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Supporting Information

Electrically Switchable Photoluminescence of Fluorescent-Molecule-Dispersed Liquid Crystal Prepared *via* Photoisomerization-Induced Phase Separation

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1. General Experimental Section

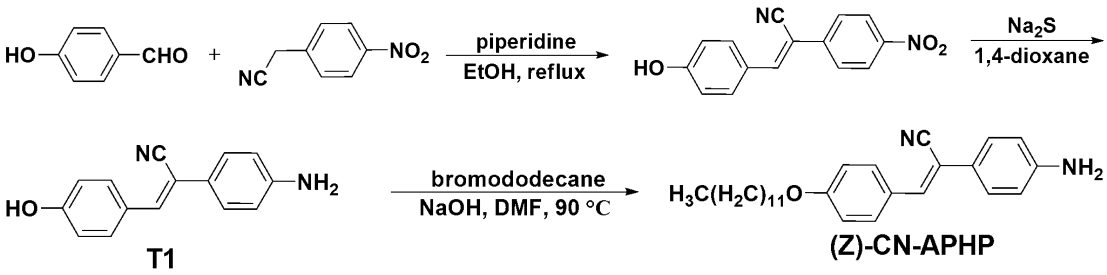
1.1 Materials and Methods

All chemicals were purchased from Sigma Aldrich Chemical Co. and used without further purification. Synthetic route and characterization of (Z)-CN-APHP are described in this Supporting Information. ^{1}H NMR spectra were recorded on Agilent VNMRS600 (600 MHz) and Bruker Avance (400 MHz). Chemcial shifts are reported in δ, ppm and the coupling constants (*J*) are given in Hz. ^{13}C NMR spectra were also measured on Bruker Avance (400 MHz). Mass spectra (MS) were obtained using an Agilent Q-TOF 6540 mass spectrometer. UV-vis absorption spectra were recorded on a TU-1901 of Beijing Purkinje General Co. PC spectrometer using samples in solutions. Fluorescence spectra were recorded on a Shimadzu RF 5301 PC fluorescence spectrometer using samples in both the solution and the solid state. Differential scanning calorimetry (DSC) was performed on a METTLER82le/400 instrument at a heating and cooling rate of 10 °C min^{-1}. The absolute photoluminescence quantum yield of solid-film was measured on HORIBA FluoroMax-4 spectrofluorometer using an integrating sphere (HORIBA Scientific, F-3092 integrating sphere). Fluorescence images were obtained by using a digital camera (Canon PowerShot G6). Polarized microscopy images were collected on a microscope (Leica DM2500M). For the measurements of electrical switching of both photoluminescence and optical transmittance, a high-voltage waveform generator (High Speed Bipolar Amplifier BA4825) was used to apply ac (1000 Hz, square-wave) electric fields through the cell.

1.2 DFT Computational Methods

The hybrid B3LYP functional[1] has been used in all calculations as incorporated in *Gaussian 09* package,[2] mixing the exact Hartree-Fock-type exchange with Becke's exchange functional[3] and that proposed by Lee-Yang-Parr for the correlation contribution.[4] We used 6-31G(d) basis set for all the atoms which provides reasonably high quality results in moderate timescales. All ground state geometry optimizations were followed by subsequent frequency test to ascertain stationary points. TD-DFT energy calculations on ground state optimized structures were performed to simulate UV-vis absorption spectra of the compounds. 1st excited state optimizations were also performed using TD-DFT method. Visualizations of the optimized structures and the MOs were performed using *Gaussview5.0*.

2. Experimental Procedures



Scheme S1. Synthetic route of (Z)-CN-APHP

Synthesis of (Z)-3-(4-hydroxyphenyl)-2-(4-nitrophenyl)acrylonitrile:

This compound was synthesized according to the method described in the literature. [5]

Synthesis of (Z)-2-(4-aminophenyl)-3-(4-hydroxyphenyl)acrylonitrile (T1):

A mixture of (Z)-3-(4-hydroxyphenyl)-2-(4-nitrophenyl)acrylonitrile (1.14 g, 4.8 mmol) dissolved in 1,4-dioxane (40 mL), water (7.5 mL) and $Na_2S \cdot 9H_2O$ (5.16 g, 20.8 mmol) was stirred at 90 °C for 4 h. Then a saturated solution of $NaHCO_3$ (120 mL) was added and the aqueous phase was extracted with EtOAc (2 × 60 mL). The combined organic layers were washed with brine and dried over $MgSO_4$. After removal of solvent in vacuo, the crude product was recrystallized from ethanol and water to give a yellow solid with a yield of 78.9%.

FT-IR (KBr, cm^{-1}): 3434 (vs), 3341 (vs), 3285 (vs), 2215 (m), 1793 (w), 1624 (m), 1605 (vs), 1521 (vs), 1447 (m), 1400 (m), 1281 (m), 1258 (s), 1179 (s), 890 (w), 825 (m).

^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 10.02 (s, 1 H, OH), 7.75 (d, 2 H, ArH, J = 8.8 Hz), 7.54 (s, 1 H, CH), 7.36 (d, 2 H, ArH, J = 8.4 Hz), 6.66 (d, 2 H, ArH, J = 8.8 Hz), 6.62 (d, 2 H, ArH, J = 8.8 Hz), 5.42 (s, 2 H, NH_2).

^{13}C NMR ($CDCl_3$, 400 MHz, ppm): δ 158.9, 149.5, 137.1, 130.5, 137.1, 129.7, 128.3, 125.4, 121.3, 118.9, 115.7, 115.6, 105.8.

Synthesis of (Z)-2-(4-aminophenyl)-3-(4-(dodecyloxy)phenyl)acrylonitrile (Z)-CN-APHP:

A mixture of compound **T1** (800 mg, 3.84 mmol) dissolved in DMF (8 mL) and NaOH (227 mg, 7.68 mmol) was stirred for 15 min at RT. Then bromododecane (1.69 g, 6.78 mmol) was added, and the mixture was sequentially stirred for 12 h at 90 °C. The mixture was poured into 500 mL water and extracted with ethyl acetate (3 ×100 mL) three times. Finally, after silica gel column chromatography (n-hexane : EtOAc = 6:1), the product was recrystallized from ethanol and water to give a yellow

powder (982 mg, 2.43 mmol), yield 63.3%.

FT-IR (KBr, cm^{-1}): 3444 (vs), 3359 (vs), 3133 (s), 2919 (vs), 2851 (s), 2215(m), 1627 (s), 1604 (vs), 1516 (s), 1472 (m), 1420 (w), 1391 (w), 1355 (w), 1284 (s), 1250 (vs), 1178 (s), 1135 (m), 1064 (m), 1032 (m), 1000 (w), 956 (w), 897 (w), 865 (w), 833 (s), 781 (w), 765 (w), 721 (w), 630 (w).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.80 (d, 2 H, ArH, J = 8.4 Hz), 7.47 (d, 2 H, ArH, J = 8.8 Hz), 7.28 (s, 1 H, CH), 6.93 (d, 2 H, ArH, J = 8.8 Hz), 6.65 (d, 2 H, ArH, J = 8.4 Hz), 4.00 (t, 2 H, CH_2, J = 6.4 Hz), 3.15 (t, 2 H, CH_2, J = 7.2 Hz), 1.77 (m, 2H, CH_2), 1.64 (m, 2 H, CH_2), 1.27 (m, 36 H, 18 × CH_2), 0.88 (t, 3 H, CH_3, J = 6.0 Hz)

^{13}C NMR ($CDCl_3$, 400 MHz): δ 155.1, 143.7, 132.3, 125.3, 121.7, 121.6, 118.2, 113.7, 109.5, 107.4, 103.6, 62.9, 36.5, 26.7, 24.4~23.9, 21.9, 20.7, 17.4, 8.9.

HRMS (ESI) m/z $[M + Na]^+$: calcd for $C_{27}H_{36}N_2O$, 427.2725, found 427.2721.

3. Sample Preparation

Irradiation Procedure of FMDLC: The nematic LC (E7) was purchased from Jiangsu Hecheng Display Technology Co., Ltd. To prepare the LC composite, weighed E7 and (Z)-CN-APHP were first dissolved in THF, a common solvent for all compounds; then, the mixture was dried in a vacuum oven to remove the solvent. To enter the mixture in a chosen ITO-coated, rubbed cell (Shenzhen Success Electronics Co., Ltd), it was heated to 100 °C and flow-filled into the cell through a capillary effect. Afterwards, the cell was taken out of the hot stage for slow cooling to room temperature to allow the aggregation of the (Z)-CN-APHP inside the predetermined LC orientational template. The cells were placed at a distance of 5 cm from the 365 nm hand-held UV lamp (0.87 mW/cm^{-2}) under atmospheric conditions at room temperature, and irradiated simultaneously for 3h.

Irradiation Procedure of powdered crystal: The finely powdered crystal samples of (Z)-CN-APHP were made into thin film in the sandwich quartz cell. The cells were placed at a distance of 5 cm from the 365 nm hand-held UV lamp (0.87 mW/cm^{-2}) under atmospheric conditions at 90 °C, and irradiated simultaneously for 2h.

4. Supplementary Figures

4.1 Gel images of CN-APHP and liquid crystal

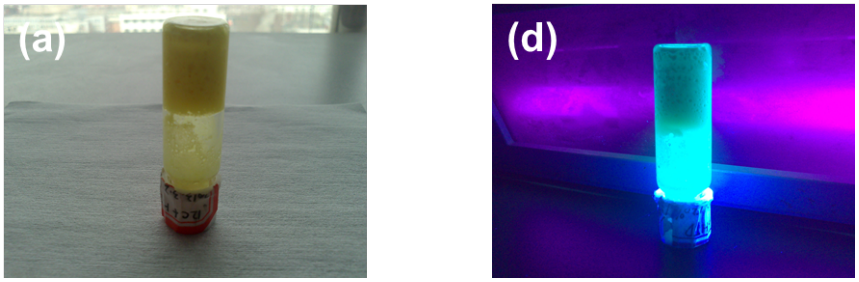


Fig. S1 Gel of the mixture of CN-APHP and liquid crystal: (a) under room light, (b) under UV light.

4.2 Polarized optical microscopy (POM) image of (Z)-CN-APHP

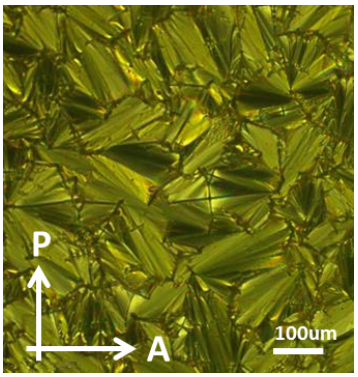


Fig. S2 Focal conic fan-shaped texture of (Z)-CN-APHP observed by POM in the smetic phase at 75 °C on the cooling process

4.3 Geometry difference between (Z)- and (E)-CN-APHP

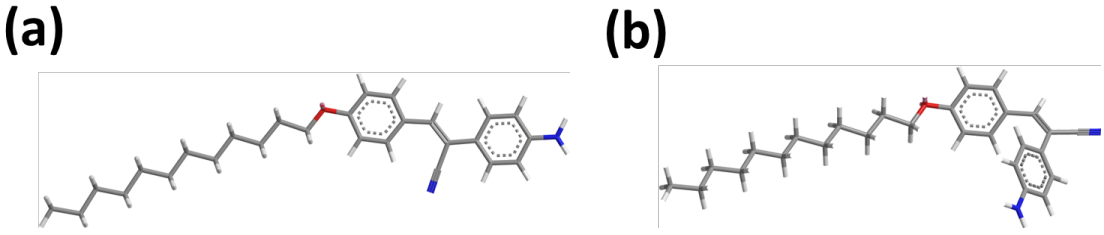


Fig. S3 Geometry optimization of (Z)- (a) and (E)-CN-APHP (b) by quantum chemical calculations based on density functional theory.

4.4 Energy levels of HOMO and LUMO and electron cloud distributions of (Z)- and (E)-CN-APHP molecules

As calculated by the B3LYP/6-31G(d) program, Eg of Z-isomer is 3.42 eV (Eg = LUMO-HOMO), which is lower than that of E-isomer (3.53 eV), so it means that it is easier for Z-isomer to convert into E-isomer in theory, which is in good agreement with the absorption spectra (**Fig. S2**).

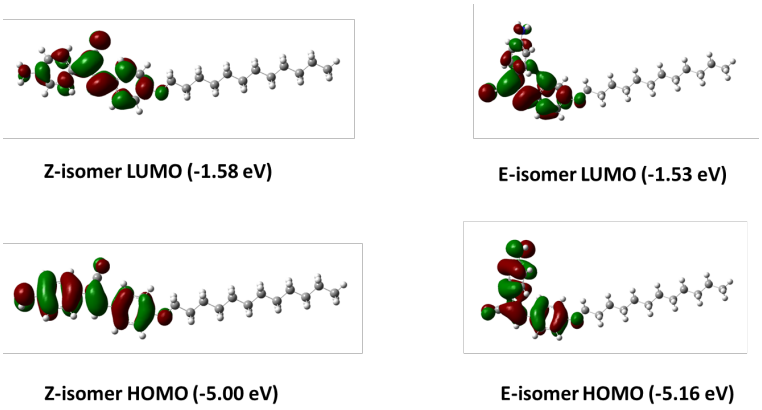


Fig. S4 Energy levels of HOMO and LUMO and electron cloud distributions of (Z)- and (E)-CN-APHP molecules calculated by the B3LYP/6-31G(d) program.

4.5 HRMS

HRMS was also studied in this paper in order to eliminate the possibility of [2+2] cycloaddition of CN-APHP in the irradiation process. As shown in **Fig. S5**, there were the same m/z peaks (found 427.2721 in MS) in different samples, which indicated that [2+2] cycloaddition of CN-APHP never occurred and only isomerization happened in the irradiation process.

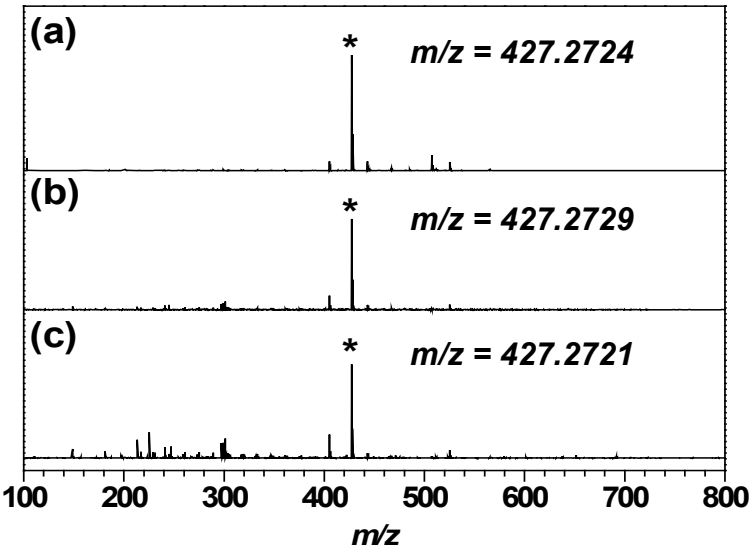


Fig. S5 HRMS of different samples with different treatments. (a) Z-isomer in DMF solution which was irradiated for 4h at 365 nm, (b) Z-isomer film in the quartz cell irradiated for 4h at 365 nm in the liquid crystalline phase, (c) pure Z-isomer powder without any treatment.

4.6 Photoisomerization of (Z)-CN-APHP in solution

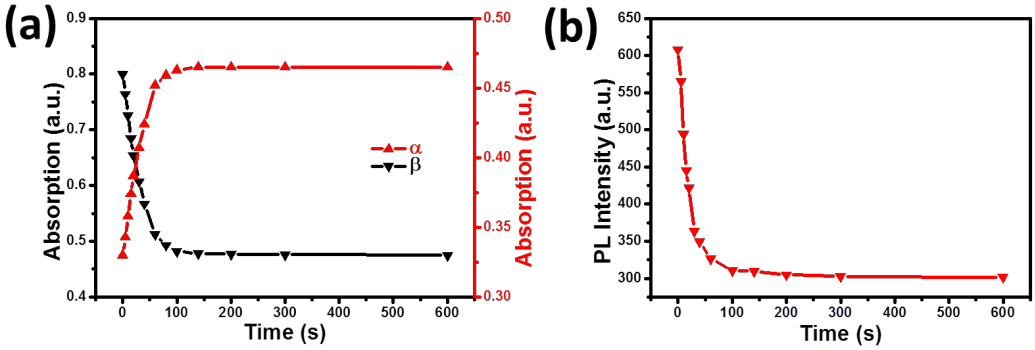


Fig. S6 (a) The influence of the irradiation time on absorption peaks of CN-APHP in DMF (2.5×10^{-5} mol L^{-1}), (b) The influence of the irradiation time on PL intensity of CN-APHP in DMF (2.5×10^{-5} mol L^{-1}).

4.7 Photoisomerization of CN-APHP in LC

The photoisomerization of (Z)-CN-APHP in liquid crystal (83.3% E7 and 16.7% (Z)-CN-APHP) was investigated by UV-vis absorption spectra in **Fig. S7a**. It is clear that the decrease of absorption was depicted as a function of exposure time. Plotted in **Fig. S7b** is the development of fluorescence intensity emitted from FMDLC as a function of applied voltage. The system displays the stronger photoluminescence in the field-off state; with an electric field applied, the photoluminescence starts to decrease at the threshold voltage of 2.3 V. It should be mentioned that after LC molecules are aligned by the electric field, further increase in voltage showed little direct effect on the photoluminescence of FMDLC. As shown in **Fig. S7b**, after the voltage reaches to 20−30 V, the fluorescence intensity becomes almost a constant. **Fig. S7c** shows the evolution of POM of CN-APHP in LC by increasing the illumination time of 365 nm light (0.87 mW/cm^{-2}).

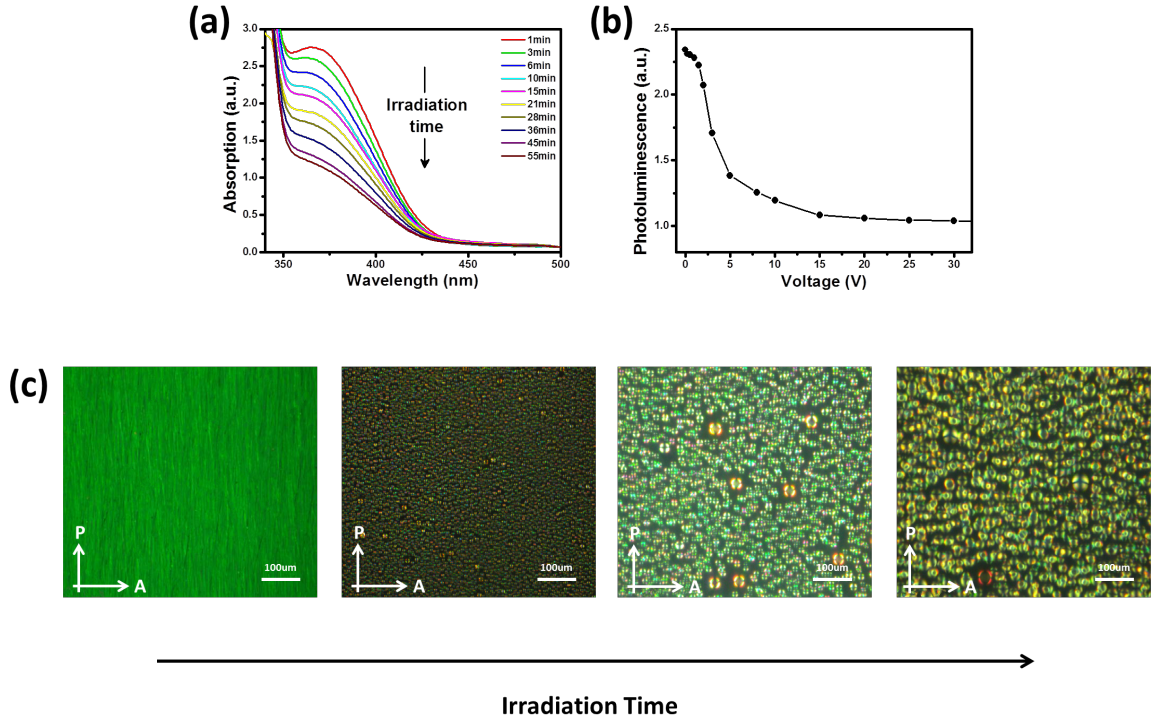


Fig. S7 (a) Development of UV-vis absorption spectra of the cell filled with the mixture of CN-APHP and liquid crystal with increasing the illumination time of 365 nm light (0.87 mW/cm^{-2}). (b) Plots of photoluminescence versus applied voltage (ac 1K Hz square-wave). (c) POM evolution of the cell filled with the mixture of CN-APHP and liquid crystal with increasing the illumination time of 365 nm light (0.87 mW/cm^{-2}).

4.8 The modulation mechanism of electrical switching of photoluminescence of FMDLC

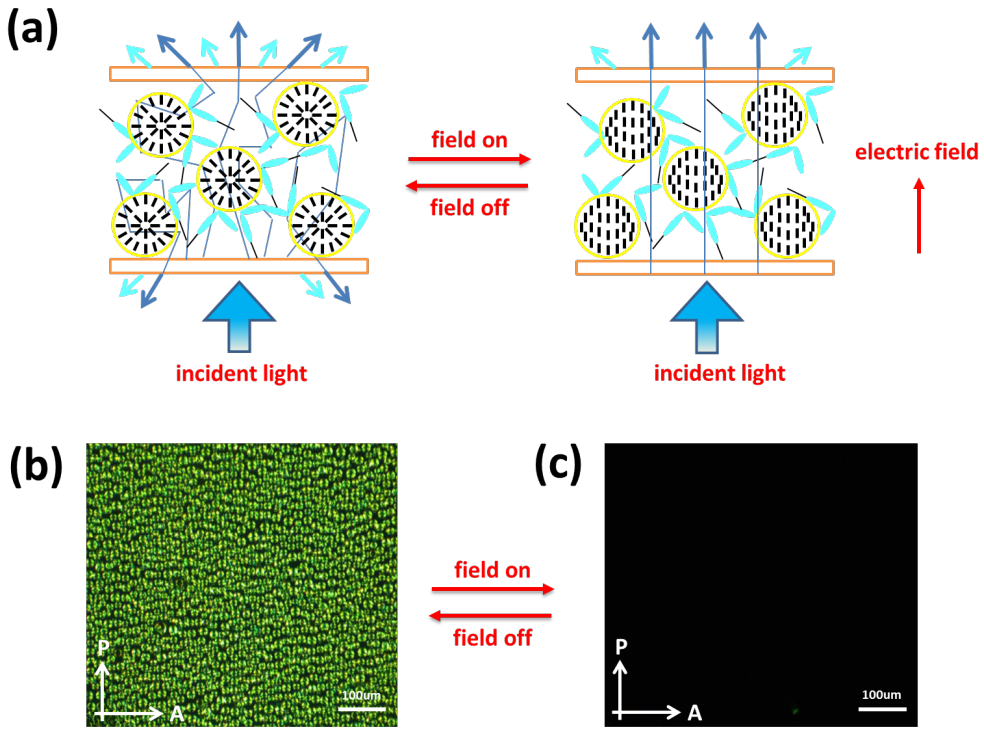


Fig. S8 (a) Schematic illustration of the mechanism for electrically switchable photoluminescence of FMDLC: different photoluminescence intensities at the field-off and field-on state are attributed to different numbers of fluorescent molecules excited by the incident light modulated by electric-field-induced orientation of LC molecules. (b) POM of FMDLC without applying an electric field (0 V). (c) POM of FMDLC with applying an electric field (30 V).

4.9 TD-DFT simulated UV-vis absorption spectra of Z, E-isomers

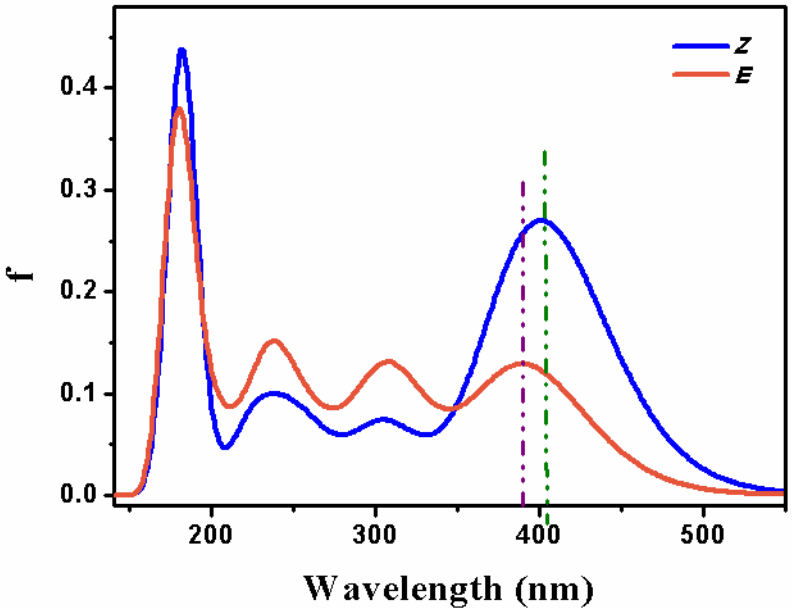


Fig. S9 TD-DFT simulated UV-vis absorption spectra of Z, E-isomers (no of states considered = 50)

Computational Data:

Z-isomers (Ground state optimized geometry)

Energy = -1234.99749094 au

Table S1: Coordinates of optimized structure of **Z-isomers** (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.848638	2.540629	-0.564097
2	6	0	2.596207	2.975420	-0.436793
3	6	0	1.585756	2.113748	0.176807
4	6	0	1.927046	0.921340	0.646708
5	6	0	3.278163	0.476371	0.536759
6	6	0	4.213248	1.218293	-0.053605
7	8	0	0.263470	2.518497	0.195440
8	6	0	-14.050796	-1.513088	-0.320079
9	6	0	-12.601432	-1.955629	-0.591921
10	6	0	-11.634415	-0.837204	-0.163363
11	6	0	-10.185516	-1.285605	-0.422855
12	6	0	-9.219375	-0.159583	-0.015649
13	6	0	-7.770312	-0.622018	-0.246079
14	6	0	-6.805788	0.518607	0.115179
15	6	0	-5.355196	0.029593	-0.030765
16	6	0	-4.403795	1.194950	0.269068
17	6	0	-2.954635	0.693136	0.302382
18	6	0	-2.030710	1.906795	0.451247
19	6	0	-0.586742	1.444342	0.610486
20	6	0	5.612251	0.721092	-0.246237
21	6	0	6.128580	-0.413320	0.264794
22	6	0	7.471596	-0.775930	-0.043955
23	6	0	5.409305	-1.295593	1.123038
24	7	0	4.830502	-2.007792	1.815176
25	6	0	7.964856	-1.884614	0.497268
26	6	0	9.319773	-2.289580	0.209187
27	6	0	10.067898	-1.551110	-0.602697
28	6	0	9.528775	-0.329960	-1.207656
29	6	0	8.281542	0.042982	-0.937999
30	7	0	11.359788	-1.942206	-0.872283
31	1	0	4.537063	3.115321	-1.006639
32	1	0	2.347263	3.888510	-0.759805
33	1	0	1.239619	0.336021	1.076659
34	1	0	3.529397	-0.415507	0.912638
35	1	0	-14.679324	-2.239376	-0.598328
36	1	0	-14.249681	-0.683004	-0.841224
37	1	0	-14.166172	-1.329013	0.656018
38	1	0	-12.403151	-2.785478	-0.070430
39	1	0	-12.486705	-2.139314	-1.568146

40	1	0	-11.826792	-0.009824	-0.690994
41	1	0	-11.755113	-0.647244	0.810996
42	1	0	-9.988620	-2.104660	0.116027
43	1	0	-10.068808	-1.489434	-1.394819
44	1	0	-9.402210	0.653133	-0.568833
45	1	0	-9.350144	0.058568	0.951464
46	1	0	-7.578133	-1.416260	0.330405
47	1	0	-7.648418	-0.869793	-1.207240
48	1	0	-6.959921	1.292468	-0.499235
49	1	0	-6.967379	0.805026	1.059632
50	1	0	-5.186153	-0.715715	0.614237
51	1	0	-5.203299	-0.295757	-0.964022
52	1	0	-4.497167	1.890252	-0.443547
53	1	0	-4.636915	1.592889	1.156342
54	1	0	-2.828518	0.074629	1.078032
55	1	0	-2.744186	0.209960	-0.547417
56	1	0	-2.106242	2.482638	-0.362775
57	1	0	-2.301162	2.432115	1.258084
58	1	0	-0.422135	0.640024	0.039562
59	1	0	-0.405662	1.217182	1.567326
60	1	0	6.220112	1.283651	-0.806692
61	1	0	7.396493	-2.439173	1.105061
62	1	0	9.693467	-3.121801	0.618729
63	1	0	10.096215	0.219999	-1.820363
64	1	0	7.903449	0.875248	-1.343432
65	1	0	11.723059	-2.770145	-0.457522
66	1	0	11.926531	-1.398517	-1.478558

Z-isomers (1st excited-state optimised geometry)

Energy = -1235.29969056 au

Table S2: Coordinates of optimized structure of **Z-isomers** (ES)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.802935	-1.985548	-0.262332
2	6	0	2.444097	-2.243346	-0.298356
3	6	0	1.526332	-1.191795	-0.144286
4	6	0	2.005222	0.112555	0.048290
5	6	0	3.374789	0.358822	0.081010
6	6	0	4.314495	-0.679164	-0.077371
7	8	0	0.213267	-1.537643	-0.192906
8	6	0	-14.848994	0.533085	0.066427
9	6	0	-13.469342	1.191535	0.168385
10	6	0	-12.310842	0.195965	0.025746
11	6	0	-10.925461	0.846977	0.126520
12	6	0	-9.767152	-0.148897	-0.016124

13	6	0	-8.382003	0.503036	0.084449
14	6	0	-7.223627	-0.492733	-0.058325
15	6	0	-5.838901	0.160174	0.041903
16	6	0	-4.681081	-0.835914	-0.101204
17	6	0	-3.297184	-0.180781	-0.001232
18	6	0	-2.145345	-1.183803	-0.145885
19	6	0	-0.779563	-0.519179	-0.045060
20	6	0	5.762948	-0.528530	-0.060475
21	6	0	6.576093	0.566619	-0.003721
22	6	0	8.056541	0.469106	0.055756
23	6	0	6.050052	1.900083	-0.019908
24	7	0	5.669081	3.001283	-0.040568
25	6	0	8.870990	1.504481	-0.436648
26	6	0	10.256510	1.414788	-0.409400
27	6	0	10.893503	0.280272	0.121858
28	6	0	10.087295	-0.751867	0.634145
29	6	0	8.702613	-0.652505	0.605640
30	7	0	12.282152	0.161220	0.101173
31	1	0	4.499648	-2.811972	-0.382674
32	1	0	2.063191	-3.249331	-0.443234
33	1	0	1.320359	0.942787	0.175555
34	1	0	3.706430	1.377856	0.235492
35	1	0	-15.653763	1.269636	0.172207
36	1	0	-14.985665	-0.224077	0.848483
37	1	0	-14.979503	0.034034	-0.901814
38	1	0	-13.376241	1.968014	-0.604321
39	1	0	-13.382427	1.711919	1.132913
40	1	0	-12.404607	-0.581483	0.798817
41	1	0	-12.398476	-0.325354	-0.939343
42	1	0	-10.832815	1.624368	-0.646572
43	1	0	-10.838940	1.368348	1.091552
44	1	0	-9.859464	-0.926174	0.757073
45	1	0	-9.853576	-0.670362	-0.981064
46	1	0	-8.289671	1.280284	-0.688750
47	1	0	-8.295447	1.024457	1.049394
48	1	0	-7.315344	-1.269829	0.715060
49	1	0	-7.309916	-1.014255	-1.023192
50	1	0	-5.747006	0.937166	-0.731529
51	1	0	-5.752235	0.681473	1.006847
52	1	0	-4.770898	-1.612514	0.672467
53	1	0	-4.766093	-1.357094	-1.066015
54	1	0	-3.207667	0.595602	-0.775264
55	1	0	-3.212170	0.339837	0.964009
56	1	0	-2.217702	-1.956606	0.630184
57	1	0	-2.213496	-1.700415	-1.111892
58	1	0	-0.658178	-0.020306	0.927260
59	1	0	-0.654271	0.238681	-0.831713
60	1	0	6.290692	-1.478070	-0.121084
61	1	0	8.409733	2.395824	-0.852102
62	1	0	10.856571	2.229486	-0.808483
63	1	0	10.555334	-1.630933	1.071822

64	1	0	8.114875	-1.451310	1.048503
65	1	0	12.791084	1.035549	0.064551
66	1	0	12.673347	-0.472237	0.787062

TD-DFT obtained Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0888 eV 401.40 nm f=0.8882 <S**2>=0.000
110 ->111 0.70515

Excited State 2: Singlet-A 4.0338 eV 307.37 nm f=0.2236 <S**2>=0.000
109 ->111 0.69126
110 ->114 -0.10868

Excited State 3: Singlet-A 4.3482 ev 285.14 nm f=0.0126 <S**2>=0.000
108 ->111 0.52195
110 ->113 -0.46310

Excited State 4: Singlet-A 4.3601 eV 284.36 nm f=0.0015 <S**2>=0.000
107 ->111 0.45737
109 ->112 0.12224
110 ->112 0.51915

Excited State 5: Singlet-A 4.6581 eV 266.17 nm f=0.0625 <S**2>=0.000
108 ->111 0.47224
108 ->114 0.11987
110 ->113 0.50669

Excited State 6: Singlet-A 4.7961 eV 258.51 nm f=0.0934 <S**2>=0.000
107 ->111 0.50239
109 ->112 0.12268
110 ->112 -0.47121

Excited State 7: Singlet-A 5.0532 eV 245.36 nm f=0.1374 <S**2>=0.000
106 ->111 0.10803
110 ->114 0.58057
110 ->115 -0.32037
110 ->116 0.14807

Excited State 8: Singlet-A 5.3075 eV 233.60 nm f=0.0630 <S**2>=0.000
106 ->111 0.54398
110 ->116 -0.43025

Excited State 9: Singlet-A 5.3874 eV 230.14 nm f=0.0555 <S**2>=0.000
106 ->111 -0.24308
108 ->113 -0.11205
109 ->112 0.12285
110 ->114 0.33446
110 ->115 0.46367
110 ->116 -0.24182

Excited State 10: Singlet-A 5.5257 eV 224.38 nm f=0.0214 <S**2>=0.000

108 ->114 -0.10114
109 ->112 0.20476
109 ->113 0.64903

Excited State 11: Singlet-A 5.5470 eV 223.51 nm f=0.0805 <S**2>=0.000
107 ->111 -0.16742
107 ->115 0.11648
109 ->112 0.60277
109 ->113 -0.19780
110 ->116 0.16090

Excited State 12: Singlet-A 5.6833 eV 218.16 nm f=0.0518 <S**2>=0.000
106 ->111 0.31556
107 ->112 -0.14644
109 ->112 -0.11979
110 ->115 0.38900
110 ->116 0.42303

Excited State 13: Singlet-A 5.7655 eV 215.05 nm f=0.0001 <S**2>=0.000
105 ->111 0.69085

Excited State 14: Singlet-A 5.8832 eV 210.74 nm f=0.0015 <S**2>=0.000
93 ->111 0.16992
96 ->111 -0.23284
97 ->111 0.29375
98 ->111 0.16181
99 ->111 -0.31107
100 ->111 0.36636
101 ->111 0.14781
105 ->111 -0.13453

Excited State 15: Singlet-A 6.0205 eV 205.94 nm f=0.0157 <S**2>=0.000
108 ->113 0.14945
109 ->114 0.64106
109 ->115 -0.17954
109 ->116 0.10443

Excited State 16: Singlet-A 6.2500 eV 198.38 nm f=0.0176 <S**2>=0.000
96 ->111 0.11365
98 ->111 -0.12207
99 ->111 0.46567
100 ->111 0.39789
101 ->111 0.20282
109 ->115 -0.12473

Excited State 17: Singlet-A 6.3061 eV 196.61 nm f=0.0040 <S**2>=0.000
108 ->112 0.70468

Excited State 18: Singlet-A 6.3849 eV 194.18 nm f=0.0301 <S**2>=0.000
99 ->111 0.10395
107 ->112 -0.13121

108 ->113 0.19642
109 ->114 0.16699
109 ->115 0.51531
109 ->116 -0.32092

Excited State 19: Singlet-A 6.4236 eV 193.01 nm f=0.0003 <S**2>=0.000
90 ->111 0.17377
92 ->111 0.10379
93 ->111 0.52480
95 ->111 -0.13628
97 ->111 0.16562
98 ->111 -0.10400
99 ->111 0.15617
100 ->111 -0.23300

Excited State 20: Singlet-A 6.5027 eV 190.67 nm f=0.0218 <S**2>=0.000
94 ->111 -0.11454
96 ->111 -0.10492
103 ->111 0.46800
107 ->112 0.21516
109 ->115 -0.18459
109 ->116 -0.36398
Excited State 21: Singlet-A 6.5076 eV 190.52 nm f=0.0338 <S**2>=0.000
100 ->111 -0.10373
101 ->111 0.18073
103 ->111 0.46267
107 ->112 -0.26009
109 ->115 0.16658
109 ->116 0.35355

Excited State 22: Singlet-A 6.5300 eV 189.87 nm f=0.0011 <S**2>=0.000
96 ->111 0.11519
100 ->111 -0.11845
101 ->111 0.22921
104 ->111 0.57504
107 ->113 -0.25646

Excited State 23: Singlet-A 6.5320 eV 189.81 nm f=0.0033 <S**2>=0.000
104 ->111 0.24357
107 ->113 0.64946

Excited State 24: Singlet-A 6.5525 eV 189.22 nm f=0.0002 <S**2>=0.000
98 ->111 -0.18923
102 ->111 0.66973

Excited State 25: Singlet-A 6.5747 eV 188.58 nm f=0.0217 <S**2>=0.000
94 ->111 0.21667
96 ->111 0.34835
97 ->111 0.24576
100 ->111 -0.16390
101 ->111 0.27687

104 ->111 -0.29272
107 ->112 0.19940

Excited State 26: Singlet-A 6.6321 eV 186.95 nm f=0.0195 <S**2>=0.000
92 ->111 -0.11505
94 ->111 -0.29043
96 ->111 -0.20019
100 ->111 -0.16292
101 ->111 0.45424
103 ->111 -0.22473
104 ->111 -0.14256
107 ->112 -0.15551

Excited State 27: Singlet-A 6.6618 eV 186.11 nm f=0.0786 <S**2>=0.000
92 ->111 -0.19992
97 ->111 0.10867
98 ->111 0.11518
100 ->113 -0.11156
106 ->113 -0.22136
108 ->114 0.53952
110 ->113 -0.10521

Excited State 28: Singlet-A 6.6730 eV 185.80 nm f=0.0124 <S**2>=0.000
95 ->111 0.12360
97 ->111 0.10730
98 ->111 0.53915
99 ->111 0.25298
102 ->111 0.18490
108 ->114 -0.19226

Excited State 29: Singlet-A 6.6975 eV 185.12 nm f=0.0189 <S**2>=0.000
89 ->111 -0.15373
90 ->111 0.14972
91 ->111 0.12774
92 ->111 0.39381
96 ->111 0.13294
97 ->111 -0.28233
98 ->111 0.27383
106 ->112 0.16660
108 ->114 0.16329

Excited State 30: Singlet-A 6.7148 eV 184.64 nm f=0.0502 <S**2>=0.000
97 ->111 0.18837
106 ->112 0.61165
108 ->113 -0.13604

Excited State 31: Singlet-A 6.7299 eV 184.23 nm f=0.1969 <S**2>=0.000
91 ->111 0.13463
92 ->111 0.34642
93 ->111 -0.22557
96 ->111 -0.23071

97 ->111 0.19723
99 ->111 0.15078
106 ->112 -0.22235
108 ->113 -0.27694

Excited State 32: Singlet-A 6.7348 eV 184.09 nm f=0.5115 <S**2>=0.000
92 ->111 0.22997
93 ->111 -0.14257
96 ->111 -0.13660
97 ->111 0.13497
108 ->113 0.49652
108 ->114 0.11001
109 ->114 -0.14734
109 ->115 -0.14128
110 ->118 0.11502

Excited State 33: Singlet-A 6.8543 eV 180.88 nm f=0.0295 <S**2>=0.000
91 ->111 -0.17571
94 ->111 0.43867
95 ->111 -0.10024
96 ->111 -0.34043
97 ->111 -0.26972
101 ->111 0.14899
107 ->112 0.14069

Excited State 34: Singlet-A 6.8864 eV 180.04 nm f=0.0396 <S**2>=0.000
94 ->111 0.12539
106 ->113 0.46547
107 ->114 -0.13947
108 ->114 0.14870
109 ->115 -0.10349
109 ->118 0.10319
110 ->118 -0.39720

Excited State 35: Singlet-A 6.9076 eV 179.49 nm f=0.1219 <S**2>=0.000
106 ->113 0.30905
107 ->114 -0.28106
108 ->113 -0.12153
109 ->118 -0.11856
110 ->118 0.48402

Excited State 36: Singlet-A 6.9143 eV 179.31 nm f=0.0390 <S**2>=0.000
106 ->113 0.28109
107 ->114 0.59099
107 ->115 -0.10995

Excited State 37: Singlet-A 6.9552 eV 178.26 nm f=0.0001 <S**2>=0.000
90 ->111 0.11738
93 ->111 0.10334
94 ->111 0.17097
95 ->111 0.64055
98 ->111 -0.12582

Excited State 38: Singlet-A 6.9825 eV 177.56 nm f=0.2878 <S**2>=0.000
88 ->111 -0.10022
89 ->111 0.11682
91 ->111 0.10735
94 ->111 -0.12689
107 ->112 0.38990
108 ->113 0.12272
108 ->115 -0.16544
108 ->116 0.16171
109 ->115 0.20032
109 ->116 0.24817
110 ->118 -0.19194

Excited State 39: Singlet-A 7.0265 eV 176.45 nm f=0.0162 <S**2>=0.000
85 ->111 -0.10479
87 ->111 0.34335
89 ->111 0.50078
92 ->111 0.10736
95 ->111 -0.12585
97 ->111 -0.11425

Excited State 40: Singlet-A 7.0658 eV 175.47 nm f=0.0356 <S**2>=0.000
106 ->113 0.11153
107 ->112 0.13537
108 ->113 0.10324
108 ->115 0.52979
108 ->116 -0.32505

Excited State 41: Singlet-A 7.1634 eV 173.08 nm f=0.0038 <S**2>=0.000
109 ->120 0.10438
110 ->117 -0.23569
110 ->119 0.32715
110 ->120 0.50705
110 ->121 0.12440
110 ->122 0.10619

Excited State 42: Singlet-A 7.2021 eV 172.15 nm f=0.0042 <S**2>=0.000
87 ->111 -0.14984
90 ->111 -0.12133
91 ->111 0.11445
93 ->111 0.10130
106 ->114 0.53041
106 ->115 -0.18507
106 ->116 0.12886

Excited State 43: Singlet-A 7.2203 eV 171.72 nm f=0.0109 <S**2>=0.000
87 ->111 0.11795
88 ->111 -0.22793
90 ->111 0.19258
91 ->111 0.47422

92 ->111 -0.24286
93 ->111 -0.12180
94 ->111 0.19999

Excited State 44: Singlet-A 7.2377 eV 171.30 nm f=0.0015 <S**2>=0.000
84 ->111 -0.13298
87 ->111 0.37037
90 ->111 0.30200
91 ->111 -0.29003
93 ->111 -0.17862
106 ->114 0.23108
106 ->115 -0.10149

Excited State 45: Singlet-A 7.2689 eV 170.57 nm f=0.0572 <S**2>=0.000
107 ->115 -0.39979
108 ->115 0.30218
108 ->116 0.44738

Excited State 46: Singlet-A 7.2797 eV 170.32 nm f=0.0545 <S**2>=0.000
106 ->114 -0.16314
107 ->115 0.47861
108 ->115 0.22581
108 ->116 0.36405

Excited State 47: Singlet-A 7.3206 eV 169.36 nm f=0.0000 <S**2>=0.000
99 ->112 -0.14311
100 ->112 0.10824
105 ->112 0.67662

Excited State 48: Singlet-A 7.3512 eV 168.66 nm f=0.0011 <S**2>=0.000
110 ->117 0.43373
110 ->119 -0.12767
110 ->120 0.14510
110 ->121 0.19847
110 ->122 0.43216
110 ->123 -0.15091

Excited State 49: Singlet-A 7.3663 eV 168.31 nm f=0.0521 <S**2>=0.000
94 ->112 -0.11568
107 ->116 0.64869

Excited State 50: Singlet-A 7.4214 eV 167.06 nm f=0.0010 <S**2>=0.000
90 ->111 -0.11939
110 ->117 0.40799
110 ->120 0.24237
110 ->122 -0.37059
110 ->123 0.28620

E-isomers (Ground state optimized geometry)

Energy = -1234.98681356 au

Table S3: Coordinates of optimized structure of **E-isomers** (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.616799	-3.186256	-0.610697
2	6	0	-3.392577	-3.631750	-0.299551
3	6	0	-2.420455	-2.725056	0.336839
4	6	0	-2.800618	-1.502519	0.668834
5	6	0	-4.123873	-1.059488	0.375475
6	6	0	-5.001473	-1.799660	-0.288410
7	8	0	-1.083609	-3.106063	0.520647
8	6	0	13.125528	1.164235	-0.492107
9	6	0	11.686789	1.649818	-0.751197
10	6	0	10.690288	0.560395	-0.313189
11	6	0	9.249739	1.068652	-0.513672
12	6	0	8.260804	-0.029204	-0.084563
13	6	0	6.812500	0.494154	-0.173081
14	6	0	5.858655	-0.645972	0.225565
15	6	0	4.396559	-0.156218	0.282406
16	6	0	3.506602	-1.378895	0.584229
17	6	0	2.026777	-0.983184	0.746794
18	6	0	1.192254	-2.284394	0.805572
19	6	0	-0.301828	-1.957977	0.942836
20	6	0	-6.393007	-1.274076	-0.696921
21	6	0	-6.933521	-0.016044	-0.712775
22	6	0	-8.319193	0.063449	-1.033509
23	7	0	-9.438474	0.128217	-1.292644
24	6	0	-6.249582	1.304670	-0.388110
25	6	0	-4.951707	1.512070	-0.589571
26	6	0	-4.293959	2.711979	-0.161729
27	6	0	-4.990906	3.657807	0.441766
28	6	0	-6.442594	3.509801	0.601821
29	6	0	-7.046478	2.392280	0.190523
30	7	0	-4.323895	4.760150	0.936554
31	1	0	-5.270222	-3.794253	-1.061778
32	1	0	-3.138500	-4.578273	-0.498756
33	1	0	-2.158690	-0.887520	1.126770
34	1	0	-4.402488	-0.150028	0.684078
35	1	0	13.772770	1.871391	-0.776414
36	1	0	13.294918	0.328513	-1.014553
37	1	0	13.244162	0.977094	0.483089
38	1	0	11.517911	2.485422	-0.228446
39	1	0	11.568664	1.836619	-1.726464
40	1	0	10.832812	-0.262060	-0.863942
41	1	0	10.835863	0.344850	0.652378
42	1	0	9.103437	1.886485	0.042976
43	1	0	9.104813	1.290812	-1.477802
44	1	0	8.363555	-0.820175	-0.687729

45	1	0	8.457028	-0.300331	0.857748
46	1	0	6.694195	1.266912	0.450440
47	1	0	6.616048	0.787060	-1.108764
48	1	0	5.930197	-1.381450	-0.448127
49	1	0	6.122044	-0.991501	1.126258
50	1	0	4.293875	0.526929	1.005422
51	1	0	4.137334	0.245655	-0.595771
52	1	0	3.586224	-2.031008	-0.169676
53	1	0	3.821896	-1.807426	1.430907
54	1	0	1.904995	-0.462785	1.591948
55	1	0	1.735931	-0.427685	-0.032178
56	1	0	1.339089	-2.807741	-0.033759
57	1	0	1.484329	-2.827401	1.592867
58	1	0	-0.526134	-1.171279	0.367727
59	1	0	-0.510787	-1.744161	1.897151
60	1	0	-7.019657	-1.987895	-1.009655
61	1	0	-4.416273	0.807356	-1.055161
62	1	0	-3.313789	2.832084	-0.319239
63	1	0	-6.978216	4.244525	1.017982
64	1	0	-8.038200	2.296896	0.276582
65	1	0	-4.819268	5.462294	1.428379
66	1	0	-3.331958	4.820290	0.841493

E-isomers (1st excited-state optimized geometry)

Energy = -1235.29531435 au

Table S4: Coordinates of optimized structure of **E-isomers** (ES)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.364162	-2.937903	0.460492
2	6	0	2.990875	-3.050885	0.602224
3	6	0	2.155370	-1.988752	0.222487
4	6	0	2.726814	-0.820441	-0.303979
5	6	0	4.109795	-0.716001	-0.427364
6	6	0	4.966002	-1.762061	-0.039352
7	8	0	0.821873	-2.191885	0.393000
8	6	0	-14.030128	1.033267	-0.071920
9	6	0	-12.609021	1.525406	-0.364565
10	6	0	-11.526091	0.502639	0.002623
11	6	0	-10.099793	0.987180	-0.287468
12	6	0	-9.017195	-0.035946	0.079928
13	6	0	-7.591001	0.448985	-0.210910
14	6	0	-6.508563	-0.574307	0.156480
15	6	0	-5.082616	-0.089162	-0.135280
16	6	0	-4.001061	-1.113026	0.232359
17	6	0	-2.575622	-0.626730	-0.060982
18	6	0	-1.500888	-1.656862	0.309720

19	6	0	-0.092431	-1.161624	0.012212
20	6	0	6.419849	-1.745919	-0.198805
21	6	0	7.302575	-0.711583	-0.300885
22	6	0	8.661292	-1.069252	-0.608808
23	7	0	9.763790	-1.336716	-0.874267
24	6	0	7.061980	0.742013	-0.100161
25	6	0	6.294915	1.216860	0.977286
26	6	0	6.108134	2.576728	1.186572
27	6	0	6.693226	3.523927	0.325630
28	6	0	7.476515	3.055895	-0.743644
29	6	0	7.661317	1.693109	-0.942583
30	7	0	6.555521	4.888301	0.567787
31	1	0	4.996649	-3.774653	0.747358
32	1	0	2.536255	-3.954455	0.995854
33	1	0	2.104304	0.006207	-0.626257
34	1	0	4.527882	0.190405	-0.849657
35	1	0	-14.779162	1.785509	-0.344670
36	1	0	-14.159350	0.805724	0.993479
37	1	0	-14.256597	0.118792	-0.634046
38	1	0	-12.521389	1.777963	-1.430964
39	1	0	-12.424940	2.460014	0.184347
40	1	0	-11.614327	0.249571	1.069860
41	1	0	-11.711069	-0.433006	-0.546152
42	1	0	-10.012633	1.240239	-1.354695
43	1	0	-9.915869	1.922961	0.261271
44	1	0	-9.103956	-0.288814	1.147168
45	1	0	-9.201131	-0.971771	-0.468568
46	1	0	-7.504145	0.701704	-1.278197
47	1	0	-7.406859	1.384816	0.337592
48	1	0	-6.594723	-0.826750	1.223814
49	1	0	-6.692600	-1.510209	-0.391728
50	1	0	-4.996167	0.162892	-1.202716
51	1	0	-4.898157	0.846698	0.413011
52	1	0	-4.085324	-1.364644	1.299713
53	1	0	-4.184100	-2.048869	-0.315633
54	1	0	-2.491569	-0.375910	-1.128722
55	1	0	-2.392578	0.309121	0.487484
56	1	0	-1.567306	-1.904787	1.376849
57	1	0	-1.667418	-2.591304	-0.241334
58	1	0	0.126138	-0.243009	0.576073
59	1	0	0.024742	-0.936816	-1.057885
60	1	0	6.861743	-2.739017	-0.263498
61	1	0	5.843506	0.508081	1.664569
62	1	0	5.520478	2.916449	2.036608
63	1	0	7.951740	3.768964	-1.413461
64	1	0	8.283448	1.358165	-1.768115
65	1	0	6.701493	5.491877	-0.231202
66	1	0	5.742355	5.158510	1.105971

TD-DFT obtained Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1698 eV 391.14 nm f=0.4200 <S**2>=0.000
110 ->111 0.70227

Excited State 2: Singlet-A 4.0025 eV 309.77 nm f=0.4017 <S**2>=0.000
109 ->111 0.68733
110 ->114 -0.12780

Excited State 3: Singlet-A 4.3038 eV 288.08 nm f=0.0158 <S**2>=0.000
107 ->111 0.12357
108 ->111 -0.40653
110 ->112 0.55033

Excited State 4: Singlet-A 4.5240 eV 274.06 nm f=0.0104 <S**2>=0.000
107 ->111 0.45935
108 ->111 0.30219
109 ->112 0.11823
110 ->112 0.15057
110 ->113 -0.39256

Excited State 5: Singlet-A 4.6404 eV 267.18 nm f=0.1550 <S**2>=0.000
107 ->111 -0.17420
108 ->111 0.48231
108 ->114 0.10129
109 ->112 -0.10383
110 ->112 0.36717
110 ->113 0.26336

Excited State 6: Singlet-A 4.8959 eV 253.24 nm f=0.0234 <S**2>=0.000
107 ->111 0.41754
109 ->112 0.18837
110 ->112 -0.15450
110 ->113 0.49906

Excited State 7: Singlet-A 5.1077 eV 242.74 nm f=0.2477 <S**2>=0.000
106 ->111 0.12933
109 ->111 0.10427
109 ->114 0.10162
110 ->114 0.63401
110 ->115 -0.16223

Excited State 8: Singlet-A 5.2612 eV 235.66 nm f=0.0871 <S**2>=0.000
107 ->111 -0.20774
108 ->114 -0.10409
109 ->112 0.62481
109 ->113 0.18015

Excited State 9: Singlet-A 5.3567 eV 231.46 nm f=0.1147 <S**2>=0.000
106 ->111 0.58961
110 ->114 -0.16596
110 ->115 -0.30496

Excited State 10: Singlet-A 5.5429 eV 223.68 nm f=0.0489 <S**2>=0.000
107 ->111 0.14017
107 ->115 -0.10780
109 ->112 -0.13756
109 ->113 0.64728

Excited State 11: Singlet-A 5.6433 eV 219.70 nm f=0.0470 <S**2>=0.000
106 ->111 0.24872
107 ->112 -0.10236
110 ->114 0.11194
110 ->115 0.52554
110 ->116 0.33357

Excited State 12: Singlet-A 5.7878 eV 214.22 nm f=0.0515 <S**2>=0.000
109 ->114 0.59904
110 ->115 -0.12535
110 ->116 0.30914

Excited State 13: Singlet-A 5.8355 eV 212.47 nm f=0.0094 <S**2>=0.000
106 ->111 -0.16958
108 ->112 -0.17749
109 ->114 -0.29121
110 ->115 -0.23248
110 ->116 0.48561

Excited State 14: Singlet-A 5.8693 eV 211.24 nm f=0.0000 <S**2>=0.000
105 ->111 0.70156

Excited State 15: Singlet-A 6.0909 eV 203.56 nm f=0.0591 <S**2>=0.000
93 ->111 0.27096
96 ->111 0.12504
102 ->111 -0.11006
103 ->111 0.49917
108 ->112 -0.29285

Excited State 16: Singlet-A 6.1337 eV 202.13 nm f=0.0811 <S**2>=0.000
93 ->111 0.14084
103 ->111 0.23223
107 ->112 0.10844
107 ->113 -0.11676
108 ->112 0.54959
108 ->113 -0.21780

Excited State 17: Singlet-A 6.2174 eV 199.41 nm f=0.0056 <S**2>=0.000
93 ->111 0.31809
94 ->111 0.18870
95 ->111 -0.13870
96 ->111 0.34080
97 ->111 0.17793
98 ->111 -0.22859

103 ->111 -0.33738

Excited State 18: Singlet-A 6.3037 eV 196.69 nm f=0.0336 <S**2>=0.000
107 ->112 0.51543
107 ->113 0.10627
108 ->113 -0.23894
109 ->115 -0.37788

Excited State 19: Singlet-A 6.4014 eV 193.68 nm f=0.0492 <S**2>=0.000
97 ->111 0.14282
107 ->112 0.20061
107 ->113 0.31943
108 ->113 -0.20899
109 ->115 0.46828
109 ->116 0.12126

Excited State 20: Singlet-A 6.4517 eV 192.17 nm f=0.0112 <S**2>=0.000
93 ->111 0.44498
95 ->111 0.27020
96 ->111 -0.11237
98 ->111 0.38149
103 ->111 -0.13048

Excited State 21: Singlet-A 6.4978 eV 190.81 nm f=0.0233 <S**2>=0.000
106 ->112 0.60141
108 ->114 -0.30792
109 ->116 -0.10064

Excited State 22: Singlet-A 6.5861 eV 188.25 nm f=0.0491 <S**2>=0.000
95 ->111 0.11697
97 ->111 0.24704
102 ->111 -0.19875
106 ->112 0.19608
107 ->113 -0.17510
108 ->114 0.40108
109 ->116 -0.21224

Excited State 23: Singlet-A 6.5899 eV 188.14 nm f=0.0487 <S**2>=0.000
95 ->111 -0.10875
97 ->111 -0.24079
102 ->111 0.23042
106 ->112 0.26657
106 ->113 -0.10852
108 ->114 0.33441
109 ->116 0.31885

Excited State 24: Singlet-A 6.6099 eV 187.57 nm f=0.0142 <S**2>=0.000
97 ->111 0.11883
100 ->111 0.25609
102 ->111 0.55671
103 ->111 0.10763

109 ->116 -0.26111

Excited State 25: Singlet-A 6.6298 eV 187.01 nm f=0.0251 <S**2>=0.000
97 ->111 0.19160
100 ->111 0.26968
104 ->111 0.53802
108 ->113 0.12581
109 ->116 0.23345

Excited State 26: Singlet-A 6.6434 eV 186.63 nm f=0.0710 <S**2>=0.000
95 ->111 -0.10077
97 ->111 -0.31985
104 ->111 0.38531
107 ->112 -0.11689
107 ->113 0.15325
108 ->113 -0.18628
109 ->116 -0.28566

Excited State 27: Singlet-A 6.6532 eV 186.35 nm f=0.0009 <S**2>=0.000
99 ->111 -0.20562
101 ->111 0.66555

Excited State 28: Singlet-A 6.7120 eV 184.72 nm f=0.0082 <S**2>=0.000
96 ->111 -0.17672
100 ->111 0.55529
102 ->111 -0.24653

104 ->111 -0.23205

Excited State 29: Singlet-A 6.7679 eV 183.20 nm f=0.1536 <S**2>=0.000
89 ->111 0.13121
95 ->111 -0.11517
99 ->111 0.31140
106 ->113 -0.11374
107 ->113 -0.12504
107 ->114 0.46430
108 ->113 -0.21846
108 ->114 -0.13044

Excited State 30: Singlet-A 6.7756 eV 182.99 nm f=0.0402 <S**2>=0.000
95 ->111 -0.11095
99 ->111 0.55704
101 ->111 0.17210
107 ->114 -0.29872
108 ->113 0.10100

Excited State 31: Singlet-A 6.7925 eV 182.53 nm f=0.2898 <S**2>=0.000
106 ->113 -0.13177
107 ->113 0.32928
107 ->114 0.34553
108 ->112 0.15817

108 ->113 0.32817
109 ->114 -0.10573

Excited State 32: Singlet-A 6.8030 eV 182.25 nm f=0.0250 <S**2>=0.000
89 ->111 0.20516
90 ->111 -0.11095
94 ->111 0.15851
95 ->111 -0.23256
96 ->111 0.22187
98 ->111 0.46593
100 ->111 0.10010
107 ->113 0.15739

Excited State 33: Singlet-A 6.8324 eV 181.47 nm f=0.0082 <S**2>=0.000
91 ->111 0.42498
92 ->111 0.48113
97 ->111 -0.11296
108 ->113 -0.11698

Excited State 34: Singlet-A 6.8698 eV 180.48 nm f=0.0223 <S**2>=0.000
106 ->113 0.63706
107 ->114 0.19270

Excited State 35: Singlet-A 6.9147 eV 179.31 nm f=0.0018 <S**2>=0.000
88 ->111 0.13767
89 ->111 0.33108
91 ->111 -0.22257
94 ->111 -0.20231
95 ->111 0.27322
96 ->111 0.19113
97 ->111 -0.27584
98 ->111 -0.15015
100 ->111 0.13321

Excited State 36: Singlet-A 6.9357 eV 178.76 nm f=0.0292 <S**2>=0.000
107 ->113 0.12377
109 ->118 -0.13652
110 ->117 0.29116
110 ->118 0.56043

Excited State 37: Singlet-A 6.9627 eV 178.07 nm f=0.2370 <S**2>=0.000
89 ->111 -0.23594
96 ->111 0.29690
97 ->111 -0.22296
100 ->111 0.10065
106 ->114 -0.19150
107 ->112 0.21542
107 ->113 -0.26320
108 ->113 0.12779
109 ->115 0.19469

Excited State 38: Singlet-A 7.0199 eV 176.62 nm f=0.1654 <S**2>=0.000
87 ->111 -0.17201
88 ->111 0.10674
89 ->111 0.32228
91 ->111 0.10314
93 ->111 0.15231
94 ->111 -0.10641
95 ->111 -0.25900
96 ->111 -0.22367
106 ->114 -0.18966
107 ->112 0.16033
107 ->113 -0.14940
108 ->113 0.11502
109 ->115 0.14616

Excited State 39: Singlet-A 7.0620 eV 175.56 nm f=0.0160 <S**2>=0.000
89 ->111 0.17041
90 ->111 -0.10976
94 ->111 0.54629
95 ->111 0.30472
96 ->111 -0.13863
99 ->111 0.11253

Excited State 40: Singlet-A 7.0693 eV 175.38 nm f=0.0813 <S**2>=0.000
106 ->114 0.58590
107 ->112 0.11581
108 ->113 0.11237
108 ->115 0.16551
109 ->116 -0.17887

Excited State 41: Singlet-A 7.1285 eV 173.93 nm f=0.0374 <S**2>=0.000
108 ->115 0.65261

Excited State 42: Singlet-A 7.2166 eV 171.80 nm f=0.0095 <S**2>=0.000
107 ->115 0.10088
110 ->117 -0.24641
110 ->119 0.30772
110 ->120 0.50702
110 ->121 -0.11218
110 ->122 0.10067

Excited State 43: Singlet-A 7.2309 eV 171.46 nm f=0.0001 <S**2>=0.000
105 ->112 0.69118

Excited State 44: Singlet-A 7.2986 eV 169.87 nm f=0.0216 <S**2>=0.000
87 ->111 -0.20066
88 ->111 0.31295
90 ->111 0.28424
91 ->111 0.30785
92 ->111 -0.29614
93 ->111 -0.14081

96 ->111 0.18429

Excited State 45: Singlet-A 7.3177 eV 169.43 nm f=0.1218 <S**2>=0.000
88 ->111 -0.13596
90 ->111 -0.13706
97 ->112 -0.14899
107 ->115 0.56801

Excited State 46: Singlet-A 7.3370 eV 168.99 nm f=0.0181 <S**2>=0.000
87 ->111 0.11877
88 ->111 0.25134
89 ->111 -0.13868
90 ->111 0.34279
91 ->111 -0.28421
92 ->111 0.26049
94 ->111 0.13994
95 ->111 -0.13512
107 ->115 0.21769

Excited State 47: Singlet-A 7.3783 eV 168.04 nm f=0.0118 <S**2>=0.000
108 ->116 -0.18232
110 ->117 0.25604
110 ->118 -0.11125
110 ->119 -0.13232
110 ->121 -0.24133
110 ->122 0.51624

Excited State 48: Singlet-A 7.3875 eV 167.83 nm f=0.0151 <S**2>=0.000
103 ->112 -0.19980
107 ->116 0.10541
108 ->116 0.59367
110 ->122 0.12873

Excited State 49: Singlet-A 7.4719 eV 165.93 nm f=0.0014 <S**2>=0.000
110 ->117 0.43928
110 ->118 -0.28372
110 ->120 0.26382
110 ->122 -0.30540
110 ->123 0.15003

Excited State 50: Singlet-A 7.4875 eV 165.59 nm f=0.0029 <S**2>=0.000
90 ->112 0.10089
94 ->112 -0.15932
95 ->112 0.25944
95 ->113 -0.13343
96 ->112 -0.18573
98 ->112 0.24792
98 ->113 -0.12477
103 ->112 0.35768
103 ->113 -0.12213
107 ->115 -0.10086

108 ->116 0.14697

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