Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supporting Information

for

Modular electron donor group tuning of frontier energy levels in 2-diarylaminofluorenone push-pull molecules.

Jamie Homnick and Paul M. Lahti*

Department of Chemistry, University of Massachusetts, Amherst, MA 01003 USA;
Tel: 1-413-545-2291; E-mail: lahti@chem.umass.edu

General Information: All solvents and commercial reagent chemicals were used as received unless otherwise stated. All new compounds were identified by ^{1}H-NMR and high resolution mass spectrometry (FAB). ^{1}H-NMR spectra were recorded on a Bruker Avance 400 MHz FT-NMR spectrometer, and the chemical shifts recorded in ppm. Mass spectral data were obtained at the University of Massachusetts Mass Spectrometry Facility, which is supported in part by the National Science Foundation. UV-Vis, photoluminescence, and FT-IR spectra were obtained at room temperature using a Shimadzu UV-3600 UV-VIS-NIR spectrophotometer, a Photon Technology International QuantaMaster 30 Phosphorescence/Fluorescence spectrophotometer, and a Bruker Alpha FT-IR spectrophotometer fitted with a Platinum ATR QuickSnap sampling module, respectively. Cyclic voltammograms were obtained using a BASi Epsilon Electrochemical Workstation equipped with platinum auxiliary and working electrodes, and an Ag/AgCl reference electrode using tetrabutylammonium hexafluorophosphate as conducting electrolyte and ferrocene as an external standard.

General Amination Procedure: To a three-necked round-bottom flask under nitrogen atmosphere were added aryl halide (ArX), aryl amine, 0.02 eq of P(*t*-butyl)$_3$, 0.02 eq of Pd_2dba_3, and 1.06 eq of *t*-BuONa. Then, 5 mL of toluene (freshly distilled from potassium) per 1 mmol of ArX was added and the reaction mixture heated to 110 ºC until the starting materials were consumed, as monitored by thin layer chromatography on silica plates. The reaction mixture was allowed to cool to room temperature, diluted with toluene, and then poured into brine and stirred for 15 min. The organic layer was separated and the aqueous layer extracted with ethyl acetate. The combined organic layers were filtered through Celite, dried over anhydrous $MgSO_4$, and concentrated in vacuo. The resulting solids were purified as described for each individual preparation.

***N,N*-Dianisylamine** (**DAA**) was prepared from *p*-anisidine and *p*-bromoanisole by the method of J. M. Kauffman and G. Koyna, J. Org. Chem., 2003, **68**, 839-853.

2,7-Dibromofluorenone was prepared by oxidizing commercially available 2,7-dibromofluorenone by the method of H. P. Rathnayake, A. Cirpan, F. E. Karasz, M. Y. Odoi, N. I. Hammer, M. D. Barnes and P. M. Lahti, *Chem. Mater.*, 2007, **19**, 3265-3270.

2-Bromofluorenone was prepared by same method as for **2,7-dibromofluorenone**, but starting with commercially available 2-bromofluorene.

2-Bromo-7-iodofluorenone was prepared by oxidation of 2-bromo-7-iodofluorene made by the method of J. J. Peterson; Y. C. Simon, E. B. Coughlin, and K. R. Carter, *Chem. Commun*., 2009, *33*, 4950-4952

[***N,N*-Di(4'-methoxyphenyl)amino)fluorenone**] (**2**) was prepared by the general amination procedure using 0.250 g (0.965 mmol) of 2,7-dibromofluorenone and 0.277 g (1.21 mmol) of **DAA**. After reacting for two days of heating, the reaction mixture was worked up using the general method. The resulting thick magenta oil was purified by dry-column chromatography on basic alumina eluted with EtOAc/hexanes (15:85). The resulting dark magenta oil was collected; it solidified after a few days to yield 0.275 g (70%) of pure product. Mp 57-59 ºC; ATR-IR (neat, cm^{-1}) 1709 (s, C=O str); ^{1}H NMR (400 MHz, DMSO-d_6, δ/ppm) 3.75 (s, 6 H), 6.85 (d, 2 H, J = 10.9 Hz), 6.95 (d, 4 H, J = 8.6 Hz), 7.09 (d, 4 H, J = 8.6 Hz), 7.22 (t, 1 H, J = 7.2 Hz), 7.48-7.52 (m, 3 H), 7.57 (d, 1 H, J = 7.3 Hz); MS (FAB$^+$, *m/z*): found *m/z* = 407.1521, calculated for $C_{27}H_{23}NO_3$ *m/z* =407.1520.

2-(*N,N*-Diphenylamino)fluorenone (**3**) was prepared by the general amination procedure using 0.250 g (0.965 mmol) of 2,7-dibromofluorenone and 0.205 g (1.21 mmol) of diphenylamine. After reacting for 1 h the reaction mixture was worked up using the general method. The

resulting red solid was purified by dry-column chromatography on silica eluted with hexanes to give a powdery red solid, yield 0.222 g (66%). Mp 122-124 ºC; ATR-IR (neat, cm^{-1}) 1706 (s, C=O str); ^{1}H NMR (400 MHz, DMSO-d_6, δ/ppm) 7.03 (d, 1 H, J = 1.5 Hz), 7.08-7.15 (m, 7 H), 7.28 (t, 1 H, J = 7.3 Hz), 7.36 (t, 4 H, J = 7.7 Hz), 7.53-7.58 (m, 2 H), 7.65 (t, 2 H, J = 7.7 Hz); MS (FAB$^+$, *m/z*): found *m/z* =347.1310, calculated for $C_{25}H_{17}NO$ *m/z* = 347.1310.

***N*-(Fluorenon-2-yl)carbazole** (**4**) was prepared by the general amination procedure using 0.250 g (0.965 mmol) of 2,7-dibromofluorenone and 0.202 g (1.21 mmol) of carbazole. After reacting for 1 h the reaction mixture was worked up using the general method. The resulting yellow solid was recrystallized from hot heptane/EtOAc to yield 0.170 g (51%) of yellow crystalline solid. Mp 196-197 ºC; ATR-IR (neat, cm^{-1}) 1705, 1716 (d, C=O str); ^{1}H NMR (400 MHz, DMSO-d_6, δ/ppm) 7.30-7.34 (m, 2 H), 7.43-7.50 (m, 5 H), 7.68-7.72 (m, 2 H), 7.77 (d, 1 H, J = 1.8 Hz), 7.89 (dd, 1 H, J = 8.0 Hz, J' = 1.8 Hz), 7.95 (d, 1 H, J = 7.6 Hz), 8.11 (d, 1 H, J = 7.8 Hz), 8.27 (d, 2 H, J = 7.8 Hz); MS (FAB$^+$, *m/z*): found *m/z* = 345.1154, calculated for $C_{25}H_{17}NO$ *m/z* = 345.1153.

(*E*)-2-bromo-7-(3',4',5'-trimethoxystyryl)fluorenone (8): To a three-necked round-bottom flask under nitrogen atmosphere were added 1.00 g (2.60 mmol) of 2-bromo-7-iodo-fluorenone, 0.504 g (2.60 mmol) of 1,2,3-trimethoxy-5-vinylbenzene, 0.52 mmol of P(*o*-tolyl)$_3$, 0.18 mmol of $Pd(OAc)_2$, and 13 mL of dry DMF. The reaction mixture was heated to 80 ºC, then stirred for 30 min. Then, 2.6 mL of triethylamine was added and the reaction stirred with continued heating for three days. The reaction mixture was allowed to cool to room temperature and then poured into acidified water and allowed to stir for 15 minutes. Solids were separated by filtration and the filtrate was extracted with $CHCl_3$. The solids were dissolved in $CHCl_3$, and the combined organic solutions were filtered through Celite, dried over $MgSO_4$, and concentrated *in vacuo*. The resulting red solid was triturated with ethanol and recrystallized from boiling dichloromethane/MeOH to yield 0.515 g (44%) of product. Mp 218-220 ºC. ^{1}H-NMR (400 MHz, $CDCl_3$): 3.88 (s, 3H), 3.93 (s, 6H), 6.75 (s, 2H), 6.98-7.02 (d, 1H), 7.09-7.13 (d, 1H) 7.50-7.52 (d, 1H), 7.55-7.59 (t, 2H), 7.74-7.76 (dd, 1H), 7.86 (s, 1H), 7.89 (s, 1H).

2-(*N,N*-Di(4'-methoxyphenyl)amino)-7-(3",4",5"-trimethoxyphenylethenyl)fluorenone (**5**) was prepared by the general amination procedure using 0.250 g (0.554 mmol) of **8** and 0.159 g (0.693 mmol) of **DAA**. After reacting for 5 h the reaction mixture was worked up using the general method. The resulting dark purple solid was purified by dry-column chromatography on silica eluted with EtOAc/hexanes (40:60) to yield 0.110 g (33%) of product. Mp 99-101 ºC; ATR-IR (neat, cm^{-1}) 1710 (s, C=O str); ^{1}H NMR (400 MHz, DMSO-d_6, δ/ppm) 3.67 (s, 3H), 3.77 (s, 6H), 3.83 (s, 6H), 6.84 (d, 1 H, J = 2.0 Hz), 6.88 (dd, 1 H, J = 8.4 Hz, J' = 2.3 Hz), 6.95-6 .98 (m, 6 H), 7.12 (d, 4 H, J = 8.8 Hz), 7.28 (d, 2H, J = 4.6 Hz), 7.53 (d, 1 H, J = 8.1 Hz), 7.59 (d, 1 H, J = 7.8 Hz), 7.68 (dd, 1H, J = 7.6 Hz, J' = 0.8 Hz), 7.78 (s, 1H); MS (FAB$^+$, *m/z*): found *m/z* = 599. 2308, calculated for $C_{38}H_{33}NO_6$ *m/z* = 599.2308.

2,7-Bis(*N,N*-Di(4'-methoxyphenyl)amino)fluorenone (**6**) was prepared by the general amination procedure using 0.250 g (1.48 mmol) of 2,7-dibromofluorenone and 0.424 g (3.70 mmol) of **DAA**. After reacting for three days the reaction mixture was worked up using the general method. The resulting very dark blue-green solid was purified by dry-column chromatography on silica gel eluted with EtOAc/hexanes (20:80) to yield 0.470 g (50%) of product. Mp 202-203 ºC; ATR-IR (neat, cm^{-1}) 1711 (s, C=O str); ^{1}H NMR (400 MHz, DMSO-d_6, δ/ppm): 3.75 (s, 12 H), 6.78 (d, 2 H, J = 2.0 Hz), 6.83 (dd, 2 H, J = 8.0 Hz, J' = 2.5 Hz), 6.94 (d, 8 H, J = 8.8 Hz), 7.06 (d, 8 H, J = 8.8 Hz), 7.35 (d, 2 H, J = 8.1 Hz); MS (FAB$^+$, *m/z*): found *m/z* = 634.2468, calculated for $C_{41}H_{34}N_2O_5$ *m/z* = 634.2468.

***N*-(*p*-Methoxyphenyl)-*N*-(3,4,5-trimethoxyphenyl)amine (MTPA)** was prepared using the general amination procedure using 3.95 g (16.0 mmol) of 5-bromo-1,2,3-trimethoxybenzene and 2.47 g (20.0 mmol) of *p*-anisidine in 40 mL toluene. After reacting for two days the reaction mixture was worked up using the general method. The resulting tan solid was purified on silica eluted with diethyl ether to yield 3.90 g (84%) of tan solid. Mp 99-100 ºC. ^{1}H-NMR (DMSO-d_6) 3.58 (s, 3H), 3.69 (s, 6H), 3.70 (s, 3H), 6.22 (s, 2H), 6.84-6.86 (d, 2H), 7.03-7.05 (d, 2H), 7.72 (s, 1H).

2,7-Bis(*N*-(4'-methoxyphenyl)-*N*-(3',4',5'-trimethoxyphenyl)amino)fluorenone (**7**) was prepared by the general amination procedure using 0.250 g (0.740 mmol) of 2,7-dibromofluorenone and 0.545 g (1.85 mmol) of **MTPA**. After reacting for 17 h the reaction mixture was worked up using the general method. The resulting very dark blue solid was purified by dry-column chromatography on silica gel eluted with Et_2O/hexanes (66:33) to yield 0.117 g (21%) of product. Mp 68-70 ºC; ATR-IR (neat, cm^{-1}) 1710 (s, C=O str); ^{1}H NMR (400 MHz, DMSO- d_6): 3.63 (s, 12 H), 3.65 (s, 6 H), 3.76 (s, 6 H), 6.35 (s, 4 H), 6.87 (d, 2 H, J = 1.5 Hz), 6.96 (d, 6 H, J = 8.8 Hz), 7.11 (d, 4H , J = 8.8 Hz), 7.42 (d, 2 H, J = 8.34 Hz); MS (FAB$^+$, *m/z*): found *m/z* = 754.2890, calculated for $C_{45}H_{42}N_2O_9$ *m/z* = 754.2892.

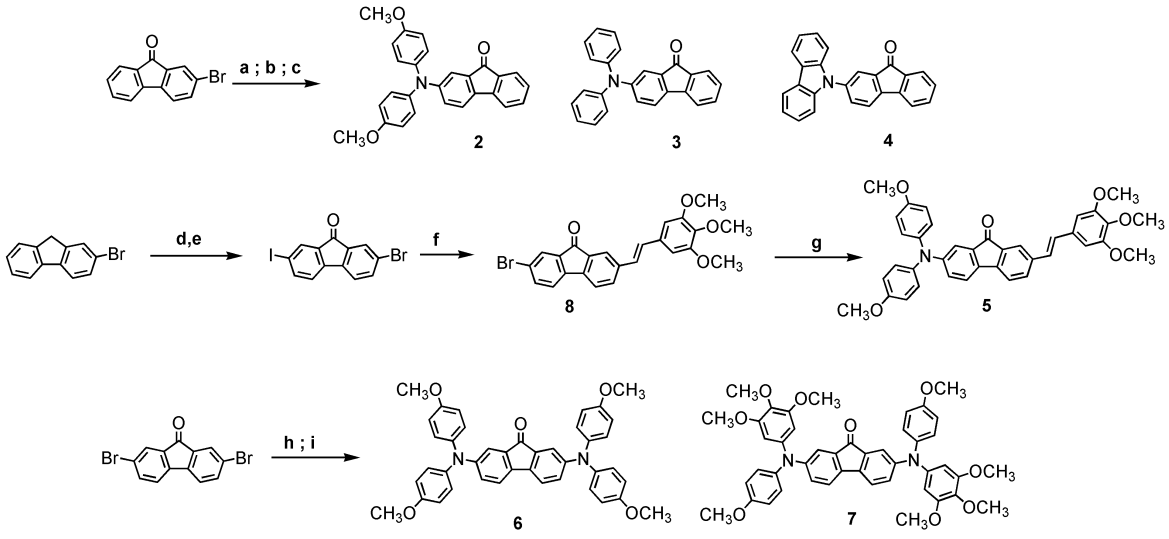


Table S1: Comparisons of absorption solvatochromism in meV.

Compound Compound	Compound	Solvatochromic Shift from Hex to MeCN (meV)
2	DAAFO	76
3	DPAFO	79
4	CzFO	20
5	DAAFOPV	83
6	BDAAFO	122
7	BTMPMPAFO	119

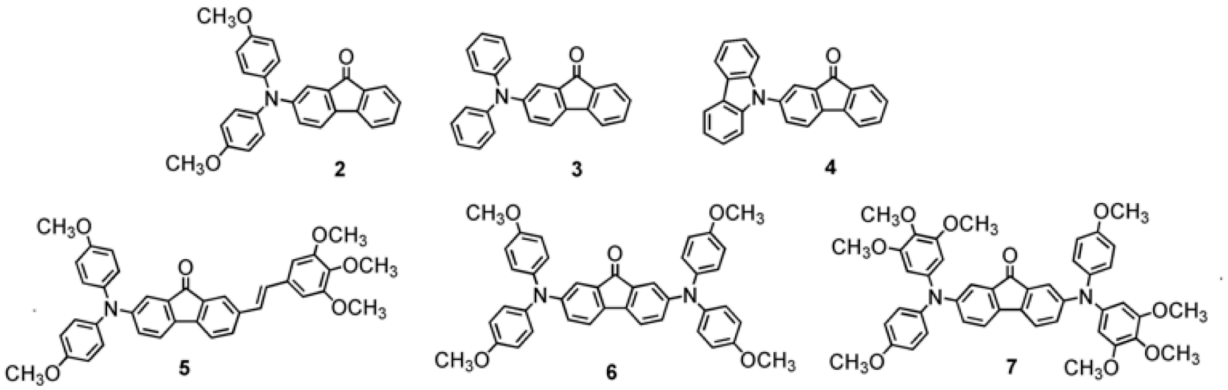


Table S2: Comparisons of fluorescence solvatochromism, Stokes shifts, computed ground state dipole moments.

Compound Number	Stokes Shift Hex (meV)	Stokes Shift MeCN (meV)	Solvatochromic Shift from Hex to MeCN (meV)	Dipole Moment[a] (B3LYP/6-31G*)	Dipole Moment[b] (M06-2X/6-311G[d,p])
2	350	N/A	Quenched	3.27 D	3.08 D
3	342	649	396	3.13 D	3.12 D
4	504	797	313	3.76 D	3.69 D
5	327	N/A	Quenched	5.27 D	5.70 D
6	331	N/A	Quenched	3.04 D[c]	2.01 D[c]
7	301	N/A	Quenched	—[d]	—[d]

Ground state dipole moments (in vacuum) were computed using geometries optimized at the same level of theory. [a]B3LYP/6-31G* dipole moments computed using Spartan 2010 for Linux (Wavefunction Inc., Irvine CA, USA). [b]M06-2X/6-311(d,p) dipole moments computed using NBO routine in Gaussian 09 for molecules optimized at the same level of theory. See page S11 for full Gaussian citation. [c]The two computed conformers of **6** were different, partly due to symmetry constraints placed on the M06-2X computation; this contributes to the difference between dipole moments at the two levels of theory. [d]Not listed, due to multiple different conformations.

Figure S1. Solutions of push-pull fluorenones in dichloromethane.

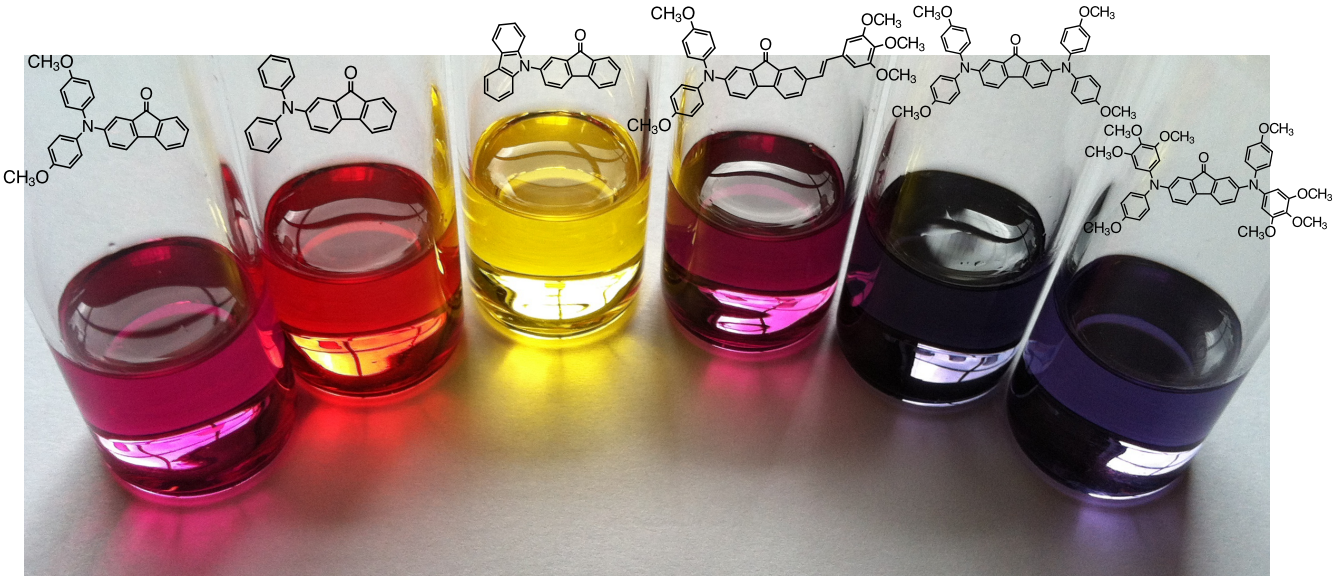


Figure S2. Cyclic voltammograms of 2-7 and individual module compounds.

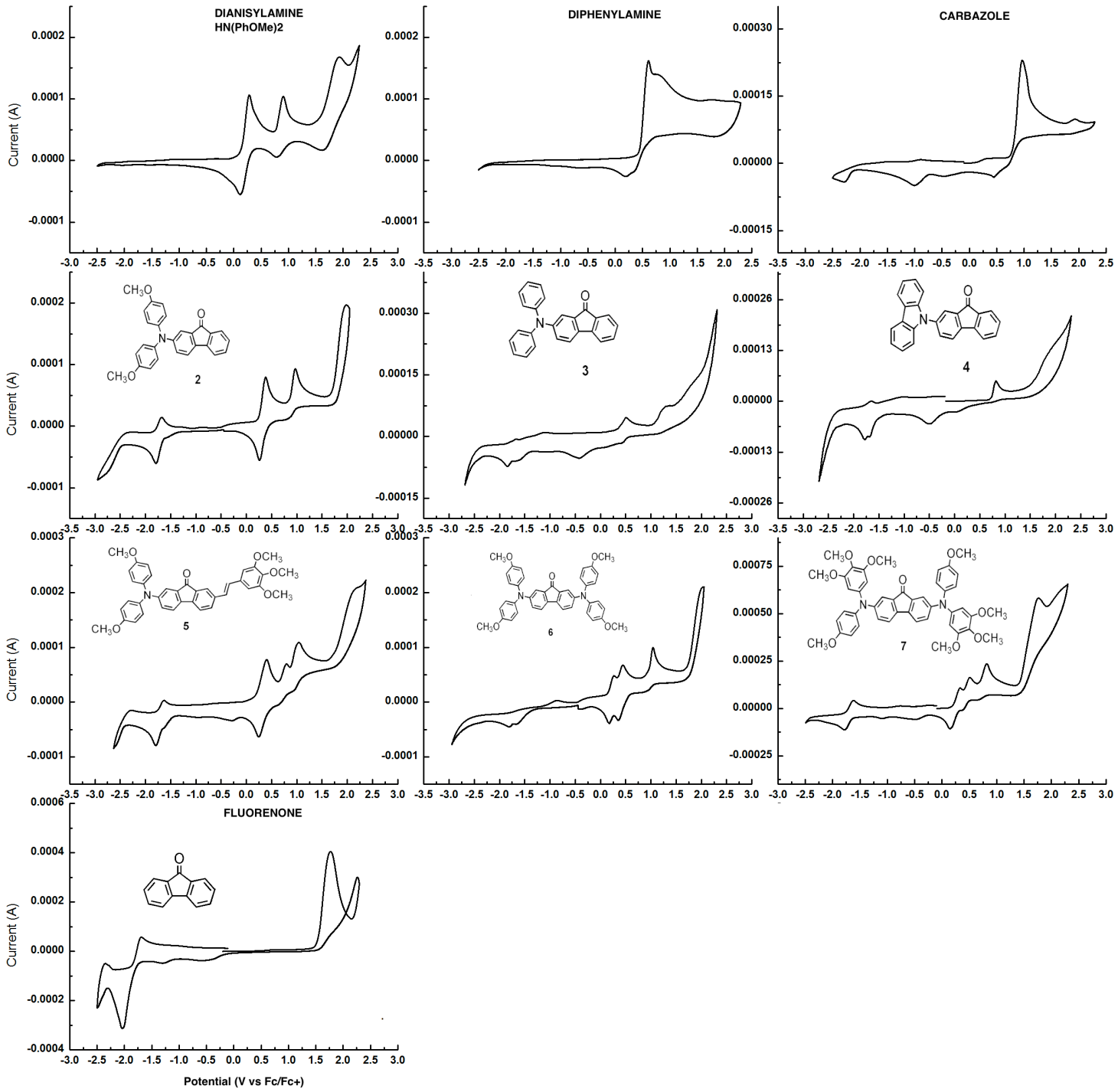


Table S3. Frontier energy levels and band gaps of **2-7** and modular donors (used in Figure 7 of main article).

Structure*	E_{HOMO} / eV	E_{LUMO} / eV	E_g /eV
DAA	-4.94	-1.38	3.56
DPA	-5.25	-1.34	3.91
Cz	-5.61	-2.00	3.61
2	-5.03	-3.02	2.01
3	-5.12	-3.01	2.11
4	-5.51	-3.05	2.46
5	-4.98	-3.05	1.93
6	-4.95	-3.21	1.74
7	-5.00	-3.18	1.82
FO	-6.72**	-2.98**	3.74**

DAA = dianisylamine, DPA = diphenylamine, Cz = carbazole, FO = fluorenone. *Donor modules electronic properties evaluated using DAA = dianisylamine, DPA = diphenylamine, Cz = carbazole, FO = fluorenone. All E_{HOMO} obtained from first oxidation onset potential. Unless otherwise stated, E_{LUMO} obtained from E_{HOMO} + E_g. **LUMO energy obtained from cyclic voltammetric reduction potential, band gap from onset of the band that maximizes at about 325 nm.

General:

$E_{redox\text{-}Fc} = E^{1/2}$ Fc = 0.0 to standardize all voltages.

E_{redox} = redox process ***onset potential***.

E_g = ICT absorption peak ***low energy onset***, in acetonitrile.

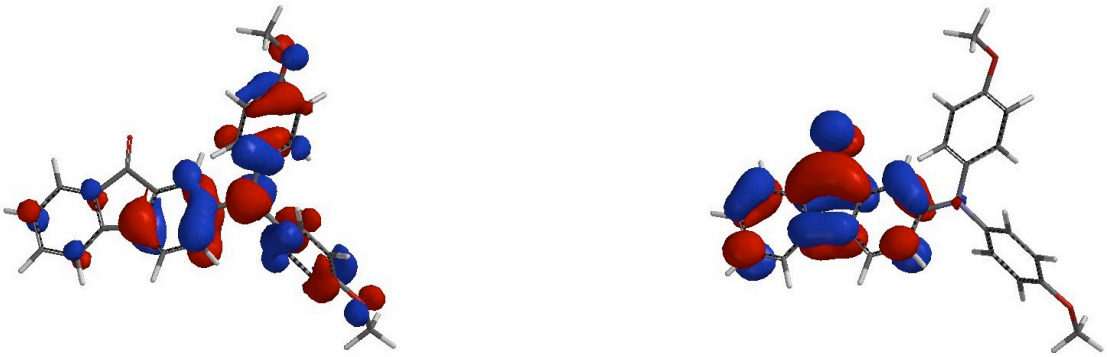
Fc/Fc^+ = 4.8 eV below vacuum, $E_{MO} = -(E_{redox} + 4.8)$ eV

Figure S3. Computed molecular orbital density maps.

These structures were optimized at the B3LYP/6-31G(d) level of theory as implemented in Spartan 2010 (Wavefunction, Irvine CA). The appropriate orbital pictures were then generated in Spartan using default settings.

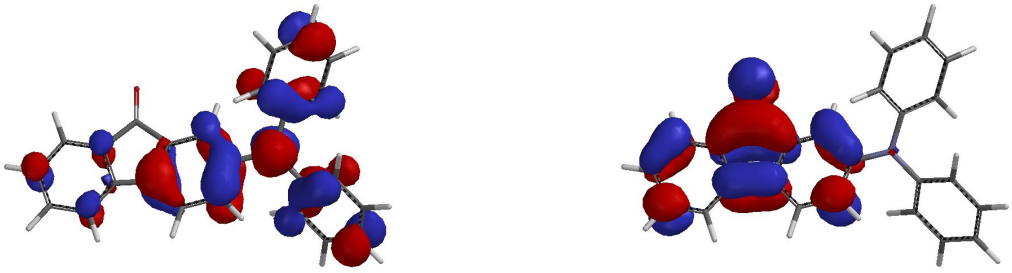
B3LYP/6-31G* HOMO (left) and LUMO (right) for compound **2** model

E = -4.74 eV E = -2.03 eV



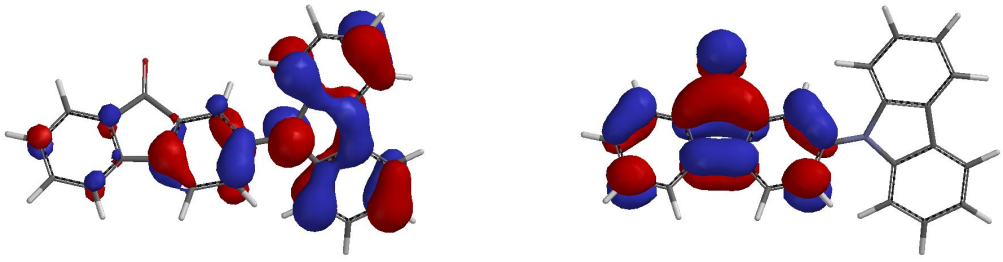
B3LYP/6-31G* HOMO (left) and LUMO (right) for compound **3** model

E = -5.05 eV E = -2.15 eV



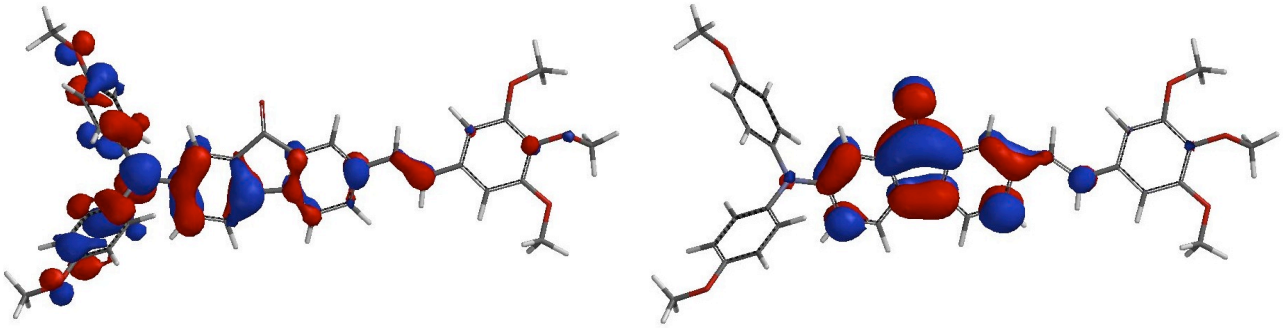
B3LYP/6-31G* HOMO (left) and LUMO (right) for compound **4** model

E = -5.41 eV E = -2.43 eV



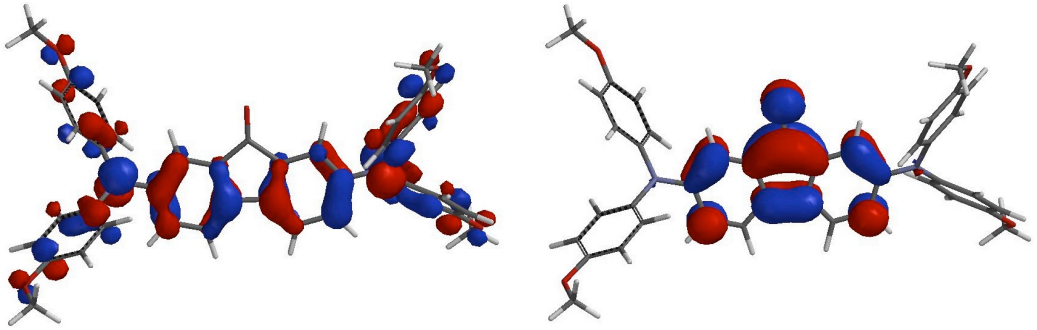
B3LYP/6-31G* HOMO (left) and LUMO (right) for compound **5** model

E = -4.66 eV E = -2.08 eV



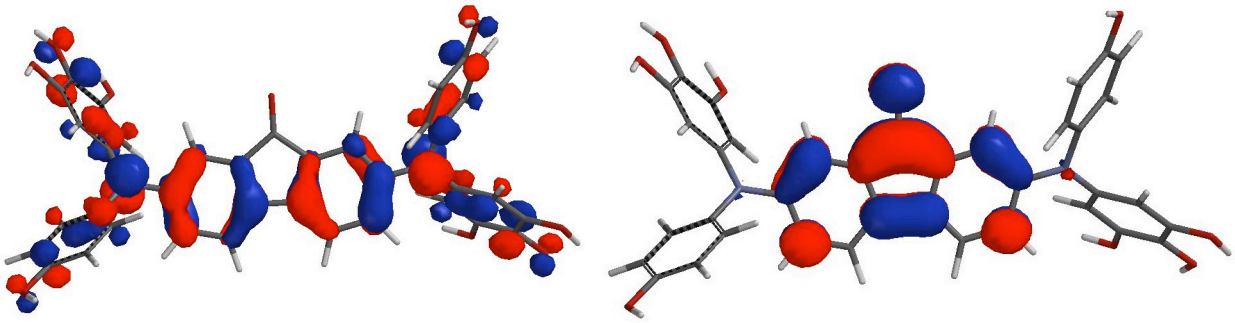
B3LYP/6-31G* HOMO (left) and LUMO (right) for compound **6** model

E = -4.44 eV E = -1.95 eV



B3LYP/6-31G* HOMO (left) and LUMO (right) for compound **7** (replace CH_3 with H)

E = -4.51 eV E = -1.97 eV



The following computations were carried out using Gaussian 09 version B.01, and were visualized using Gaussview version 5 with default settings for surfaces. The geometries for were optimized at the same level of theory as was used to generate the MO diagrams.

Full citation for Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.,; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian 09 Revision B.01 ed.; Gaussian, Inc: Wallingford CT, 2010.

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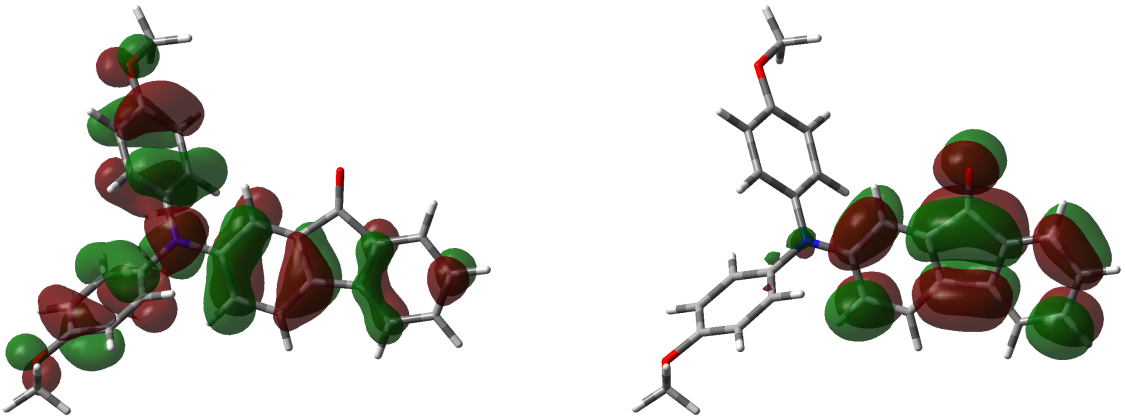
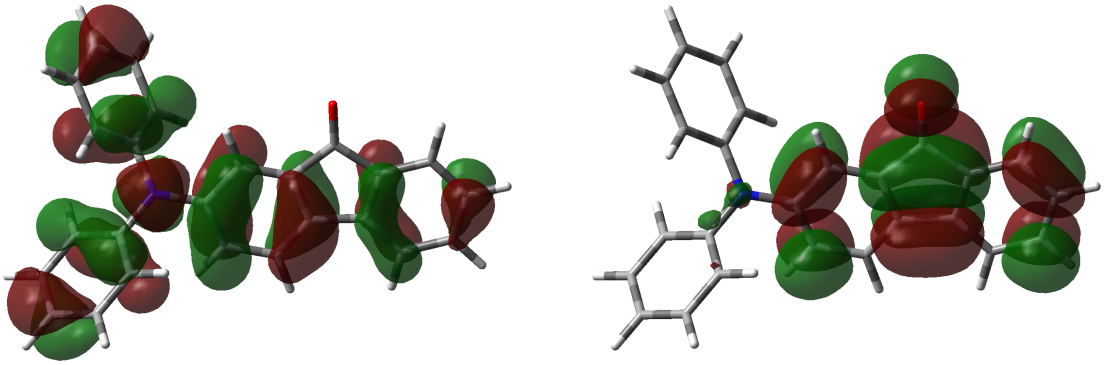
M06-2X/6-311G(d,p) (left, E = -6.149 eV), LUMO (right, E = -1.390 eV), compound **2**



M06-2X/6-311G(d,p) HOMO (left, E = -6.484 eV); LUMO (right, E = -1.462 eV), compound **3**



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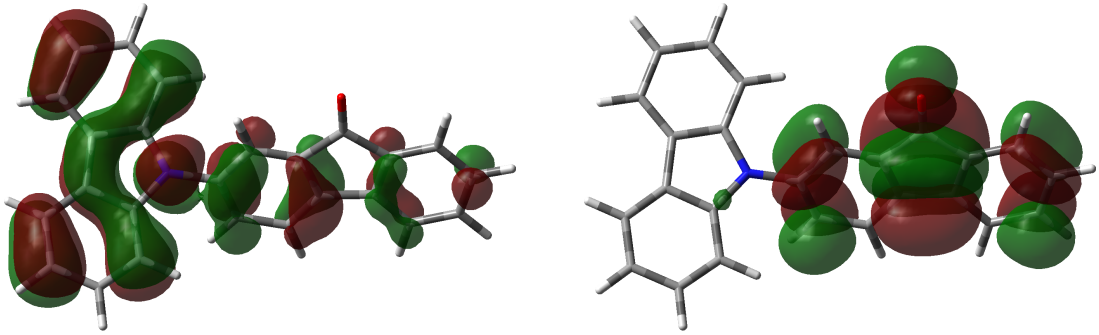
M06-2X/6-311G(d,p) HOMO (left, E = -6.885 eV); LUMO (right, E = -1.730 eV), compound **4**



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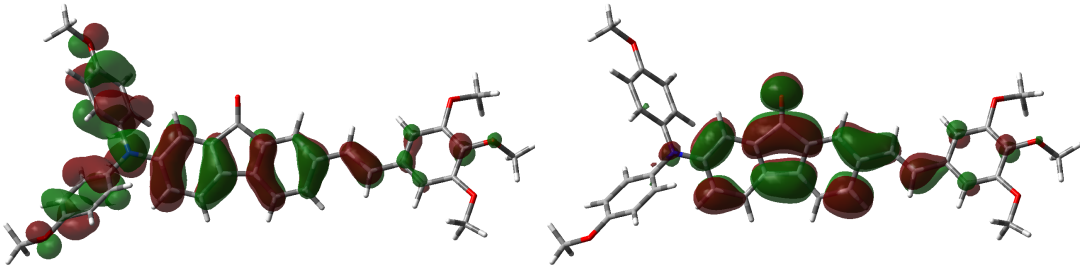
M06-2X/6-311G(d,p) HOMO (left, E = -6.082 eV); LUMO (right, E = -1.439 eV), compound **5**



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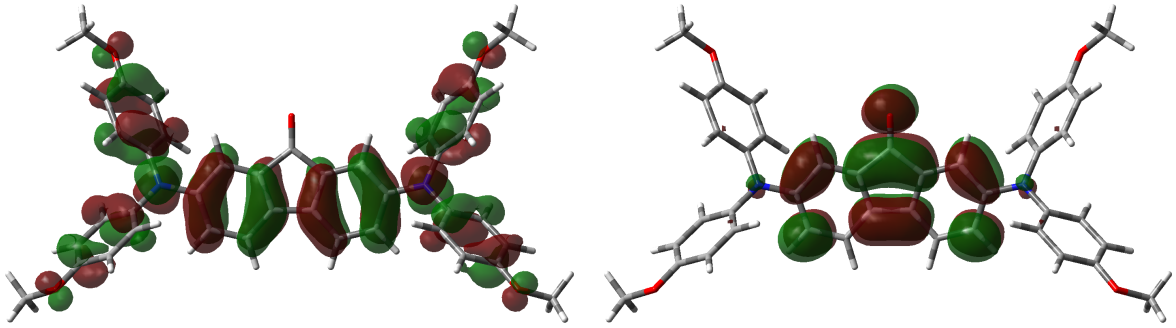
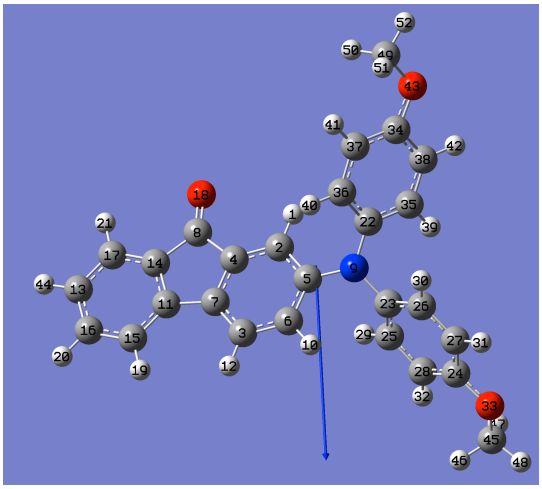
M06-2X/6-311G(d,p) HOMO (left, E = -5.790 eV); LUMO (right, E = -1.212 eV), compound **6**

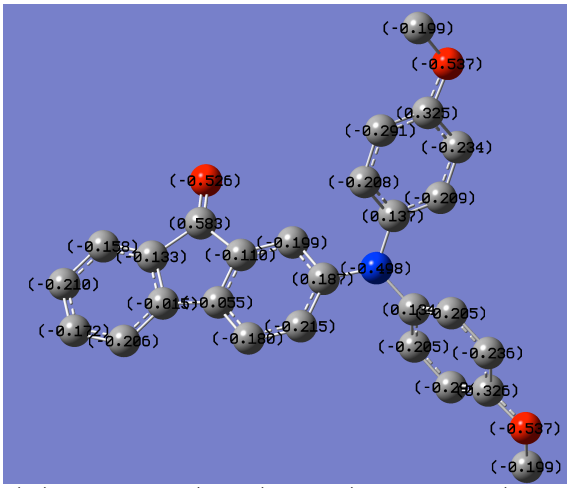


Archival output for Gaussian 09 computations

[All charge populations by NBO method, A. E. Reed, L. A. Curtiss and F. Weinhold, *Chem. Rev*., 1988, **88**, 899–926.)



Compound **2**, M06-2X/6-311G(d,p), Dipole moment vector (above), NBO populations (below)

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1\1\GINC-SKYNET\FOpt\RM062X\6-311G(d,p)\C27H21N1O3\LAHTI\30-Jun-2012\0
 \\#p opt 6-311g(d,p) direct gfinput iop(6/7=3) m062x test\\DAAFO with
 Truhlar functional opt\\0,1\H,-0.881730764,-1.5672175167,-0.5722298066
 \C,-0.3433932241,-0.6788041754,-0.8826231685\C,1.0272173609,1.63011657
 18,-1.7447031834\C,-0.1914511217,-0.383963497,-2.2190185908\C,0.212749
 8864,0.2024453105,0.0618961644\C,0.8952415425,1.3432193046,-0.38800728
 6\C,0.4805763271,0.7577672115,-2.6711547241\C,-0.6961081176,-1.1518422
 433,-3.4084893769\N,0.083947573,-0.0468832454,1.4384529955\H,1.3253953
 386,2.01224929,0.3475416681\C,0.4448926608,0.7777243743,-4.1518603494\
 H,1.5627646817,2.5205276316,-2.054391291\C,0.0598062212,0.304522618,-6
 .8657638038\C,-0.2551867599,-0.3516408657,-4.5983495489\C,0.958581483,
 1.6790156168,-5.0698668321\C,0.7579048121,1.4276621153,-6.4300692153\C
 ,-0.458352864,-0.6040361841,-5.9401998327\O,-1.3157067178,-2.182475322
 9,-3.4061851569\H,1.5031305926,2.5601089702,-4.7504573915\H,1.15378729
 8,2.1230636686,-7.1612873829\H,-1.0055959035,-1.486982899,-6.250607672
 1\C,0.0479405092,-1.3769039713,1.9337262763\C,-0.0771144345,1.03269634
 01,2.347777221\C,-0.4038136068,3.1545624884,4.1459003558\C,-0.96108586
 37,2.068998411,2.0685855302\C,0.6418288133,1.0637316676,3.5478641048\C
 ,0.4724482917,2.1061987539,4.4391670368\C,-1.1193533773,3.1348360518,2
 .9503525417\H,-1.527333354,2.0473450284,1.1444052091\H,1.3284906983,0.
 2566075837,3.7758311342\H,1.0201974797,2.1432003878,5.3725737161\H,-1.
 8117188365,3.9261625123,2.6974877193\O,-0.4874422378,4.1370850821,5.07
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99539448\C,-0.0241093045,-4.0002036572,2.9157362203\C,-0.8684434288,-1
.7398065644,2.9272704161\C,0.9263993456,-2.3406275081,1.4495875498\C,0
.8864466722,-3.6499947687,1.9214126888\C,-0.895477165,-3.0307781956,3.
4188243683\H,-1.5556764618,-0.9962669403,3.3135957615\H,1.6447284802,-
2.0695154567,0.6845498333\H,1.5777233573,-4.3744663918,1.5132831061\H,
-1.5971234672,-3.3241940236,4.1895659425\O,-0.1403662665,-5.2410463528
,3.4555274652\H,-0.0798147734,0.1374445712,-7.9266810701\C,-1.36641782
94,5.2102637904,4.8210178598\H,-1.0814033956,5.7462321779,3.9096827495
\H,-2.4010789637,4.8635552171,4.7305748139\H,-1.2834679163,5.880104832
,5.6738201279\C,0.7180210537,-6.2483849142,2.965281543\H,0.5599335869,
-6.4185071165,1.895239319\H,1.7686053879,-5.9953445658,3.1421464649\H,
0.4673849115,-7.1521760022,3.515734175\\Version=EM64L-G09RevB.01\State
=1-A\HF=-1321.7184246\RMSD=8.438e-09\RMSF=5.185e-06\Dipole=0.5831383,1
.0494577,0.1595581\Quadrupole=-8.3928622,10.8290325,-2.4361703,-9.5546
851,-5.9407322,-4.4449583\PG=C01 [X(C27H21N1O3)]\\@

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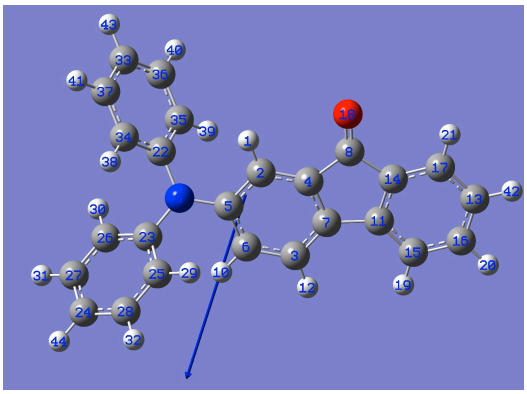
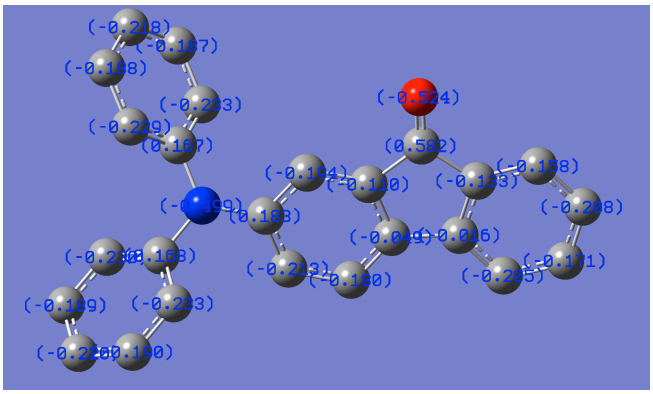


Compound **3**, M06-2X/6-311G(d,p), Dipole moment vector (above), NBO populations (below)



1\1\GINC-SKYNET\SP\RM062X\6-311G(d,p)\C25H17N1O1\LAHTI\29-Jun-2012\0\\
 #P GFINPUT IOP(6/7=3) DIRECT TEST pop=nboread m062x/6-311G(d,p)\\DPAFO
  with Truhlar functional opt\\0,1\H,0,-1.0278293384,-1.5753423259,-0.3
 698145773\C,0,-0.4734568363,-0.6947000677,-0.674382394\C,0,0.945430135
 1,1.5911555484,-1.518186154\C,0,-0.276840279,-0.4175247953,-2.00811767
 14\C,0,0.0673674687,0.1888557244,0.2759624574\C,0,0.7733568372,1.31762
 91904,-0.1620026833\C,0,0.4202984131,0.7128384749,-2.4510984533\C,0,-0
 .7430038656,-1.2002485275,-3.2032183413\N,0,-0.0978721953,-0.064259814
 9,1.6513725243\H,0,1.1916717271,1.9887040226,0.5786790682\C,0,0.439184
 3212,0.7098994121,-3.9333835548\H,0,1.4971216815,2.4736237104,-1.82150
 45792\C,0,0.1618601073,0.187209217,-6.6510078463\C,0,-0.2482308158,-0.
 4241937291,-4.3870882192\C,0,0.9921760703,1.5927764555,-4.8462208636\C
 ,0,0.8452851042,1.3168037603,-6.2084648274\C,0,-0.3973681545,-0.701672
 6508,-5.7310174235\O,0,-1.3728526878,-2.2241408144,-3.206990442\H,0,1.
 5280253288,2.4769372622,-4.5209889354\H,0,1.2736270833,1.996837187,-6.
 9356135757\H,0,-0.9359856317,-1.5876808018,-6.0473002343\C,0,-0.085184

4395,-1.3976408932,2.1383580181\C,0,-0.2120795154,1.005495953,2.575674
1479\C,0,-0.4489947682,3.0956958303,4.4164869369\C,0,-1.0279049801,2.1
037452379,2.2931347242\C,0,0.4841087119,0.9617511369,3.7855135723\C,0,
0.3566608371,1.9982870833,4.7005981743\C,0,-1.1352716715,3.1435524422,
3.2071264766\H,0,-1.5735945308,2.1341091342,1.3571891913\H,0,1.1166210
641,0.1089971411,4.0021221895\H,0,0.9004413882,1.9507527915,5.63661821
63\H,0,-1.7724463275,3.9894070278,2.9777573281\C,0,-0.0601488479,-4.01
26456107,3.1220267366\C,0,-0.9895140283,-1.785745814,3.1289807627\C,0,
0.8330020182,-2.3266363851,1.6443573737\C,0,0.8348565248,-3.6278723578
,2.1296055224\C,0,-0.9679664996,-3.0837385326,3.6207129208\H,0,-1.7006
740194,-1.0616967314,3.5092861628\H,0,1.5377467066,-2.0236490071,0.878
8088992\H,0,1.5493945646,-4.34115645,1.7363164081\H,0,-1.6737544875,-3
.3732284406,4.390054632\H,0,0.0652619693,0.0009009527,-7.71346868\H,0,
-0.0506773539,-5.0264022244,3.5025251282\H,0,-0.5428467888,3.904211278
4,5.1306018833\\Version=EM64L-G09RevB.01\State=1-A\HF=-1092.7001118\RM
SD=3.610e-09\Dipole=0.6408213,0.9751903,0.3813077\Quadrupole=-8.136332
3,-0.4171512,8.5534835,-1.3596273,-4.8039242,-6.1520569\PG=C01 [X(C25H
17N1O1)]\\@

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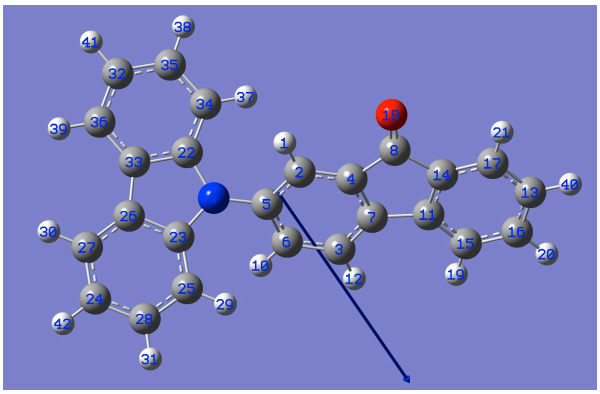
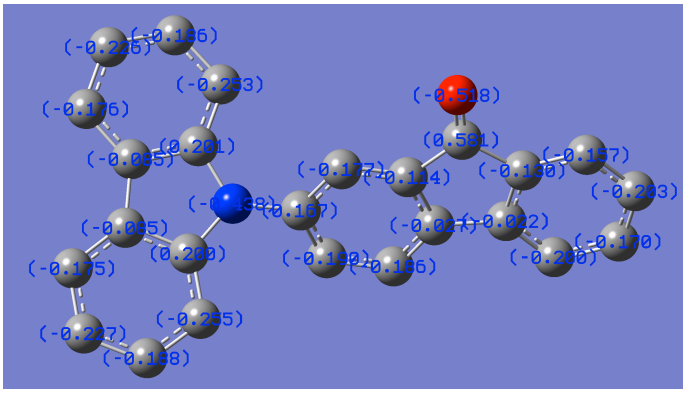


Compound **4**, M06-2X/6-311G(d,p), Dipole moment vector (above), NBO populations (below)



1\1\GINC-SKYNET\SP\RM062X\6-311G(d,p)\C25H15N1O1\LAHTI\29-Jun-2012\0\\
#P GFINPUT IOP(6/7=3) DIRECT TEST pop=nboread m062x/6-311G(d,p)\\CzFO
with Truhlar functional opt\\0,1\H,0,-1.1940923997,-1.4433063994,-0.37
93004806\C,0,-0.5413139374,-0.6379382975,-0.697461849\C,0,1.1036954283
,1.495768951,-1.5477108551\C,0,-0.3371064905,-0.3722788659,-2.03446883
07\C,0,0.1106383867,0.1753537513,0.2368895889\C,0,0.9276769354,1.22423
15443,-0.1910488431\C,0,0.4692550547,0.6843333146,-2.4733977697\C,0,-0
.9015277927,-1.0844496206,-3.2321158296\N,0,-0.0525006949,-0.066453128
6,1.6185973041\H,0,1.4375600047,1.821293968,0.5560171577\C,0,0.4638854
081,0.7006532488,-3.9570841796\H,0,1.7412253646,2.3154772326,-1.857515
8411\C,0,0.0918746385,0.2568615275,-6.673611569\C,0,-0.3477418862,-0.3
456131073,-4.4135337096\C,0,1.0957678644,1.5350104133,-4.8632597727\C,
0,0.8999787884,1.2991437818,-6.226894497\C,0,-0.5458857917,-0.58318609
78,-5.7592226902\O,0,-1.6328530853,-2.0376713768,-3.2357678309\H,0,1.7
270980619,2.3516778621,-4.5331083459\H,0,1.3875066001,1.9404782019,-6.

9517078314\H,0,-1.1794702509,-1.401787227,-6.0808280504\C,0,0.14114754
94,-1.2924571178,2.2548494917\C,0,-0.3987419127,0.8826009927,2.5792893
345\C,0,-1.0702356953,2.3500996405,4.8249261435\C,0,-0.7217329773,2.22
97227946,2.4196385408\C,0,-0.4299550759,0.26070473,3.8439233398\C,0,-0
.7660644062,1.0064425491,4.9730457852\C,0,-1.0528482416,2.948828782,3.
5582877733\H,0,-0.7265793999,2.6962225902,1.4425569923\H,0,-0.79222136
88,0.5383785593,5.9503440656\H,0,-1.3075302462,3.9974884885,3.46227817
65\C,0,0.4352357223,-3.4450809228,3.9639868878\C,0,-0.0867956484,-1.13
05941071,3.6361949725\C,0,0.5368881883,-2.5162696025,1.7171449903\C,0,
0.6760777882,-3.5842728307,2.5906849703\C,0,0.0592461442,-2.2210495423
,4.4930796433\H,0,0.7383496588,-2.6314796044,0.6596748046\H,0,0.980887
7403,-4.5472622158,2.1992568492\H,0,-0.1153017138,-2.1082164644,5.5569
624143\H,0,-0.0402040564,0.0996595736,-7.737049741\H,0,0.5509120675,-4
.3019231652,4.61574853\H,0,-1.332204323,2.9438571958,5.691710761\\Vers
ion=EM64L-G09RevB.01\State=1-A\HF=-1091.524386\RMSD=5.614e-09\Dipole=0
.8288403,1.0438935,-0.5791738\Quadrupole=-11.3817681,-0.0897813,11.471
5494,-0.0504458,-5.9444684,-6.5938249\PG=C01 [X(C25H15N1O1)]\\@

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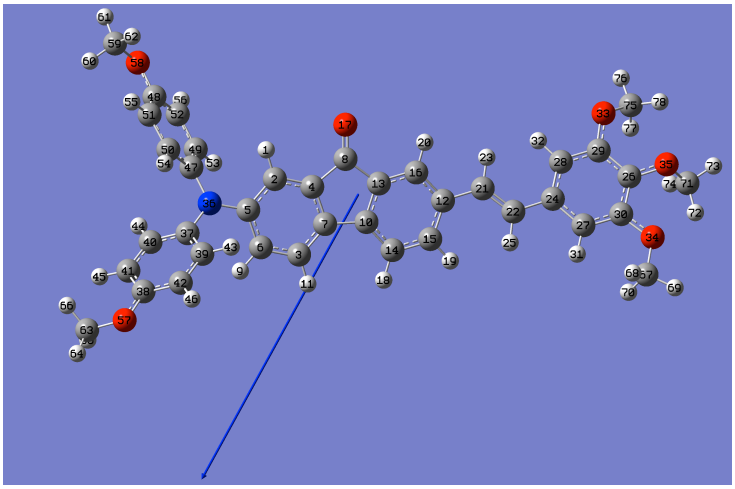
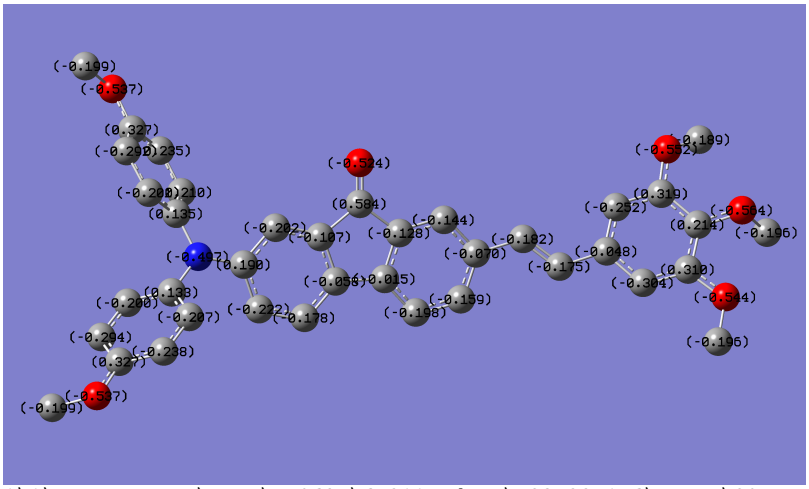


Compound **5**, M06-2X/6-311G(d,p), Dipole moment vector (above), NBO populations (below)



1\1\GINC-SKYNET\FOpt\RM062X\6-311G(d,p)\C38H33N1O6\LAHTI\30-Jun-2012\0
 \\#P GFINPUT IOP(6/7=3) DIRECT TEST OPT m062x/6-311G(d,p)\\DPAFO with
 Truhlar functional opt\\0,1\H,2.8853773872,-1.4778837094,0.8405943948\
 C,2.5827724676,-0.5818872572,0.3106651959\C,1.7368536677,1.7450149727,
 -1.0370605816\C,1.2496864958,-0.2814611689,0.1533456668\C,3.5359921364
 ,0.2993762725,-0.2348370476\C,3.0926417782,1.4518333763,-0.9029930205\

C,0.8027670951,0.8684776405,-0.5105472038\C,0.0566563208,-1.0606417884
,0.6309248938\H,3.8288840792,2.1228436183,-1.3282360035\C,-0.676573450
9,0.8789855278,-0.4984228193\H,1.433349963,2.6432200092,-1.5629789186\
C,-3.4193867459,0.3584712739,-0.1856480364\C,-1.129187813,-0.262530119
8,0.1753061945\C,-1.6023426066,1.7677079306,-1.0259280541\C,-2.9588888
564,1.4940991771,-0.8691082763\C,-2.4695387333,-0.5353968063,0.3365916
387\O,0.0540358298,-2.0969311812,1.2400442686\H,-1.2861581628,2.653453
4378,-1.564963167\H,-3.6790767632,2.1737017675,-1.3097201163\H,-2.7812
931256,-1.4319337309,0.8632735251\C,-4.8441286882,0.0559756741,-0.0080
190068\C,-5.8681412825,0.8945149838,-0.2091293137\H,-5.0528552142,-0.9
499772493,0.3462832022\C,-7.2898888059,0.5651866237,-0.0399810663\H,-5
.6651903668,1.9227924255,-0.4976111\C,-10.0272141973,0.0251178968,0.31
29018821\C,-8.2177388843,1.6151350482,0.0177833689\C,-7.7464551965,-0.
7441634991,0.0571098108\C,-9.1010756062,-1.0193162747,0.229265296\C,-9
.5680992291,1.3496018673,0.2033081908\H,-7.8615862553,2.6338154272,-0.
0580075605\H,-7.0788925083,-1.5920139624,-0.0198964355\O,-9.4353850224
,-2.3291633438,0.3573327522\O,-10.5270846723,2.304795178,0.3239238663\
O,-11.3377186768,-0.2483325233,0.5795924171\N,4.9058784894,0.026793677
4,-0.1118350742\C,5.8562825087,1.0834435381,-0.1006206789\C,7.74370156
2,3.1508729269,-0.0555251958\C,5.6853673315,2.1831631466,0.7480250182\
C,6.9805361455,1.032992914,-0.9160295148\C,7.9296693796,2.0524169225,-
0.8915953808\C,6.6108048417,3.2086992433,0.7621255156\H,4.8131871414,2
.2262785881,1.3905735405\H,7.1214453247,0.1805540822,-1.5706226675\H,8
.7959544534,1.9773493449,-1.5346871825\H,6.4911872742,4.0660879976,1.4
125237541\C,5.3776791565,-1.3128899033,-0.0568733907\C,6.3405006587,-3
.9410961427,0.0368503944\C,4.8761647627,-2.2857686053,-0.9294938678\C,
6.3663066587,-1.6728364178,0.8513408517\C,6.8582519736,-2.9747700569,0
.8968771997\C,5.342322315,-3.5850558635,-0.8740186055\H,4.1091597538,-
2.0143777337,-1.6458045246\H,6.763921772,-0.9225318004,1.5251339195\H,
7.6310655573,-3.2184971731,1.612961677\H,4.9567400429,-4.3492632356,-1
.5372293008\O,8.5972737172,4.2027507951,0.0390903558\O,6.7380506969,-5
.2391230318,0.0051262695\C,7.7158543405,-5.6438578764,0.9387279481\H,8
.6565206649,-5.1032661967,0.7895909642\H,7.8788093376,-6.7049263152,0.
7647893766\H,7.3689806555,-5.4929727422,1.9662217919\C,9.7429277951,4.
1894521429,-0.7850726253\H,10.2800623323,5.1102649723,-0.5702062239\H,
9.4691383531,4.1667562775,-1.8449877982\H,10.3859722104,3.3327552278,-
0.5576048218\C,-10.1133810503,3.6550792283,0.2967195418\H,-9.403659832
9,3.866066112,1.1023304925\H,-11.0137945624,4.2471796789,0.4434211049\
H,-9.6604893443,3.9122908663,-0.6661613781\C,-12.2710839197,0.10855529
66,-0.4355468561\H,-12.4065500975,1.1886696628,-0.4808300944\H,-13.210
9004159,-0.3719438154,-0.1662861763\H,-11.9386271561,-0.2611887947,-1.
4110828566\C,-10.6231420878,-2.8027438973,-0.2634938278\H,-10.47084976
21,-3.8702053576,-0.4177332779\H,-10.7725830025,-2.3186799985,-1.23366
37743\H,-11.4957723325,-2.6379651981,0.367416542\\Version=EM64L-G09Rev
B.01\State=1-A\HF=-1973.6369072\RMSD=7.965e-09\RMSF=3.110e-06\Dipole=1
.0218551,1.5229878,-1.289723\Quadrupole=41.0792613,-11.1304192,-29.948
8421,-13.6364468,13.7175061,-4.7818128\PG=C01 [X(C38H33N1O6)]\\@

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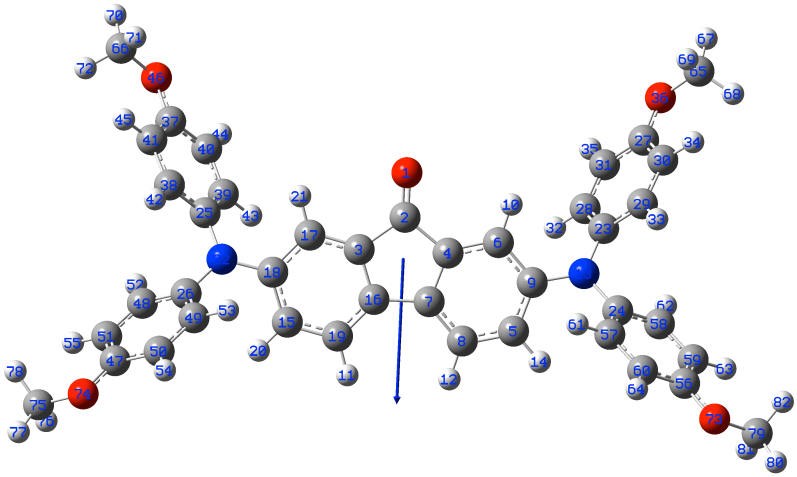
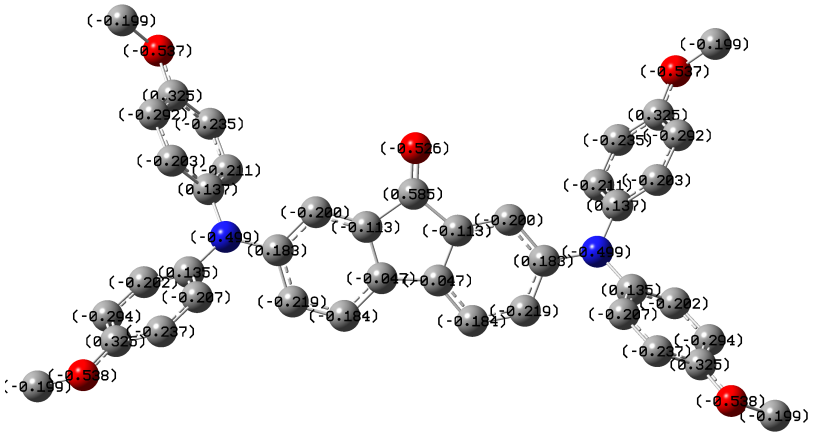


Compound **6**, M06-2X/6-311G(d,p), Dipole moment vector (above), NBO populations (below)



1\1\GINC-SKYNET\SP\RM062X\6-311G(d,p)\C41H34N2O5\LAHTI\29-Jun-2012\0\\
#P GFINPUT IOP(6/7=3) DIRECT TEST pop=nboread m062x/6-311G(d,p) guess=
read geom=check\\BDAAFO with Truhlar functional opt\\0,1\O,0,-2.046670
984,1.1191197987,0.0000000037\C,0,-0.9802523229,0.5640550051,0.0000000
018\C,0,-0.1680367563,0.1398177165,1.1903218696\C,0,-0.1680367607,0.13
98177165,-1.190321869\C,0,1.6340708738,-0.800056046,-3.029235789\C,0,-
0.4645910082,0.2964032416,-2.5252408518\C,0,1.0131238746,-0.4645139841
,-0.7397577855\C,0,1.9243248294,-0.9320118378,-1.6721024483\C,0,0.4524
652032,-0.1896481067,-3.4752842097\H,0,-1.3852850929,0.7807154874,-2.8
306011625\H,0,2.8480075475,-1.410408474,1.366672894\H,0,2.8480075425,-
1.410408474,-1.3666729044\N,0,0.1872193484,-0.0640804597,-4.8494718488
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