Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Content:

Table S1-1. Photophysical parameters of B1 upon various solvents.

solvent (polarity)	λ_{abs} (nm)	λ_{em} (nm)	FWHM(nm)	Φ	τ (ns)
Hexane (0.06)	570	N/A	N/A	N/A	N/A
Toluene (2.4)	574	N/A	N/A	N/A	N/A
CH_2Cl_2 (3.4)	577	N/A	N/A	N/A	N/A
THF (4.2)	573	N/A	N/A	N/A	N/A
MeCN (6.2)	568	N/A	N/A	N/A	N/A

Table S1-2. Photophysical parameters of B2 upon various solvents.

solvent (polarity)	λ_{abs} (nm)	λ_{em} (nm)	FWHM(nm)	Φ	τ (ns)
Hexane (0.06)	755	N/A	N/A	N/A	N/A
Toluene (2.4)	760	N/A	N/A	N/A	N/A
CH_2Cl_2 (3.4)	767	788	24.2	<0.01	N/A
THF (4.2)	762	N/A	N/A	N/A	N/A
MeCN (6.2)	764	N/A	N/A	N/A	N/A

Table S1-3. Photophysical parameters of B3 upon various solvents.

solvent (polarity)	λ_{abs} (nm)	λ_{em} (nm)	FWHM(nm)	Φ	τ (ns)
Hexane (0.06)	762	N/A	N/A	N/A	N/A
Toluene (2.4)	769	N/A	N/A	N/A	N/A
CH_2Cl_2 (3.4)	780	793	24.8	0.02	3.2
THF (4.2)	773	796	25.0	<0.01	N/A
MeCN (6.2)	775	N/A	N/A	N/A	N/A

Table S1-4. Photophysical parameters of B4 upon various solvents.

solvent (polarity)	λ_{abs} (nm)	λ_{em} (nm)	FWHM(nm)	Φ	τ^a (ns)
Hexane (0.06)	611	624	22.0	0.79	29.4
Toluene (2.4)	617	629	21.2	0.97	35.8
CH_2Cl_2 (3.4)	626	648	21.8	0.99	36.4
THF (4.2)	620	645	23.0	0.85	31.1
MeCN (6.2)	619	646	23.6	0.77	28.5

a, fitted with single exponential decay equation $y=y_0+c*e^{(-x/t)}$

Table S1-5. Photophysical parameters of B5 upon various solvents.

solvent (polarity)	λ_{abs} (nm)	λ_{em} (nm)	FWHM(nm)	Φ	τ^a (ns)
Hexane (0.06)	611	625	22.6	0.69	24.5
Toluene (2.4)	619	631	23.5	0.94	33.1
CH_2Cl_2 (3.4)	621	636	22.0	0.97	34.9
THF (4.2)	618	632	25.0	0.81	29.4

MeCN (6.2)	614	635	24.6	0.62	22.0

a, fitted with single exponential decay equation $y=y_0+c*e^{(-x/t)}$

Figure S1-1. Absorption spectra of B1 upon various solvents.

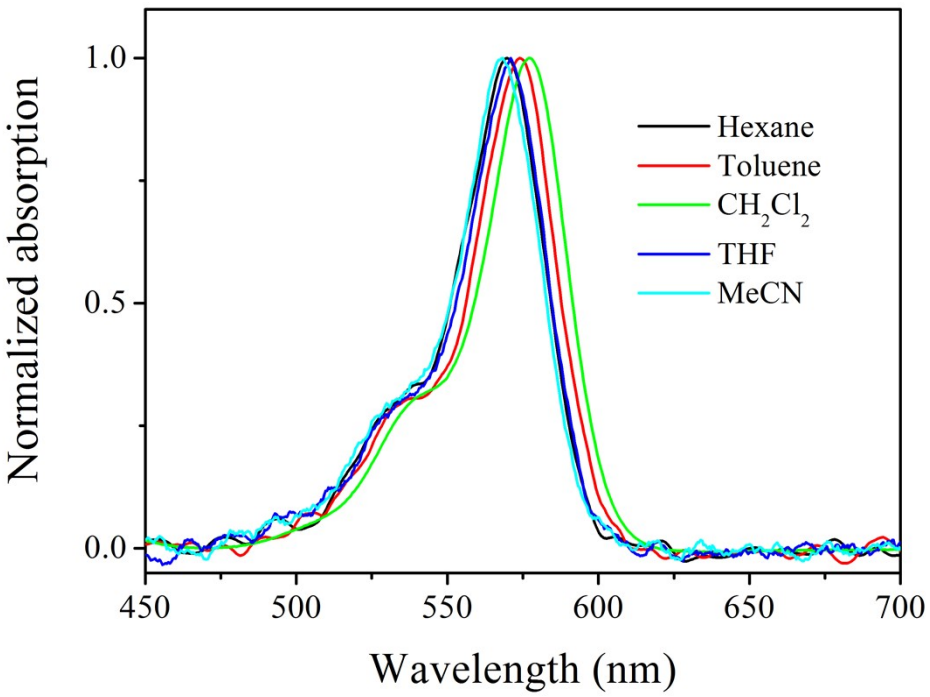


Figure S1-2. Absorption spectra of B2 upon various solvents.

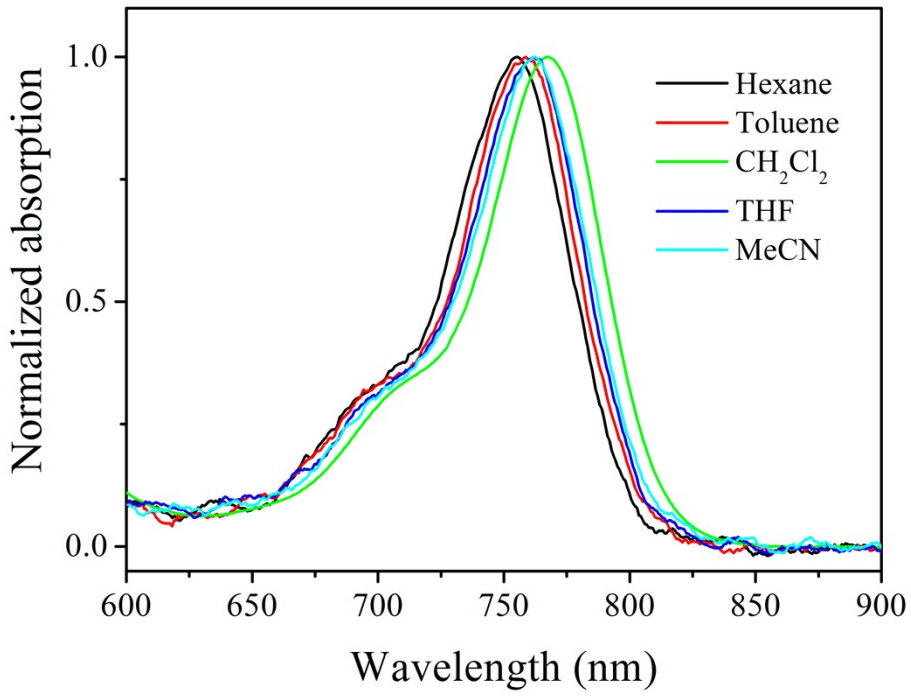


Figure S1-3. Absorption spectra of B3 upon various solvents.

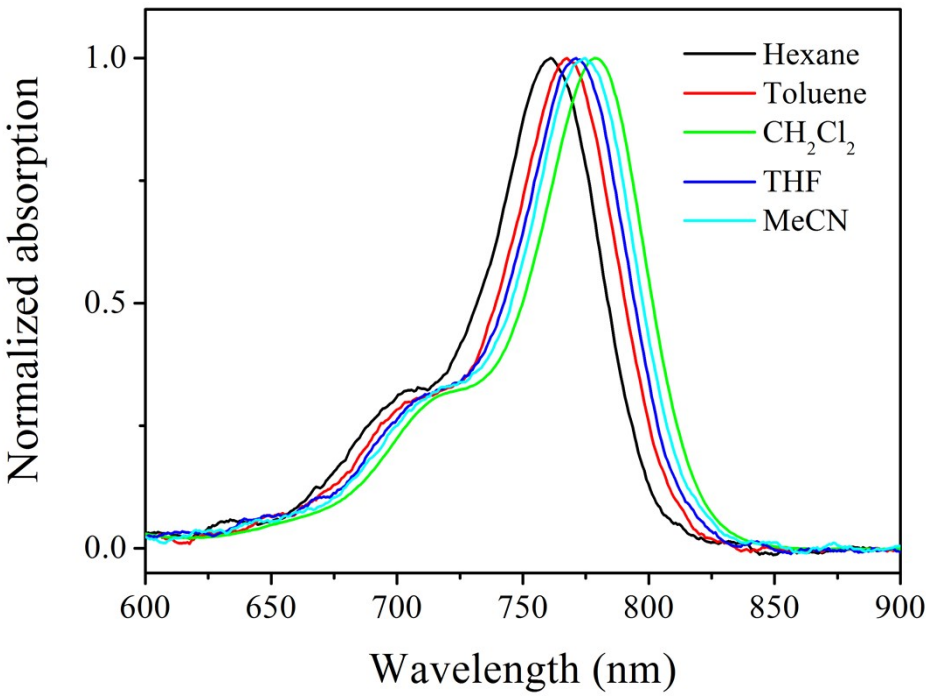


Figure S1-4. Absorption spectra of B4 upon various solvents.

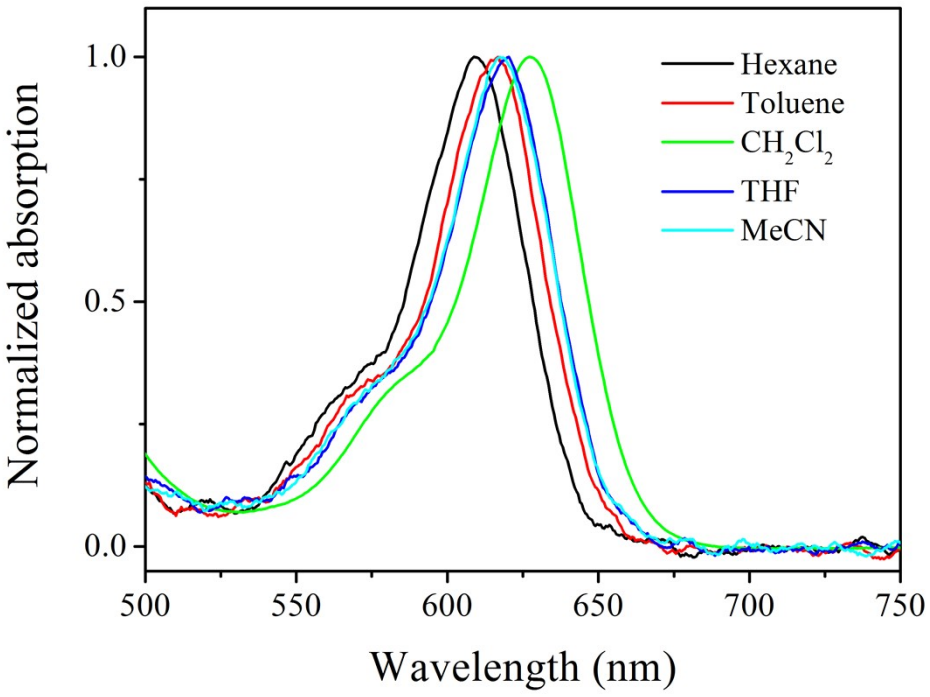


Figure S1-5. Absorption spectra of B5 upon various solvents.

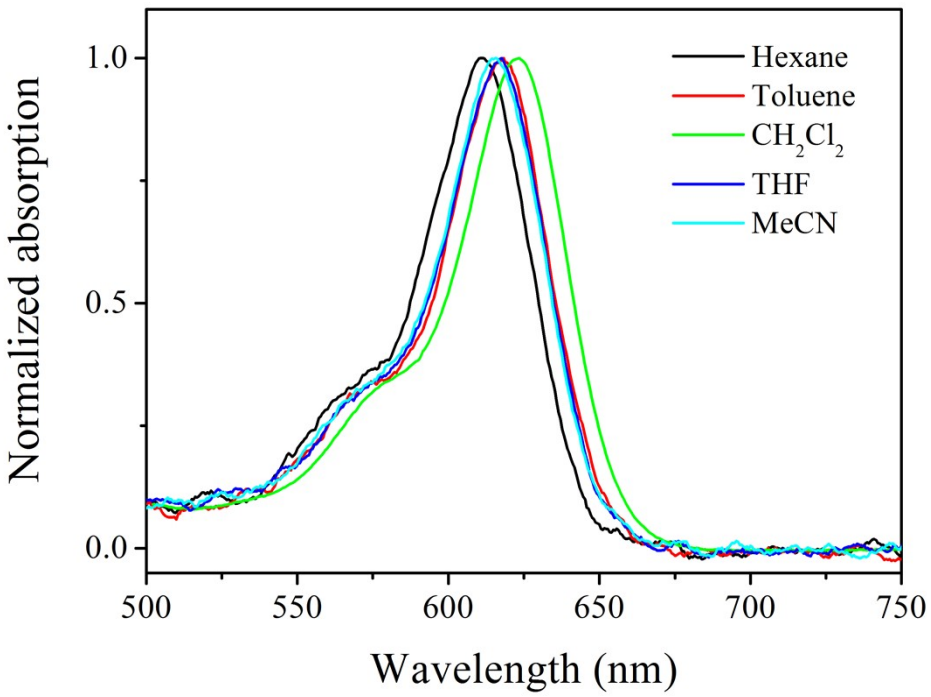


Figure S2-1. Emission spectra of B3 upon various solvents.

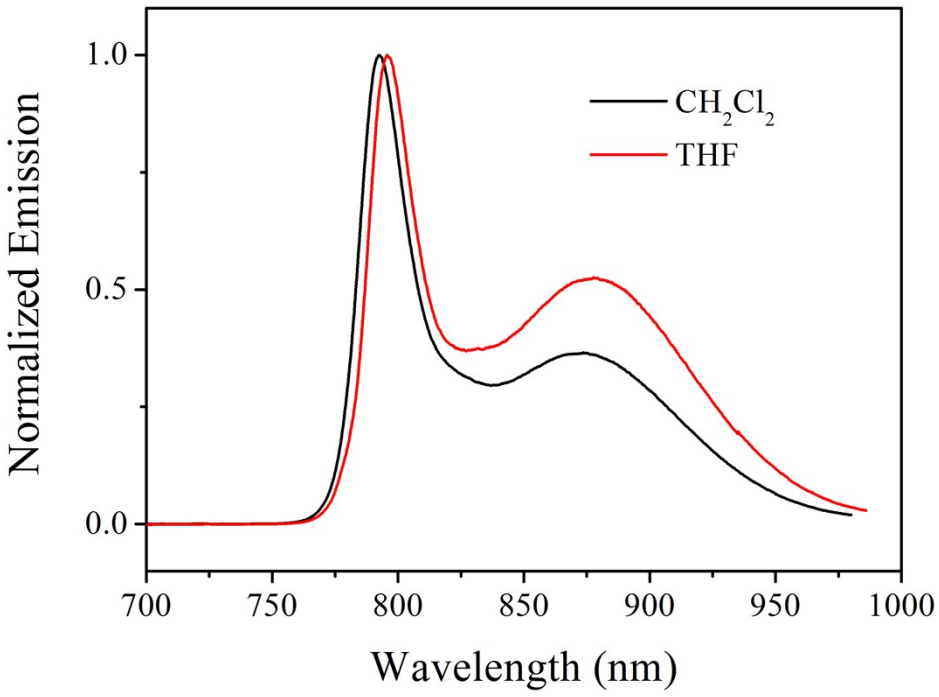


Figure S2-2. Emission spectra of B4 upon various solvents.

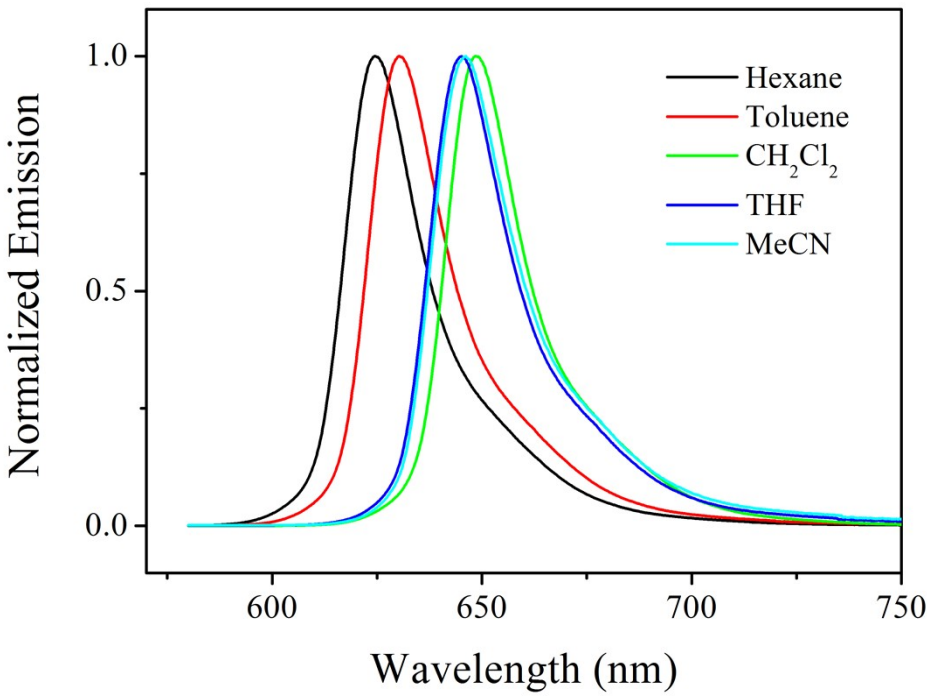


Figure S2-3. Emission spectra of B5 upon various solvents.

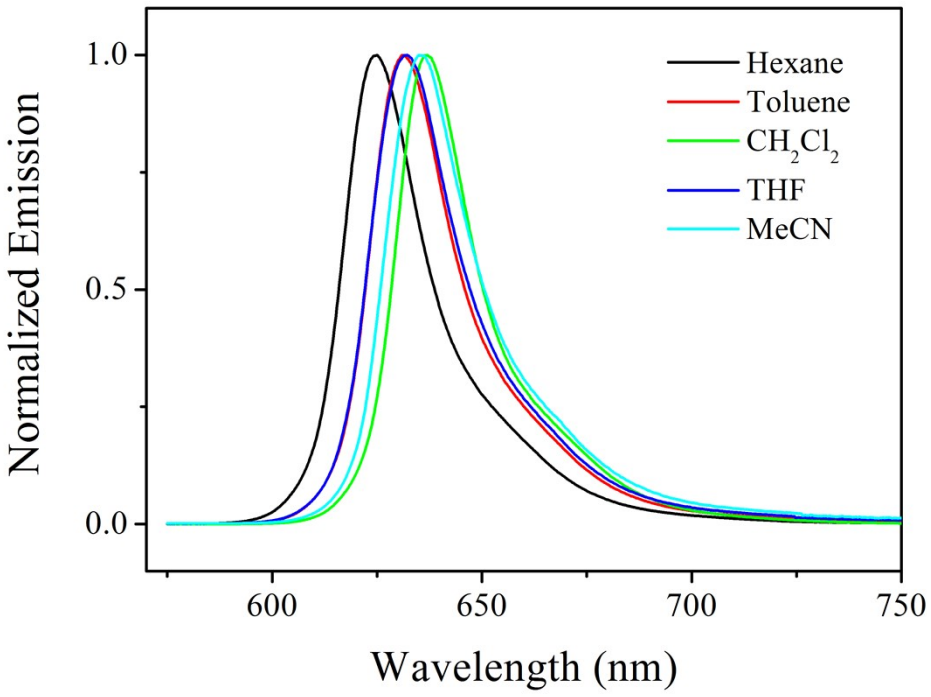


Table S2. OPA ($S_0 \rightarrow S_n$) and TPA ($TPA_{m,n}$) values of B1, B2, B4, and B5 calculated by TD-DFT at B3LYP/6-31G(d) level in vacuum. m and n denote state. See Supporting Information for a detailed result.

Transition	B1 energy (eV)	B1 oscillator strength	B2 energy (eV)	B2 oscillator strength	B4 energy (eV)	B4 oscillator strength	B5 energy (eV)	B5 oscillator strength
$S_0 \rightarrow S_1$	2.701	0.5304	1.880	0.3171	2.413	0.7787	2.420	0.3566
$S_0 \rightarrow S_2$	2.813	0.0074	2.175	0.0240	2.800	0.0966	2.453	0.4878
$S_0 \rightarrow S_3$	2.941	0.0453	2.217	0.6791	2.836	0.0271	2.753	0.0713
$S_0 \rightarrow S_4$	3.224	0.0118	2.801	0.0153	3.023	0.0091	2.885	0.0725
$S_0 \rightarrow S_5$	3.249	0.0031	3.064	0.0080	3.181	0.0361	3.117	0.0076
$TPA_{1,2}$	0.112	0.0115	0.295	0.2182	0.387	0.0272	0.033	0.0130
$TPA_{1,3}$	0.241	0.0181	0.336	0.0011	0.423	0.0847	0.333	0.0174
$TPA_{1,4}$	0.523	0.0098	0.920	0.4828	0.610	0.2121	0.465	0.0347
$TPA_{1,5}$	0.549	0.0095	1.184	0.0203	0.768	0.0453	0.697	0.0987
$TPA_{2,3}$	0.129	0.0867	0.042	0.0120	0.036	0.0270	0.300	0.0059
$TPA_{2,4}$	0.411	0.0017	0.626	0.0071	0.223	0.0296	0.432	0.0585
$TPA_{2,5}$	0.437	0.0014	0.889	0.0201	0.380	0.0171	0.664	0.1017
$TPA_{3,4}$	0.282	0.0011	0.584	0.3449	0.187	0.0032	0.132	0.1169
$TPA_{3,5}$	0.308	0.0005	0.848	0.0010	0.344	0.0123	0.364	0.0408
$TPA_{4,5}$	0.026	0.0073	0.264	0.0116	0.158	0.1782	0.233	0.0058

Emission decay fitting of B3.

B3 needed more explanation words to explain its decay behavior as follows. We tried three exponential decay equations to fit the decay data of B3 (first order, second order, and third order). As shown in Figure S1, the first order fitting (corresponding to mono-exponential) within 26-200 ns showed a bad R^2 value of 0.8843. The second order fitting (corresponding to bi-exponential) within 26-200 ns showed an R^2 value of 0.98357. The third order fitting (corresponding to tri-exponential) within 26-200 ns showed an R^2 value of 0.98778. The τ1 (2.87988 ns) and τ2 (2.87897 ns) values for the third order fitting were rather similar to each other. So, the tri-exponential decay was degraded as bi-exponential decay. Thus, the second order fitting should be good enough to fit B3 decay data. On the other hand, the calculated weighted mean lifetime of B3 $[=(A_1\tau1^2+ A_2\tau2^2)/(A_1\tau1+ A_2\tau2)]$ was only 3.2 ns. This short lifetime compared to those of B4 (36.4 ns) and B5 (34.9 ns) was clearly inconsistent with their comparable decay curves, especially within decay region of 30-200 ns. We found sharp intensity decrease for B3 within decay region of 26-30 ns, but after 30 ns, B3 tended to follow a mono-exponential decay, and this statement was supported by the first order fitting of B3 within 30-200 ns (starting from 30 ns, not 26 ns). An R^2 value of 0.987 was observed. Thus, we stated in the manuscript that this sharp intensity decrease was caused by either geometric relaxation in excited state or energy transfer to the secondary emissive centre peaking at 876 nm. And the geometric relaxation in excited state is assumed as the major factor considering the low emission quantum yield of B3 (0.02).

Figure S3-1. Decay data of B3 and its mono-exponential decay within 26-200 ns.

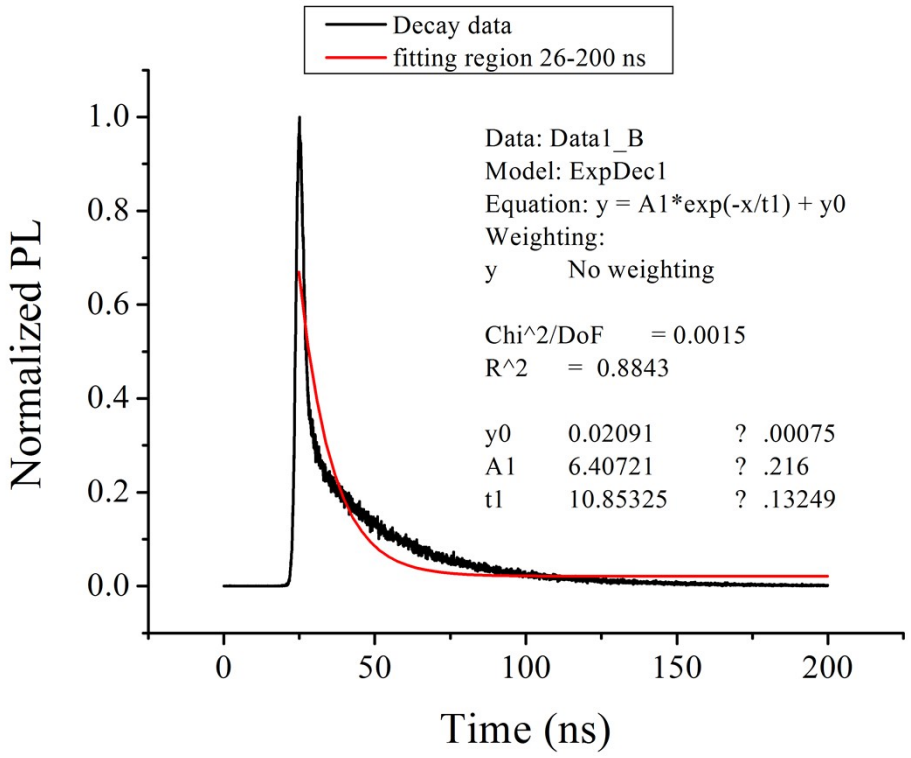


Figure S3-2. Decay data of B3 and its bi-exponential decay within 26-200 ns. The weighted mean lifetime was calculated by $[(A_1\tau1^2+ A_2\tau2^2)/(A_1\tau1+ A_2\tau2)]$=3.2 ns

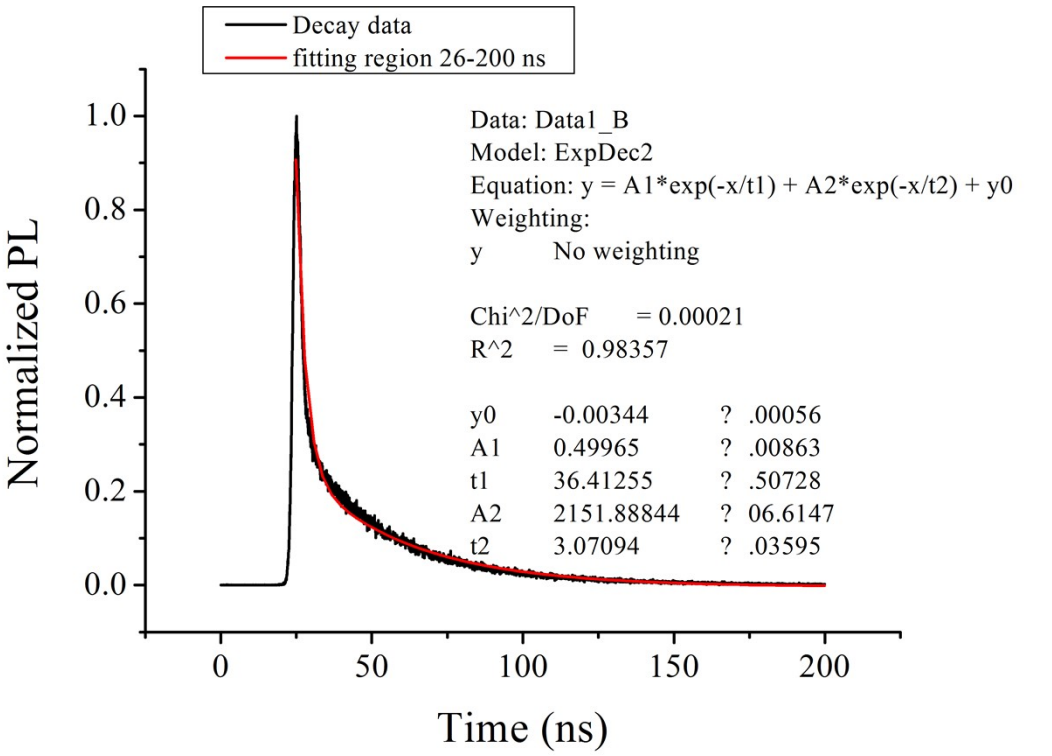


Figure S3-3. Decay data of B3 and its tri-exponential decay within 26-200 ns. τ1 (2.87988)≈τ2 (2.87897). So, the tri-exponential decay is degraded as bi-exponential decay.

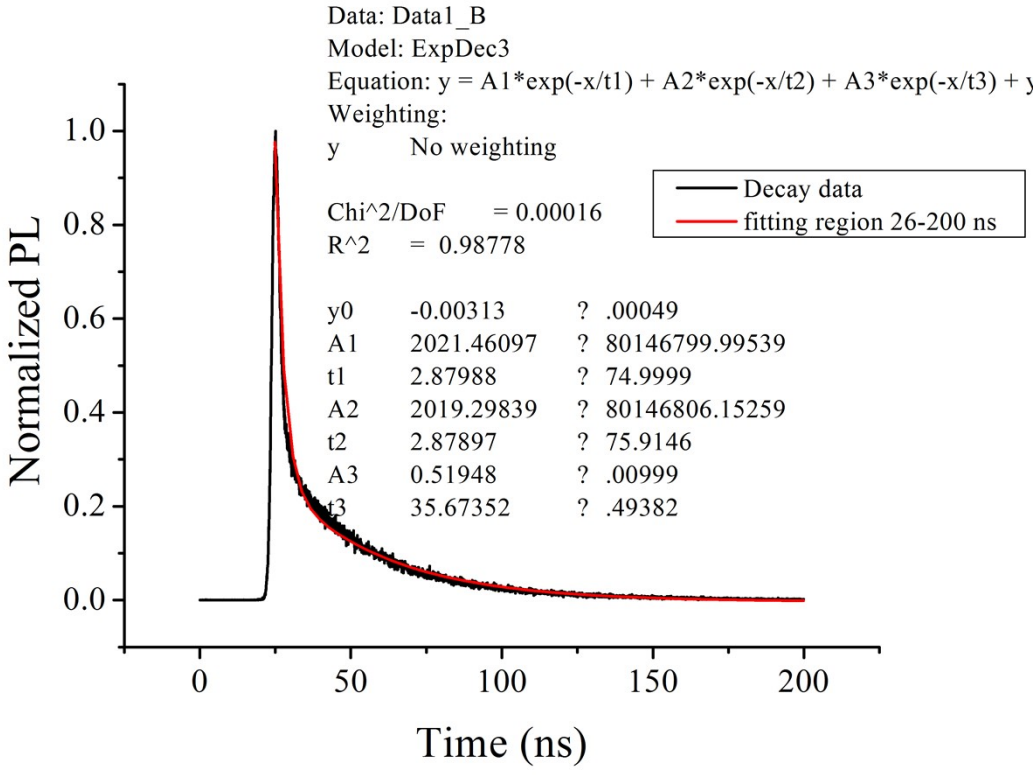


Figure S3-4. Decay data of B3 and its mono-exponential decay within 30-200 ns (starting from 30 ns, not 26 ns).

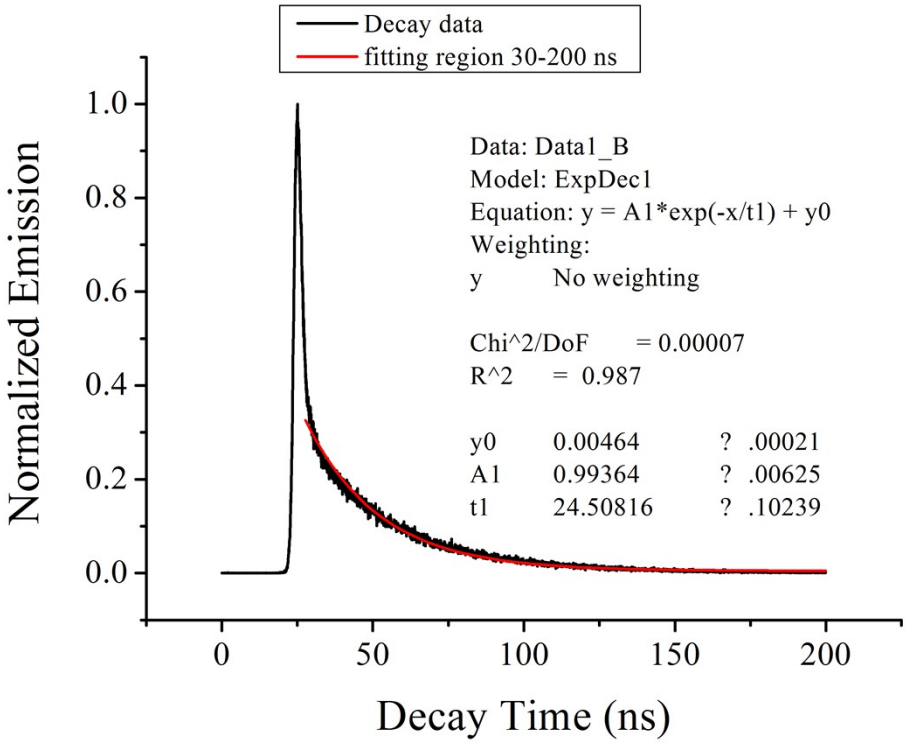


Figure S4. Decay data of B4 and its mono-exponential decay within 26-200 ns.

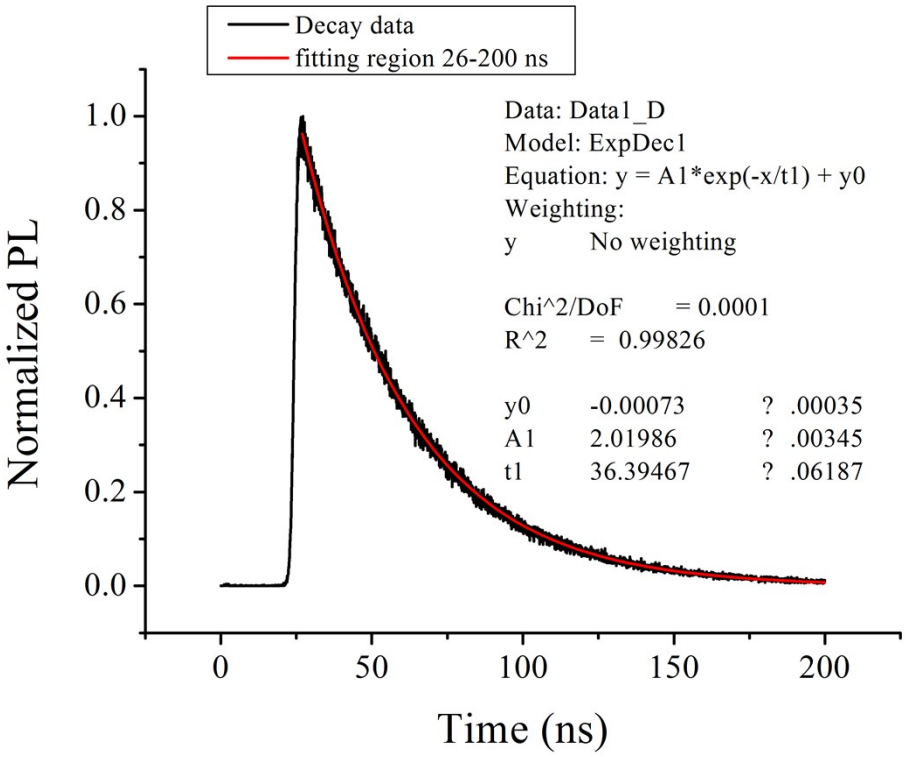
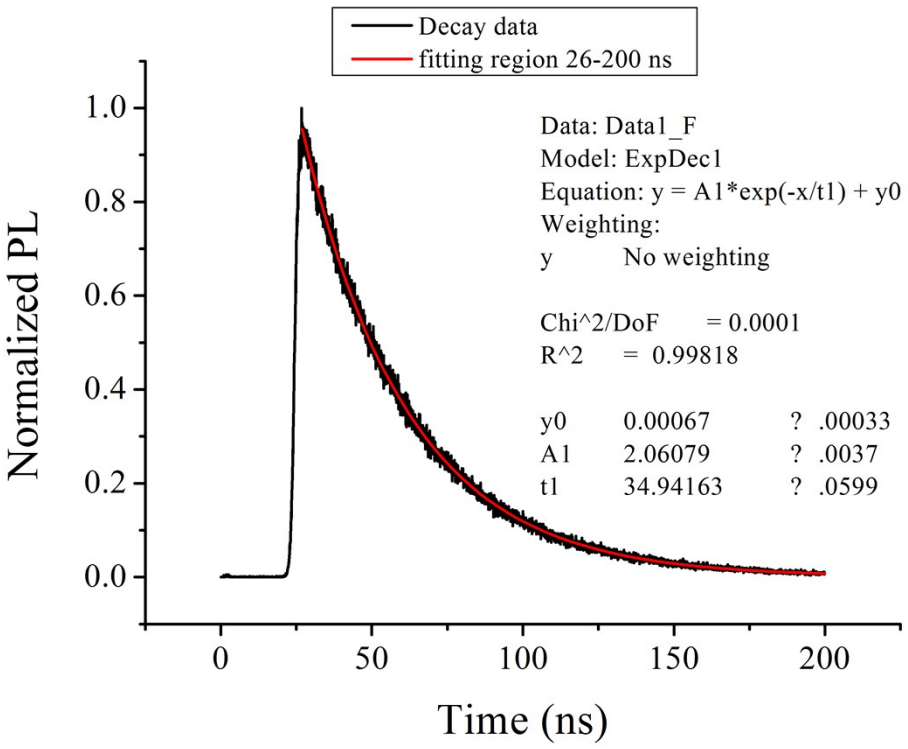
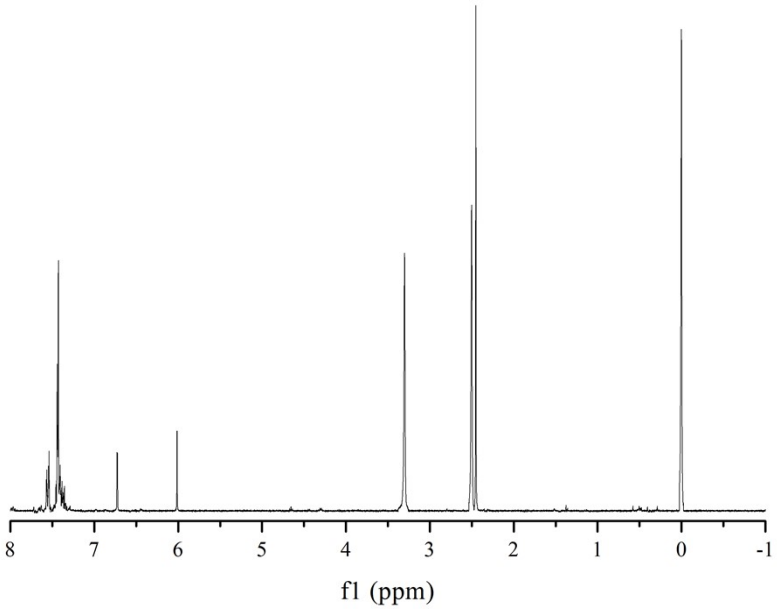


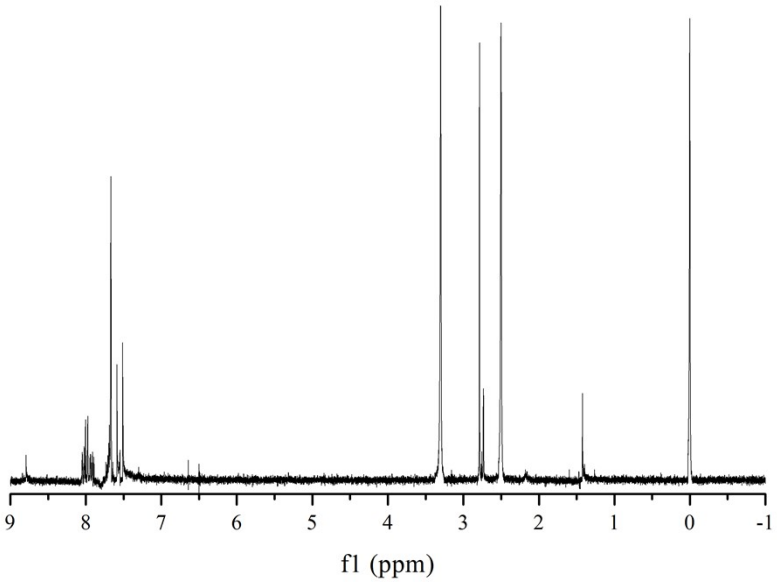
Figure S5. Decay data of B5 and its mono-exponential decay within 26-200 ns.



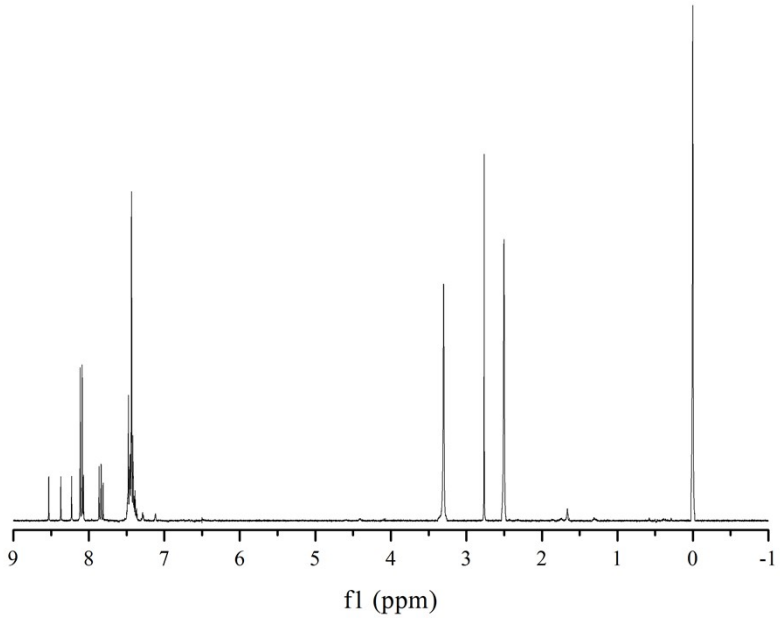
^{1}HNMR of B1



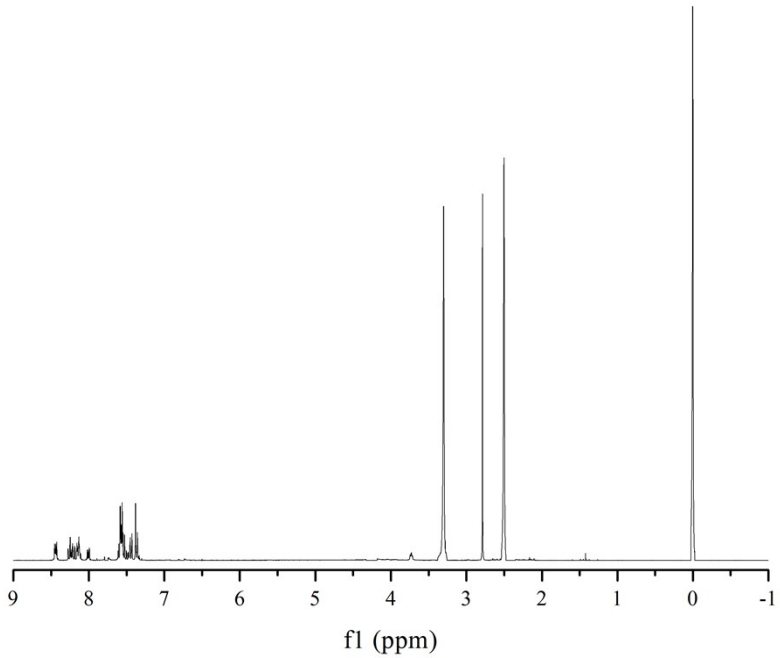
^{1}HNMR of B2



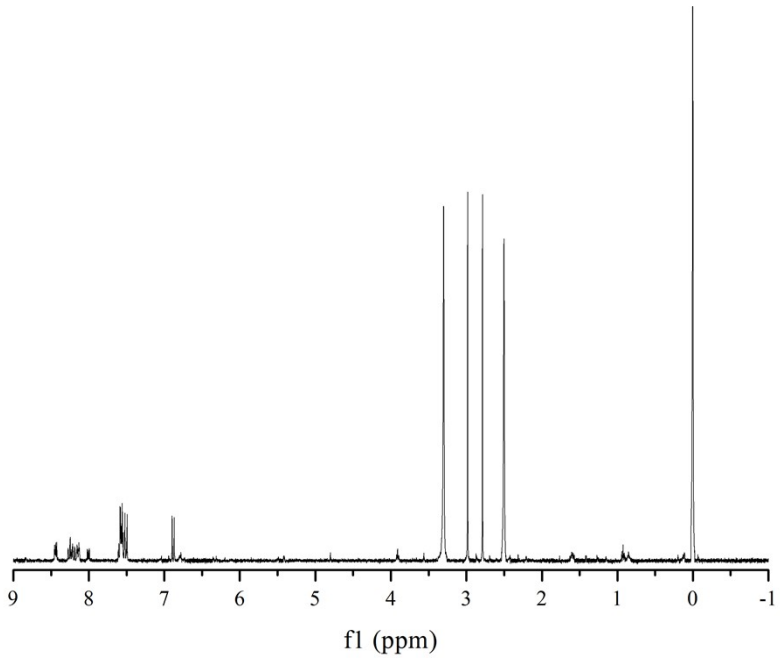
^{1}HNMR of B3



^{1}HNMR of B4



^{1}HNMR of B5



One photon absorption (OPA) and two photon absorption (OPA) TD-DFT calculation result of B1, B2, B4, and B5 calculated at RB3LYP/6-31G(d) level.

Result of B1

SINGLET EXCITATIONS

STATE # 1 ENERGY = 2.700529 EV
OSCILLATOR STRENGTH = 0.530411
LAMBDA DIAGNOSTIC = 0.721 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

		EXCITATION	DE-EXCITATION
OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
107	114	-0.034497	-0.006454
108	114	0.146488	0.016780
110	114	0.067616	0.008450
112	114	-0.227489	-0.005894
113	114	0.968840	-0.183809
111	115	0.031960	0.008054
108	120	-0.033964	-0.017962
112	120	-0.039827	-0.013981

STATE # 2 ENERGY = 2.812749 EV
OSCILLATOR STRENGTH = 0.007427
LAMBDA DIAGNOSTIC = 0.471 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

		EXCITATION	DE-EXCITATION
OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
108	114	0.104815	-0.013550
111	114	0.101549	0.000034
112	114	0.963197	-0.023863
113	114	0.214974	-0.048232

STATE # 3 ENERGY = 2.941398 EV
OSCILLATOR STRENGTH = 0.045295
LAMBDA DIAGNOSTIC = 0.422 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

		EXCITATION	DE-EXCITATION

OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
111	114	0.991629	-0.017013
112	114	-0.104812	0.004808

STATE # 4 ENERGY = 3.223681 EV
OSCILLATOR STRENGTH = 0.011829
LAMBDA DIAGNOSTIC = 0.184 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

		EXCITATION	DE-EXCITATION
OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
110	114	-0.996076	0.002597
113	114	0.068702	-0.021804

STATE # 5 ENERGY = 3.249410 EV
OSCILLATOR STRENGTH = 0.003084
LAMBDA DIAGNOSTIC = 0.177 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

		EXCITATION	DE-EXCITATION
OCC	VIR	AMPLITUDE	AMPLITUDE
I	A	X(I->A)	Y(A->I)
109	114	-0.998021	0.002341

SUMMARY OF TDDFT RESULTS

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE, A.U.			OSCILLATOR
0 ->	HARTREE	EV	X	Y	Z	STRENGTH
0 A	-1558.2931267666	0.000				
1 A	-1558.1938841329	2.701	-2.6379	-0.9475	-0.4004	0.5304
2 A	-1558.1897601348	2.813	-0.3119	0.1016	0.0142	0.0074
3 A	-1558.1850323609	2.941	0.2630	-0.7441	-0.0752	0.0453
4 A	-1558.1746586681	3.224	-0.3841	-0.0417	-0.0222	0.0118
5 A	-1558.1737131339	3.249	0.0892	0.1476	0.0948	0.0031

TRANSITION	EXCITATION	TRANSITION DIPOLE, A.U.			OSCILLATOR
	EV	X	Y	Z	DIP STRENGTH
1 -> 2	0.112	0.1484	-2.0156	-0.2999	2.0432 0.0115
1 -> 3	0.241	1.6818	0.3788	0.2994	1.7497 0.0181
1 -> 4	0.523	0.6768	-0.5482	0.0716	0.8739 0.0098

1	->	5	0.549	0.6340	0.5443	0.0978	0.8413	0.0095
2	->	3	0.129	-4.9710	-1.4681	-0.8029	5.2451	0.0867
2	->	4	0.411	0.3857	-0.0897	-0.1061	0.4099	0.0017
2	->	5	0.437	0.2443	0.2117	0.1687	0.3646	0.0014
3	->	4	0.282	-0.3778	0.0415	-0.1363	0.4037	0.0011
3	->	5	0.308	0.1162	0.2154	-0.0758	0.2562	0.0005
4	->	5	0.026	-3.1949	-0.9996	-0.5701	3.3959	0.0073

SELECTING EXCITED STATE 1 E= -1558.1938841329 AS THE STATE OF INTEREST.

..... DONE WITH TD-DFT EXCITATION ENERGIES .....
STEP CPU TIME = 4891.00 TOTAL CPU TIME = 6601.1 (110.0 MIN)
TOTAL WALL CLOCK TIME= 6840.0 SECONDS, CPU UTILIZATION IS 96.51%

TWO-PHOTON ABSORPTION (TPA) CALCULATIONS (A.U.):

EXCITED STATE # 1

SUBCOMPONENT 1 HAS CONVERGED: 17 9.7276E-05
SUBCOMPONENT 2 HAS CONVERGED: 19 5.5282E-05
SUBCOMPONENT 3 HAS CONVERGED: 17 2.2674E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 3.1131
S(2,1) = -10.1103
S(2,2) = -15.2544
S(3,1) = -4.0790
S(3,2) = -5.5146
S(3,3) = -1.7570

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 6.4387 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 18.1336 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 85.4118 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 95.9241 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.1231

EXCITED STATE # 2

SUBCOMPONENT 1 HAS CONVERGED: 17 9.1415E-05
SUBCOMPONENT 2 HAS CONVERGED: 19 1.4188E-05
SUBCOMPONENT 3 HAS CONVERGED: 21 1.1052E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -32.8940
S(2,1) = 68.8766
S(2,2) = 66.4205
S(3,1) = 6.4941
S(3,2) = 19.4435
S(3,3) = 3.9191

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 46.7393 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 527.9165 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 2205.1447 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 3074.0205 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.3940

EXCITED STATE # 3

SUBCOMPONENT 1 HAS CONVERGED: 17 9.1971E-05
SUBCOMPONENT 2 HAS CONVERGED: 19 1.4630E-05
SUBCOMPONENT 3 HAS CONVERGED: 21 5.1747E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -87.0244
S(2,1) = 0.5663
S(2,2) = -67.2787
S(3,1) = -11.6376
S(3,2) = -12.3391
S(3,3) = -2.9558

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 824.3450 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 422.8139 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 3339.9454 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 888.1933 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 0.2659

EXCITED STATE # 4

SUBCOMPONENT 1 HAS CONVERGED: 17 1.0686E-04
SUBCOMPONENT 2 HAS CONVERGED: 17 2.2832E-04
SUBCOMPONENT 3 HAS CONVERGED: 19 2.9921E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -10.0708
S(2,1) = 2.0776
S(2,2) = 8.9211
S(3,1) = -6.3617

S(3,2) = 1.5432
S(3,3) = -1.2697

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 0.1951 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 9.2319 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 37.3179 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 55.0013 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.4739

EXCITED STATE # 5

SUBCOMPONENT 1 HAS CONVERGED: 17 1.0919E-04
SUBCOMPONENT 2 HAS CONVERGED: 17 2.2010E-04
SUBCOMPONENT 3 HAS CONVERGED: 19 2.5584E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -12.5773
S(2,1) = -11.3478
S(2,2) = 3.2977
S(3,1) = -0.9206
S(3,2) = 5.6457
S(3,3) = 2.2678

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 1.6388 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 16.5732 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 69.5703 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 96.1613 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.3822

..... DONE WITH TD-DFT TPA-CROSS SECTIONS .....

Result of B2

SINGLET EXCITATIONS

STATE # 1 ENERGY = 1.880200 EV
OSCILLATOR STRENGTH = 0.317060
LAMBDA DIAGNOSTIC = 0.706 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
129	138	0.033557	-0.004863
131	138	0.050387	0.021422
133	138	0.050147	0.014976
136	138	0.544473	-0.001967
137	138	0.839367	-0.127302
132	139	-0.030946	-0.009392
135	139	-0.034453	0.007043
136	140	0.039242	0.010541

STATE # 2 ENERGY = 2.174943 EV
OSCILLATOR STRENGTH = 0.024034
LAMBDA DIAGNOSTIC = 0.666 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
130	138	0.044629	0.002111
132	138	-0.057377	-0.011566
134	138	-0.058331	0.001496
135	138	-0.986359	0.043443
136	138	-0.085790	0.005002
137	138	0.034065	-0.007468

133	139	0.043993	0.009487
137	139	0.054194	0.000871
132	140	0.037946	0.008723
137	143	0.031486	0.015118

STATE # 3 ENERGY = 2.216666 EV
OSCILLATOR STRENGTH = 0.679085
LAMBDA DIAGNOSTIC = 0.673 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
---	---	--------	--------
131	138	-0.080400	-0.028373
135	138	-0.090066	0.005057
136	138	0.830110	-0.061149
137	138	-0.554284	0.122622
132	139	-0.030928	-0.008014
134	139	-0.042695	-0.004480
136	144	0.032090	0.012771

STATE # 4 ENERGY = 2.800600 EV
OSCILLATOR STRENGTH = 0.015278
LAMBDA DIAGNOSTIC = 0.640 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
---	---	--------	--------
132	138	0.031343	-0.000034
134	138	-0.955767	0.030776
135	138	0.068770	-0.002542
137	139	0.266763	0.030000
134	140	-0.037883	-0.006647
135	144	-0.037537	-0.013986

STATE # 5 ENERGY = 3.064317 EV
OSCILLATOR STRENGTH = 0.007988
LAMBDA DIAGNOSTIC = 0.498 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
---	---	--------	--------

129	138	0.037267	0.000241
131	138	0.221176	-0.001571
132	138	0.043130	-0.000890
133	138	-0.957566	0.016703
136	138	0.031732	-0.011380
135	139	0.096068	-0.001395
133	140	-0.030498	-0.011085
136	140	0.074777	-0.002265
137	140	0.033632	-0.004804
134	141	0.053001	0.016823
131	142	-0.032131	-0.011783
136	142	0.030875	0.006332
137	142	-0.067677	-0.012920

SUMMARY OF TDDFT RESULTS

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE, A.U.			OSCILLATOR
0 ->	HARTREE	EV	X	Y	Z	STRENGTH
0 A	-1862.9938604209	0.000				
1 A	-1862.9247643427	1.880	-0.0470	-0.5284	-2.5694	0.3171
2 A	-1862.9139327500	2.175	0.0742	-0.6638	-0.0705	0.0240
3 A	-1862.9123994559	2.217	0.0793	0.6865	3.4680	0.6791
4 A	-1862.8909402490	2.801	-0.0663	-0.4481	0.1321	0.0153
5 A	-1862.8812488530	3.064	-0.0088	0.0040	-0.3261	0.0080

TRANSITION	EXCITATION	TRANSITION DIPOLE, A.U.				OSCILLATOR
	EV	X	Y	Z	DIP	STRENGTH
1 -> 2	0.295	0.0928	1.1306	5.3789	5.4972	0.2182
1 -> 3	0.336	0.0418	-0.1400	0.3329	0.3636	0.0011
1 -> 4	0.920	-0.0956	-0.9529	-4.5268	4.6270	0.4828
1 -> 5	1.184	-0.0532	0.7916	-0.2666	0.8369	0.0203
2 -> 3	0.042	0.0640	0.7544	3.3385	3.4232	0.0120
2 -> 4	0.626	0.1185	-0.6544	-0.1451	0.6806	0.0071
2 -> 5	0.889	-0.0256	-0.2612	-0.9232	0.9598	0.0201
3 -> 4	0.584	0.1198	0.9810	4.8095	4.9100	0.3449
3 -> 5	0.848	0.0554	-0.1999	0.0856	0.2244	0.0010
4 -> 5	0.264	0.0278	0.2714	1.3092	1.3373	0.0116

SELECTING EXCITED STATE 1 E= -1862.9247643427 AS THE STATE OF INTEREST.

..... DONE WITH TD-DFT EXCITATION ENERGIES .....
STEP CPU TIME = 9445.17 TOTAL CPU TIME = 12172.9 (202.9 MIN)
TOTAL WALL CLOCK TIME= 12188.2 SECONDS, CPU UTILIZATION IS 99.87%

TWO-PHOTON ABSORPTION (TPA) CALCULATIONS (A.U.):

EXCITED STATE # 1

SUBCOMPONENT 1 HAS CONVERGED: 19 5.4712E-06
SUBCOMPONENT 2 HAS CONVERGED: 17 1.0334E-04
SUBCOMPONENT 3 HAS CONVERGED: 19 9.5578E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 0.5104
S(2,1) = 1.6790
S(2,2) = -21.4811
S(3,1) = 13.5525
S(3,2) = -49.1844
S(3,3) = 25.6299

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 0.7236 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 210.9928 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 845.4184 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 1264.5095 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.4957

EXCITED STATE # 2

SUBCOMPONENT 1 HAS CONVERGED: 19 6.0801E-06

SUBCOMPONENT 2 HAS CONVERGED: 19 9.2465E-05
SUBCOMPONENT 3 HAS CONVERGED: 19 1.6564E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -0.4552
S(2,1) = 0.4342
S(2,2) = 9.2525
S(3,1) = -0.8225
S(3,2) = -17.2556
S(3,3) = -82.5668

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 181.3976 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 250.0112 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 1362.8401 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 1137.2720 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 0.8345

EXCITED STATE # 3

SUBCOMPONENT 1 HAS CONVERGED: 19 6.2608E-06
SUBCOMPONENT 2 HAS CONVERGED: 19 3.3158E-05
SUBCOMPONENT 3 HAS CONVERGED: 19 1.8781E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -0.0908
S(2,1) = -1.6478
S(2,2) = -21.7681
S(3,1) = -1.5742
S(3,2) = -52.2911

S(3,3) = 13.6099

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 2.2682 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 204.6068 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 822.9635 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 1223.1043 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.4862

EXCITED STATE # 4

SUBCOMPONENT 1 HAS CONVERGED: 19 1.8351E-05
SUBCOMPONENT 2 HAS CONVERGED: 19 1.5827E-04
SUBCOMPONENT 3 HAS CONVERGED: 21 2.9691E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 0.5730
S(2,1) = 3.4675
S(2,2) = 58.6041
S(3,1) = 14.5973
S(3,2) = 129.4395
S(3,3) = 649.1651

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 16724.9532 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 15293.6486 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 94624.5006 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 58311.9851 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 0.6162

EXCITED STATE # 5

SUBCOMPONENT 1 HAS CONVERGED: 23 1.9648E-05
SUBCOMPONENT 2 HAS CONVERGED: 21 3.6938E-04
SUBCOMPONENT 3 HAS CONVERGED: 21 3.0768E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 0.1966
S(2,1) = -0.1803
S(2,2) = -20.1823
S(3,1) = 4.6323
S(3,2) = -47.7394
S(3,3) = 28.4354

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 2.3800 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 193.9004 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 780.3616 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 1158.6427 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.4848

..... DONE WITH TD-DFT TPA-CROSS SECTIONS .....

Result of B4

SINGLET EXCITATIONS

STATE # 1 ENERGY = 2.412915 EV
OSCILLATOR STRENGTH = 0.778720
LAMBDA DIAGNOSTIC = 0.698 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
149	156	0.042536	0.014917
151	156	0.092951	0.023714
154	156	0.121575	0.017108
155	156	0.989223	-0.134901
152	160	0.034266	0.007201
155	164	0.030836	0.018654

STATE # 2 ENERGY = 2.800330 EV
OSCILLATOR STRENGTH = 0.096614
LAMBDA DIAGNOSTIC = 0.547 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
143	156	-0.030951	0.006587
152	156	0.118119	-0.003918
153	156	0.374287	-0.013082
154	156	0.902642	-0.027064
155	156	-0.115949	0.033891
152	157	0.047309	0.009535
155	157	-0.070261	-0.005346
155	158	0.058163	0.005447

STATE # 3 ENERGY = 2.836301 EV
OSCILLATOR STRENGTH = 0.027068
LAMBDA DIAGNOSTIC = 0.545 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)

144	156	-0.034660	0.003273
150	156	0.099285	0.004206
151	156	0.038136	-0.001303
152	156	-0.123909	0.005140
153	156	0.910093	-0.026539
154	156	-0.352563	0.007645
155	157	0.070736	0.004679
151	158	0.032558	0.008318
152	158	0.040472	0.009593
155	158	0.044801	0.004026
155	162	0.036321	0.005956

STATE # 4 ENERGY = 3.023182 EV
OSCILLATOR STRENGTH = 0.009127
LAMBDA DIAGNOSTIC = 0.538 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

		EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
OCC I	VIR A	X(I->A)	Y(A->I)
151	156	-0.035109	-0.001269
152	156	-0.971187	0.015044
153	156	-0.073712	0.000720
154	156	0.156103	-0.001493
155	156	-0.036757	0.012891
154	157	0.082486	0.013790
155	157	0.057808	0.002465
153	158	0.063840	0.012182
155	161	-0.030980	-0.005551

STATE # 5 ENERGY = 3.180731 EV
OSCILLATOR STRENGTH = 0.036143
LAMBDA DIAGNOSTIC = 0.518 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

		EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
OCC I	VIR A	X(I->A)	Y(A->I)
149	156	0.045417	0.005982
150	156	-0.060308	-0.001077
151	156	-0.980568	0.014407
153	156	0.033530	0.001775
154	156	-0.038540	0.006094
155	156	0.096582	-0.039442

153	157	0.039810	0.005027
154	157	-0.045705	-0.005350
155	157	-0.056083	-0.001452
153	158	0.081655	0.012742
155	161	0.034158	0.007497

SUMMARY OF TDDFT RESULTS

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE, A.U.			OSCILLATOR
0 ->	HARTREE	EV	X	Y	Z	STRENGTH
0 A	-1911.1694365051	0.000				
1 A	-1911.0807635091	2.413	0.7302	-2.5854	2.4404	0.7787
2 A	-1911.0665262754	2.800	-0.3715	0.6657	-0.9094	0.0966
3 A	-1911.0652043718	2.836	0.5063	-0.1041	-0.3498	0.0271
4 A	-1911.0583365944	3.023	0.0119	0.2396	-0.2563	0.0091
5 A	-1911.0525467771	3.181	0.1151	-0.4252	0.5194	0.0361

TRANSITION	EXCITATION	TRANSITION DIPOLE, A.U.				OSCILLATOR
	EV	X	Y	Z	DIP	STRENGTH
1 -> 2	0.387	-0.2136	1.1654	-1.2079	1.6920	0.0272
1 -> 3	0.423	1.0604	-2.2121	1.4647	2.8571	0.0847
1 -> 4	0.610	-1.3435	2.6180	-2.3503	3.7660	0.2121
1 -> 5	0.768	1.2032	0.1702	-0.9661	1.5525	0.0453
2 -> 3	0.036	1.5118	-3.6720	3.8566	5.5356	0.0270
2 -> 4	0.223	-0.1289	-1.5958	1.6917	2.3292	0.0296
2 -> 5	0.380	1.1051	-0.7102	0.3233	1.3529	0.0171
3 -> 4	0.187	0.4350	-0.5608	0.4441	0.8372	0.0032
3 -> 5	0.344	0.1828	0.1921	-1.1762	1.2058	0.0123
4 -> 5	0.158	0.7240	-4.6892	4.8636	6.7947	0.1782

SELECTING EXCITED STATE 1 E= -1911.0807635091 AS THE STATE OF INTEREST.

..... DONE WITH TD-DFT EXCITATION ENERGIES .....
STEP CPU TIME = 16660.50 TOTAL CPU TIME = 21018.7 (350.3 MIN)
TOTAL WALL CLOCK TIME= 21032.9 SECONDS, CPU UTILIZATION IS 99.93%

TWO-PHOTON ABSORPTION (TPA) CALCULATIONS (A.U.):

EXCITED STATE # 1

SUBCOMPONENT 1 HAS CONVERGED: 17 1.2936E-04
SUBCOMPONENT 2 HAS CONVERGED: 19 1.8867E-04
SUBCOMPONENT 3 HAS CONVERGED: 17 1.5992E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 14.6149
S(2,1) = -15.4971
S(2,2) = -27.0737
S(3,1) = 8.4093
S(3,2) = 40.3485
S(3,3) = -49.6724

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 128.6765 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 243.0562 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 1229.5776 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 1200.9841 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 0.9767

EXCITED STATE # 2

SUBCOMPONENT 1 HAS CONVERGED: 17 3.4648E-04
SUBCOMPONENT 2 HAS CONVERGED: 17 1.6886E-04
SUBCOMPONENT 3 HAS CONVERGED: 21 4.8617E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 25.4978

S(2,1) = -24.3747
S(2,2) = -48.0591
S(3,1) = 21.5470
S(3,2) = 65.0116
S(3,3) = -86.2918

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 394.9658 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 699.1963 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 3586.7170 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 3405.2464 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 0.9494

EXCITED STATE # 3

SUBCOMPONENT 1 HAS CONVERGED: 17 3.8664E-04
SUBCOMPONENT 2 HAS CONVERGED: 17 1.5654E-04
SUBCOMPONENT 3 HAS CONVERGED: 21 2.3365E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 7.0935
S(2,1) = -39.7642
S(2,2) = 85.2170
S(3,1) = 31.7691
S(3,2) = -43.2514
S(3,3) = -4.1319

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 259.1821 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 541.7216 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 2685.2505 (A.U.)

D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 2731.9654 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.0174

EXCITED STATE # 4

SUBCOMPONENT 1 HAS CONVERGED: 19 4.7534E-04
SUBCOMPONENT 2 HAS CONVERGED: 17 1.4276E-04
SUBCOMPONENT 3 HAS CONVERGED: 19 6.7998E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -18.6207
S(2,1) = 71.8829
S(2,2) = -169.3061
S(3,1) = -71.7154
S(3,2) = 162.4836
S(3,3) = -155.1447

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 3923.2690 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 4216.7837 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 24713.6727 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 17454.1642 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 0.7063

EXCITED STATE # 5

SUBCOMPONENT 1 HAS CONVERGED: 21 9.4567E-05

SUBCOMPONENT 2 HAS CONVERGED: 17 1.6859E-04
SUBCOMPONENT 3 HAS CONVERGED: 19 6.7151E-05

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 17.7558
S(2,1) = -35.2749
S(2,2) = -21.7792
S(3,1) = 19.6189
S(3,2) = 47.0786
S(3,3) = -59.2980

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 133.6534 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 399.9025 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 1866.9167 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 2132.1083 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.1420

..... DONE WITH TD-DFT TPA-CROSS SECTIONS .....

Result of B5

SINGLET EXCITATIONS

STATE # 1 ENERGY = 2.420341 EV
OSCILLATOR STRENGTH = 0.356597
LAMBDA DIAGNOSTIC = 0.540 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
160	168	-0.030747	-0.009487
162	168	0.055280	0.015743
164	168	0.070251	-0.001519
165	168	-0.071517	-0.003907
166	168	-0.723416	0.020337
167	168	0.678147	-0.087362

STATE # 2 ENERGY = 2.453279 EV
OSCILLATOR STRENGTH = 0.487828
LAMBDA DIAGNOSTIC = 0.558 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
160	168	-0.032445	-0.010378
162	168	0.064858	0.016833
164	168	-0.097353	-0.001381
165	168	-0.042435	-0.005692
166	168	0.674916	-0.024151
167	168	0.726341	-0.099153
161	171	-0.031404	-0.010789

STATE # 3 ENERGY = 2.753295 EV
OSCILLATOR STRENGTH = 0.071275
LAMBDA DIAGNOSTIC = 0.642 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
155	168	0.033488	-0.006921
164	168	-0.084809	0.001925
165	168	-0.985768	0.035449
167	168	-0.086964	0.022273
163	169	0.034927	0.008829
167	170	0.066044	0.008729

STATE # 4 ENERGY = 2.884975 EV
OSCILLATOR STRENGTH = 0.072543

LAMBDA DIAGNOSTIC = 0.637 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
156	168	0.035038	0.000201
161	168	0.045953	0.000164
163	168	0.036923	0.001964
164	168	0.976475	-0.032270
165	168	-0.082260	0.003739
166	168	0.115419	-0.006649
162	169	0.034130	0.009234
167	169	0.087548	0.007535
163	170	0.042060	0.010105
165	171	0.030174	0.018943
167	173	0.050674	0.007518

STATE # 5 ENERGY = 3.117476 EV
OSCILLATOR STRENGTH = 0.007567
LAMBDA DIAGNOSTIC = 0.484 (RYDBERG/CHARGE TRANSFER CHARACTER)
SYMMETRY OF STATE = A

OCC	VIR	EXCITATION AMPLITUDE	DE-EXCITATION AMPLITUDE
I	A	X(I->A)	Y(A->I)
161	168	0.038935	0.006667
163	168	0.987685	-0.010345
164	168	-0.034610	0.002803
165	169	0.074028	0.013138
164	170	-0.066885	-0.012293
165	170	0.053642	0.009731
162	171	0.032204	-0.003266

SUMMARY OF TDDFT RESULTS

STATE 0 ->		ENERGY HARTREE	EXCITATION EV	TRANSITION DIPOLE, A.U. X	Y	Z	OSCILLATOR STRENGTH
0	A	-2045.0181410621	0.000				
1	A	-2044.9291951460	2.420	-1.7650	-1.6105	-0.5520	0.3566
2	A	-2044.9279847104	2.453	-0.5879	-2.6653	-0.8167	0.4878
3	A	-2044.9169593389	2.753	0.5835	0.6186	0.5775	0.0713
4	A	-2044.9121201863	2.885	0.7819	-0.6136	-0.1959	0.0725
5	A	-2044.9035759173	3.117	-0.2561	0.1767	0.0475	0.0076

TRANSITION	EXCITATION	TRANSITION DIPOLE, A.U.			OSCILLATOR
	EV	X	Y	Z	DIP STRENGTH
1 -> 2	0.033	3.5386	-1.8482	-0.3813	4.0104 0.0130
1 -> 3	0.333	-0.0886	-1.3550	-0.5348	1.4594 0.0174
1 -> 4	0.465	-0.1755	-1.7202	-0.2391	1.7456 0.0347
1 -> 5	0.697	-1.9301	-1.2411	-0.7151	2.4035 0.0987
2 -> 3	0.300	0.7239	0.3641	0.3890	0.8988 0.0059
2 -> 4	0.432	-1.7053	-1.5975	-0.2743	2.3527 0.0585
2 -> 5	0.664	-0.3912	-2.2937	-0.9133	2.4997 0.1017
3 -> 4	0.132	-2.7356	-5.0124	-1.9042	6.0194 0.1169
3 -> 5	0.364	0.6170	2.0324	0.2450	2.1380 0.0408
4 -> 5	0.233	-0.9510	-0.2408	-0.2291	1.0075 0.0058

SELECTING EXCITED STATE 1 E= -2044.9291951460 AS THE STATE OF INTEREST.

..... DONE WITH TD-DFT EXCITATION ENERGIES .....
STEP CPU TIME = 20507.61 TOTAL CPU TIME = 25686.3 (428.1 MIN)
TOTAL WALL CLOCK TIME= 25702.3 SECONDS, CPU UTILIZATION IS 99.94%

TWO-PHOTON ABSORPTION (TPA) CALCULATIONS (A.U.):

EXCITED STATE # 1

SUBCOMPONENT 1 HAS CONVERGED: 19 6.8027E-05
SUBCOMPONENT 2 HAS CONVERGED: 99 4.6498E-04
SUBCOMPONENT 3 HAS CONVERGED: 15 1.4285E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 54.0954
S(2,1) = -109.5086
S(2,2) = 14.8455
S(3,1) = -32.3275
S(3,2) = -5.8039

S(3,3) = -6.8450

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 128.5301 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 977.8432 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 4168.4331 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 5609.9993 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.3458

EXCITED STATE # 2

SUBCOMPONENT 1 HAS CONVERGED: 19 6.0595E-05
SUBCOMPONENT 2 HAS CONVERGED: 21 1.7464E-05
SUBCOMPONENT 3 HAS CONVERGED: 15 1.4629E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -115.2470
S(2,1) = 55.3137
S(2,2) = 44.8453
S(3,1) = 15.8397
S(3,2) = 18.9228
S(3,3) = 9.6215

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 123.1408 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 757.4235 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 3275.9756 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 4298.2594 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.3121

EXCITED STATE # 3

SUBCOMPONENT 1 HAS CONVERGED: 19 3.8694E-05
SUBCOMPONENT 2 HAS CONVERGED: 19 7.8057E-05
SUBCOMPONENT 3 HAS CONVERGED: 15 2.0640E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = -57.6966
S(2,1) = -32.1087
S(2,2) = 59.6488
S(3,1) = -17.7858
S(3,2) = 9.6400
S(3,3) = -1.0374

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 0.0279 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 325.6139 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 1302.5115 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 1953.6278 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.4999

EXCITED STATE # 4

SUBCOMPONENT 1 HAS CONVERGED: 17 4.4806E-04
SUBCOMPONENT 2 HAS CONVERGED: 17 3.3941E-04
SUBCOMPONENT 3 HAS CONVERGED: 15 2.5228E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 2.6466
S(2,1) = 66.3183
S(2,2) = 68.2211
S(3,1) = 2.7483
S(3,2) = -9.2101
S(3,3) = -16.7200

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 97.7322 (A.U.)
DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 464.0556 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 2051.6867 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 2588.8690 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 1.2618

EXCITED STATE # 5

SUBCOMPONENT 1 HAS CONVERGED: 19 7.5322E-05
SUBCOMPONENT 2 HAS CONVERGED: 17 4.6232E-04
SUBCOMPONENT 3 HAS CONVERGED: 17 1.0541E-04

TPA TRANSITION (SYMMETRIC) TENSOR ELEMENTS (A.U.):

S(1,1) = 99.4449
S(2,1) = 107.4230
S(2,2) = 230.1245
S(3,1) = 43.4204
S(3,2) = 91.4765
S(3,3) = 32.4574

DF = (SUM_{I,J} S(I,I)*S(J,J))/30 = 4368.7786 (A.U.)

DG = (SUM_{I,J} S(I,J)*S(I,J))/30 = 3582.8675 (A.U.)

D (LINEAR POLARIZATION) = 2*DF+4*DG = 23069.0274 (A.U.)
D (CIRCULAR POLARIZATION) = -2*DF+6*DG = 12759.6478 (A.U.)

R (POLARIZATION RATIO) = (-DF+3*DG)/(DF+2*DG) = 0.5531

..... DONE WITH TD-DFT TPA-CROSS SECTIONS .....