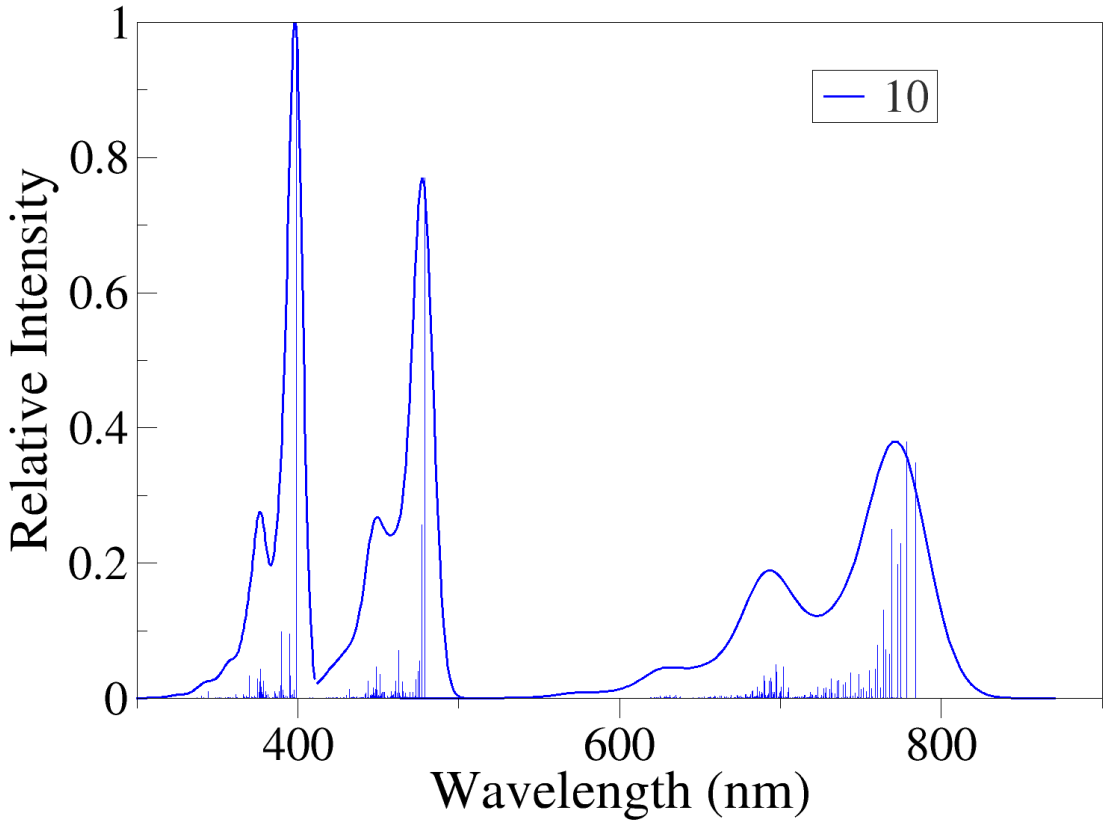

5
5 (exp)
Absorbance
0
0.1
0.2
0.3
0.4
0.5
300
400
500
600
700
800
Wavelength (nm)

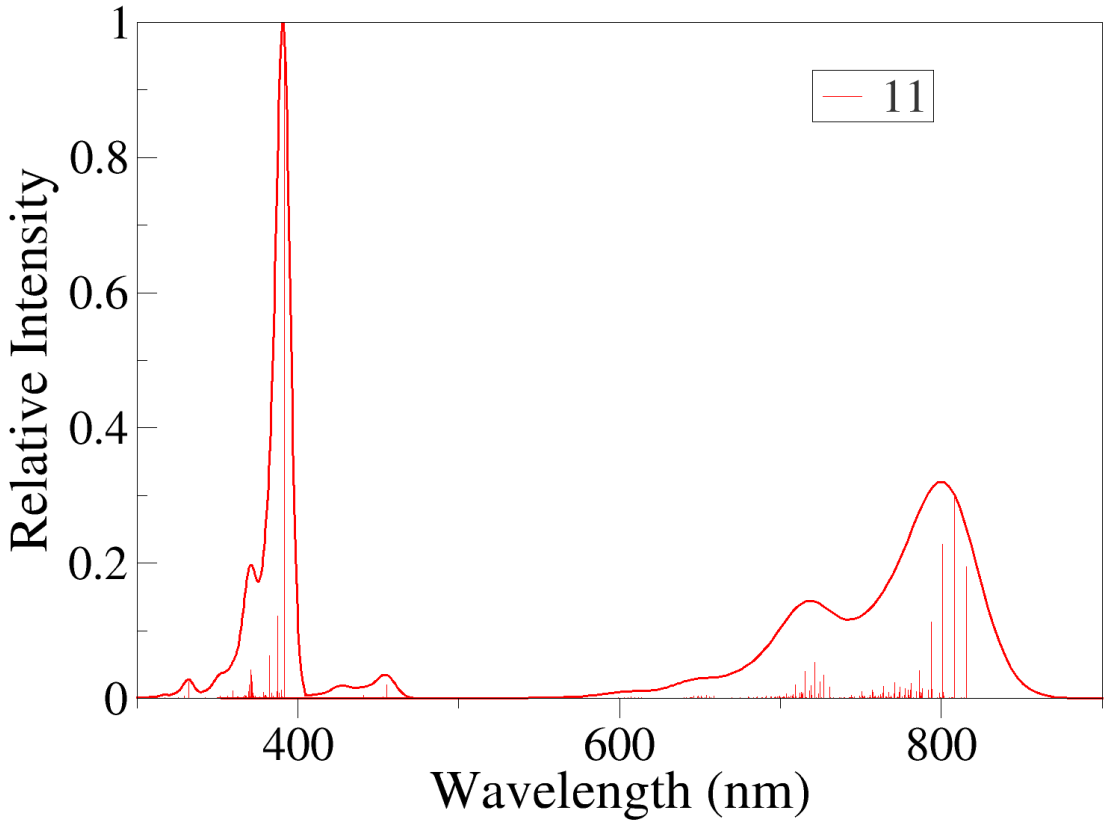

0.8
0.6
0.4
0.2
0
Absorbance
300
400
500
600
700
800
900
Wavelength (nm)
6 (exp)
6

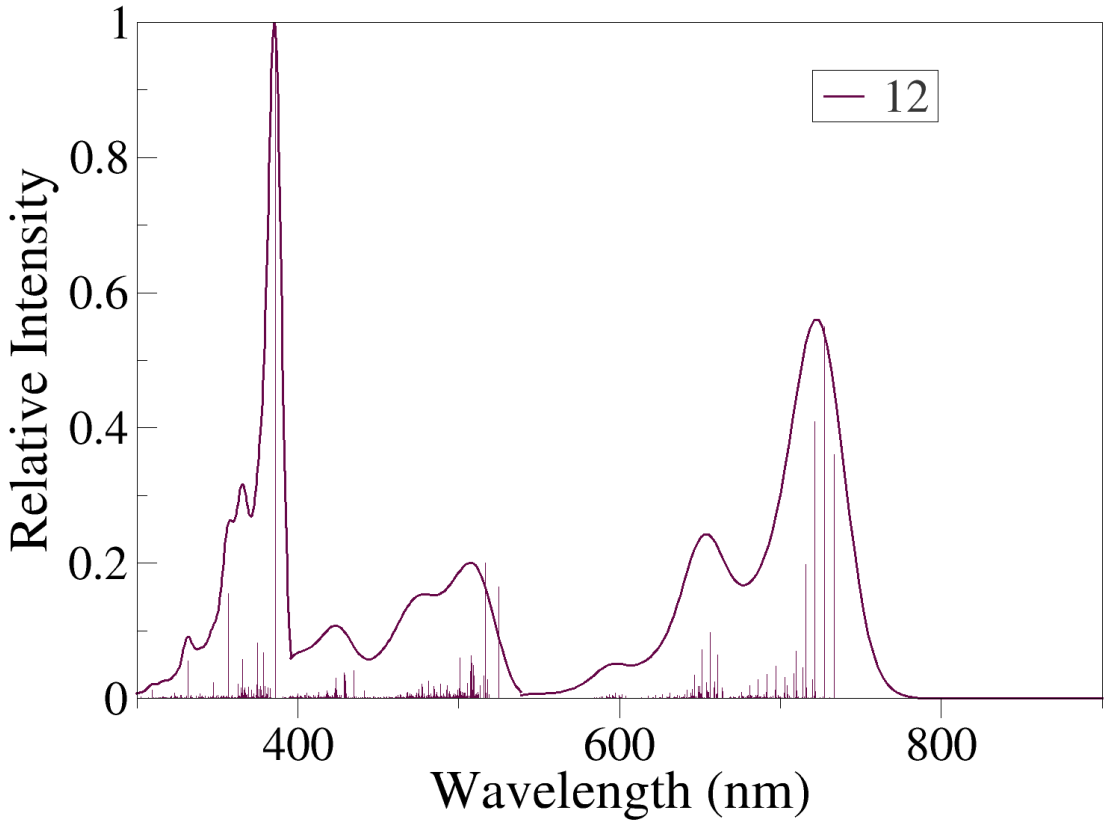

Relative Intensity
1
0.8
0.6
0.4
0.2
0
400
600
800
Wavelength (nm)
7

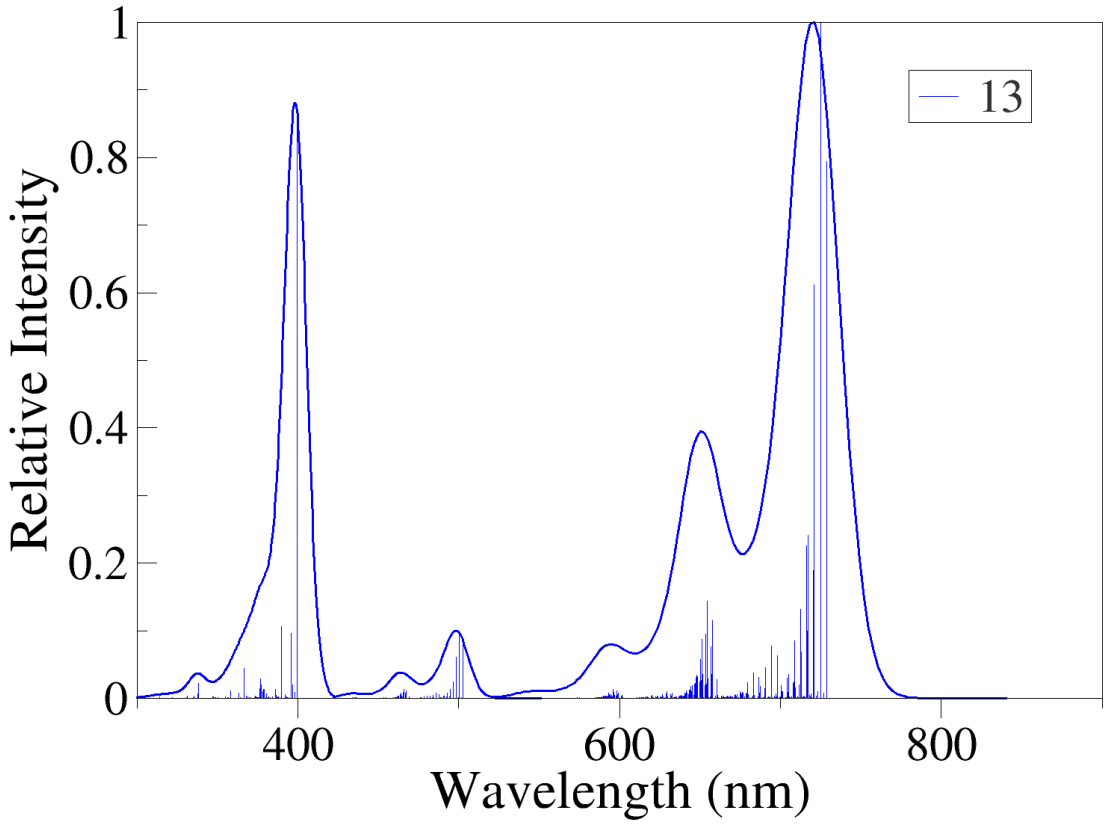

1
0.8
0.6
0.4
0.2
0
Relative Intensity
400
600
800
1000
Wavelength (nm)
8

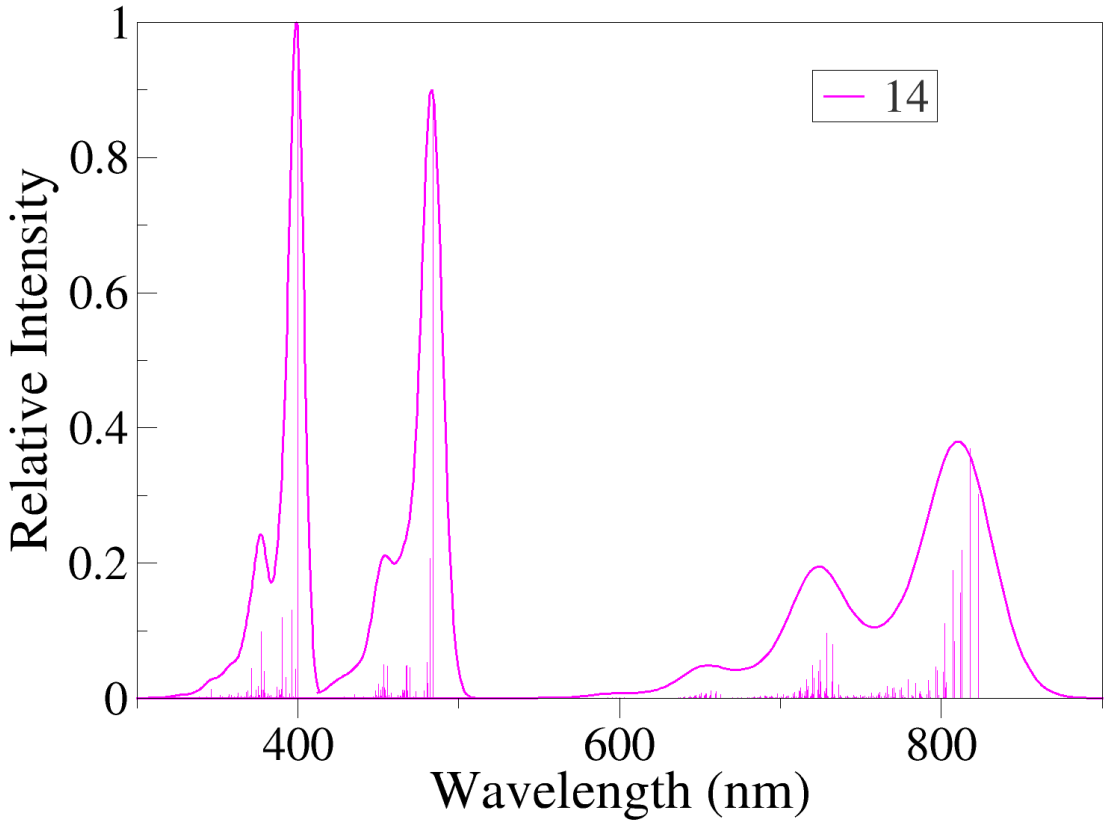

1
0.8
0.6
0.4
0.2
0
Relative Intensity
400
600
800
Wavelength (nm)
— 9

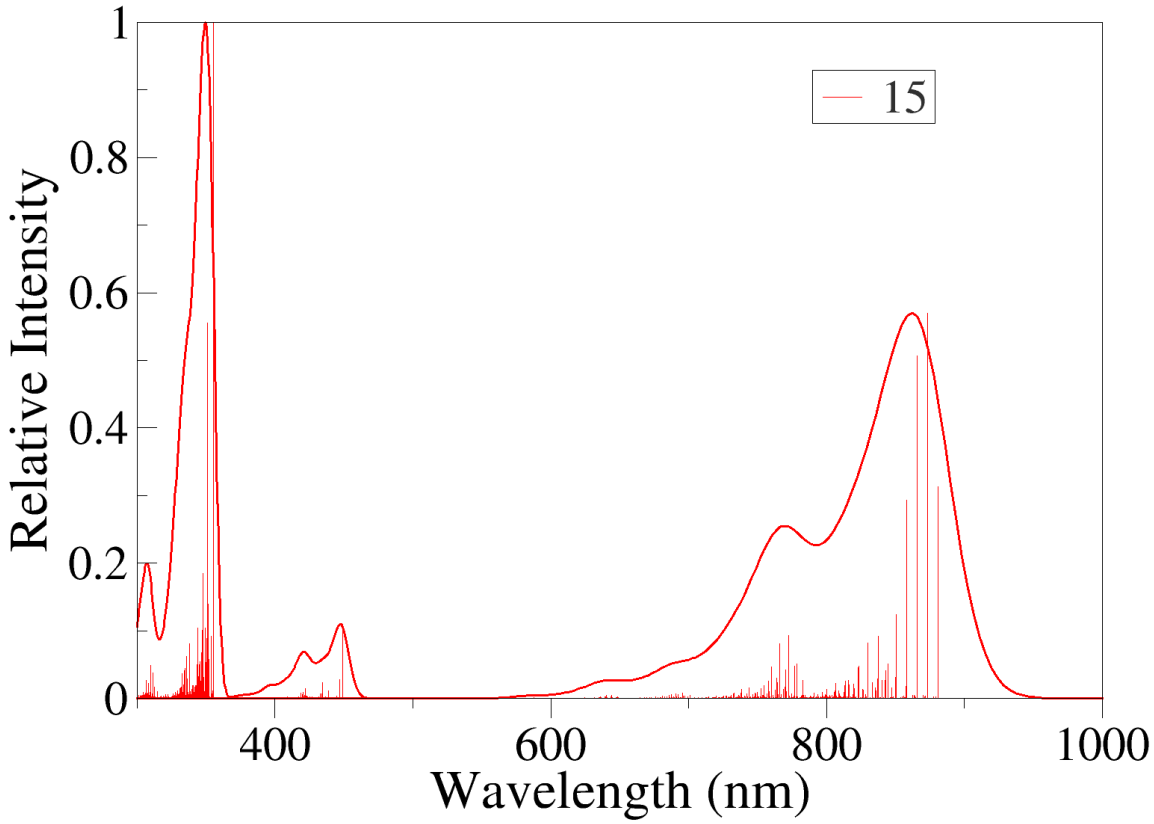

1
0.8
0.6
0.4
0.2
0
Relative Intensity
400
600
800
Wavelength (nm)
10

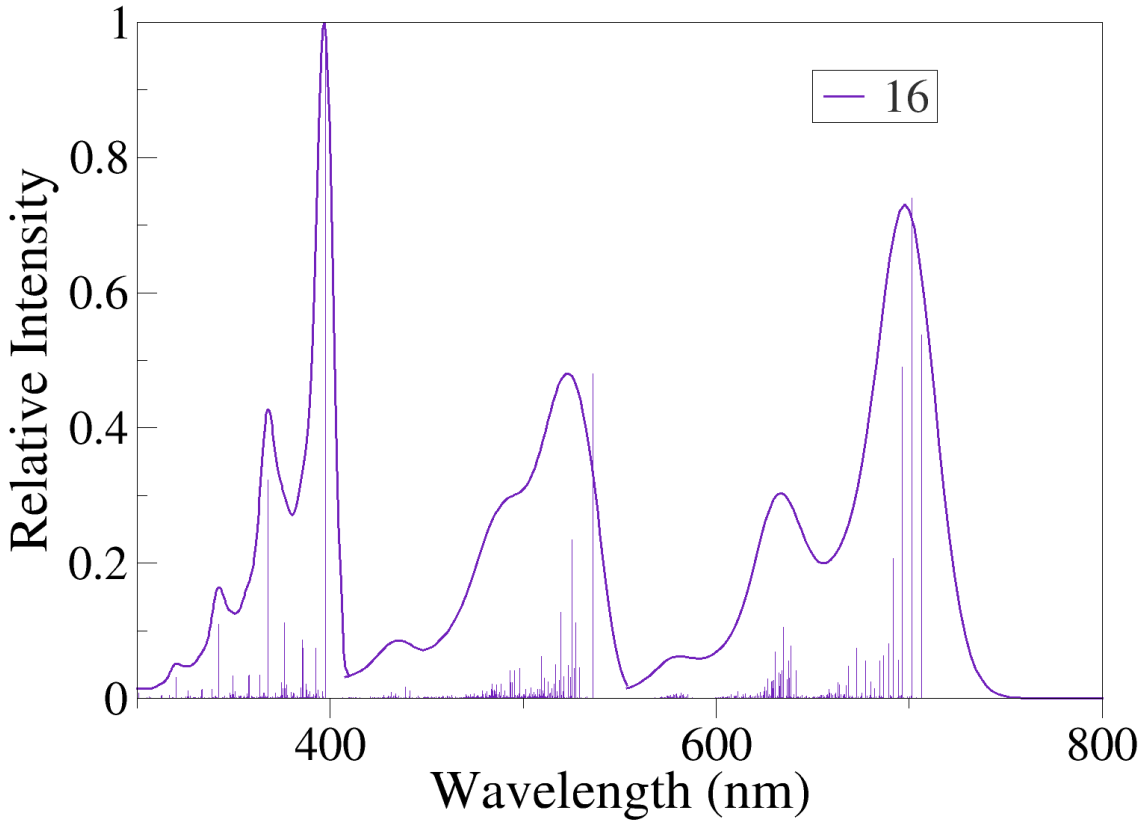

1
0.8
0.6
0.4
0.2
0
Relative Intensity
11
400
600
800
Wavelength (nm)


1
0.8
0.6
0.4
0.2
0
Relative Intensity
400
600
800
Wavelength (nm)
12


1
0.8
0.6
0.4
0.2
0
Relative Intensity
400
600
800
Wavelength (nm)
13


1
0.8
0.6
0.4
0.2
0
Relative Intensity
400
600
800
Wavelength (nm)
14


15
Relative Intensity
Wavelength (nm)
0
0.2
0.4
0.6
0.8
1
400
600
800
1000


16
Relative Intensity
1
0.8
0.6
0.4
0.2
0
400
600
800
Wavelength (nm)

References

(1) Zissimou, G. A.; Kourtellaris, A.; Koutentis, P. A. *J. Org. Chem.* **2018**, *83*, 4754–4761.