Supporting Information

Density Functional Theory Calculation on the Structural, Electronic and Optical Properties of Fluorene Based Azo Compounds

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Figures (from DFT-B3LYP/6-31+G(d,p) calculation)

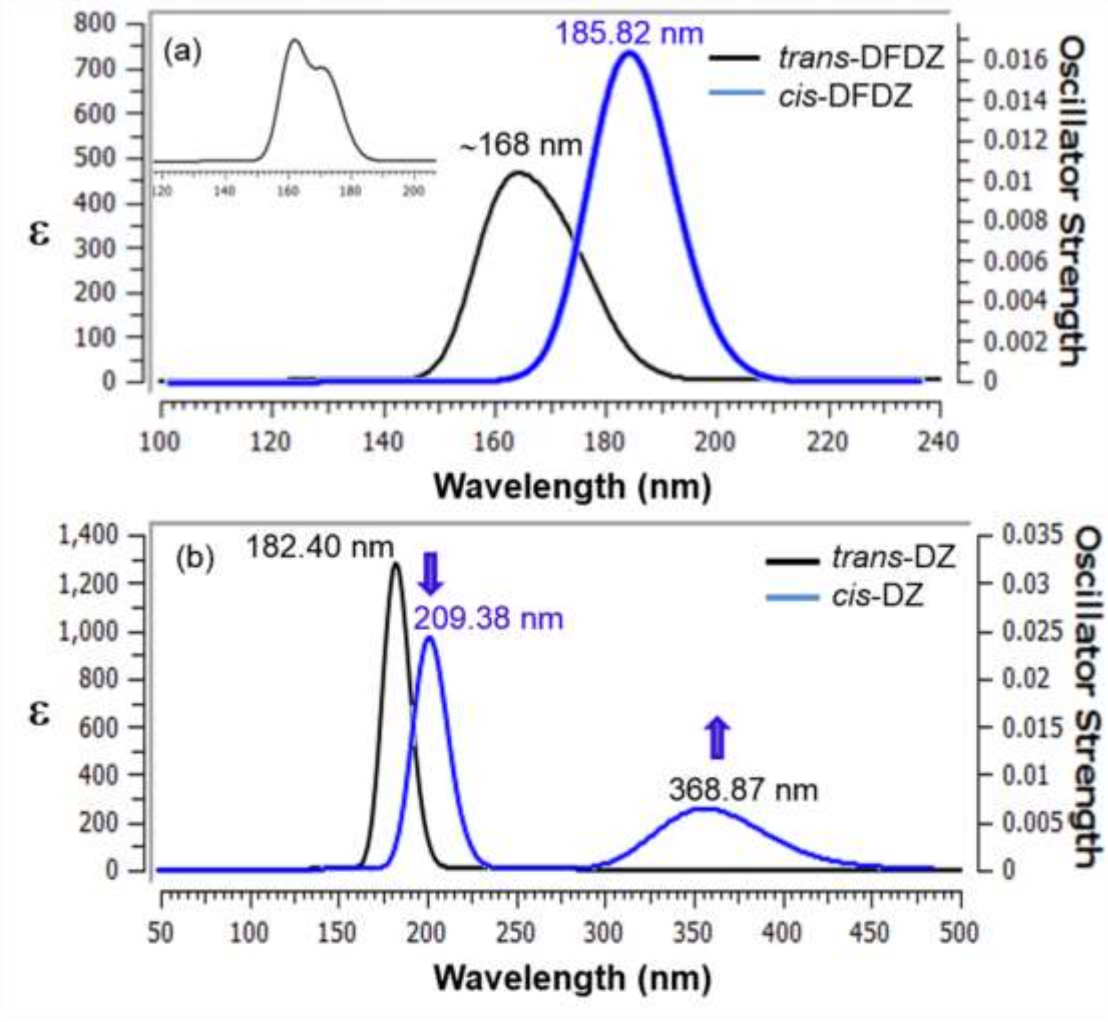


Figure S1. Electronic UV-Vis spectra of (a) DFDZ; (b) DZ by TD-DFT from B3LYP/6-31+G(d,p) calculation by using different initial HF/6-31+G(d,p) geometry. The calculated UV-Vis spectra are represented with a Gaussian UV-Vis peak half-width at half height 0.333 eV. The inset spectrum of *trans*-DFDZ (a) is shown from Gaussian UV-Vis peak half-width at half height 0.233 eV.

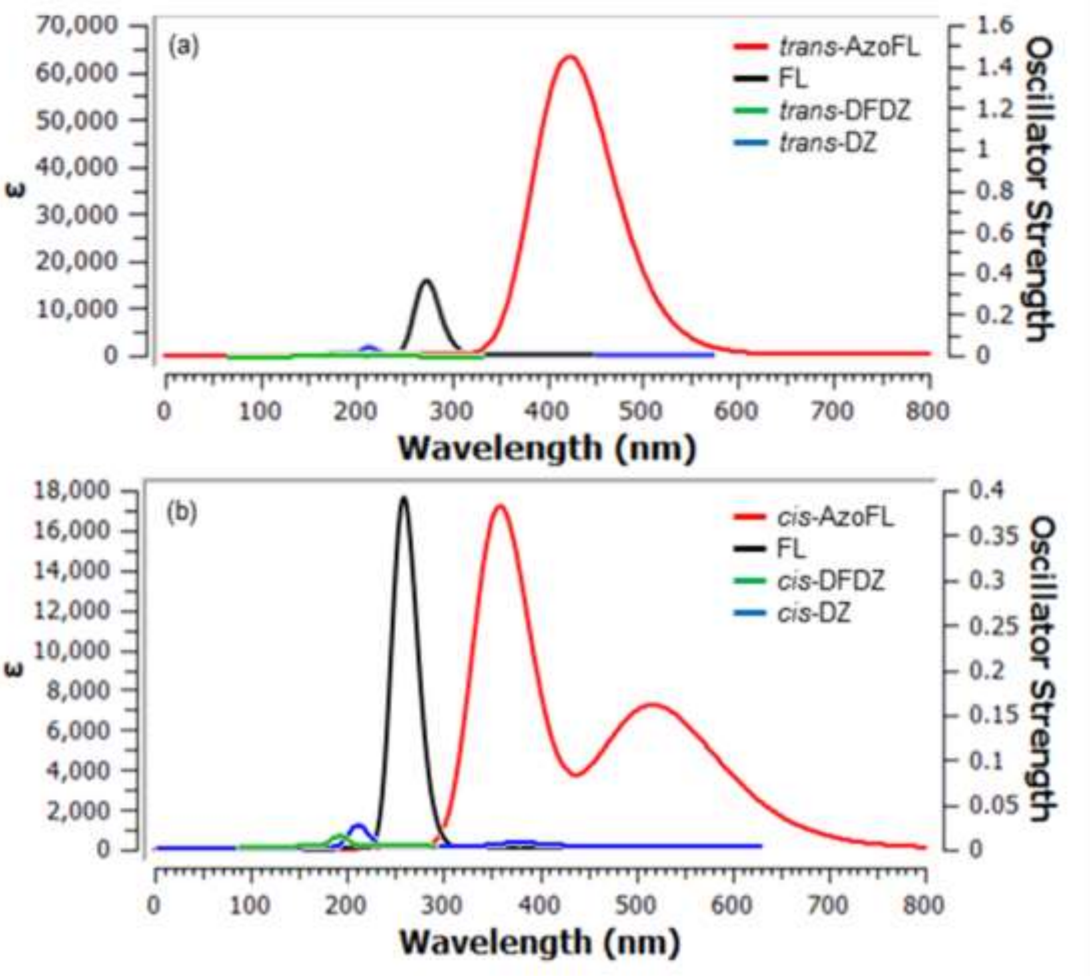
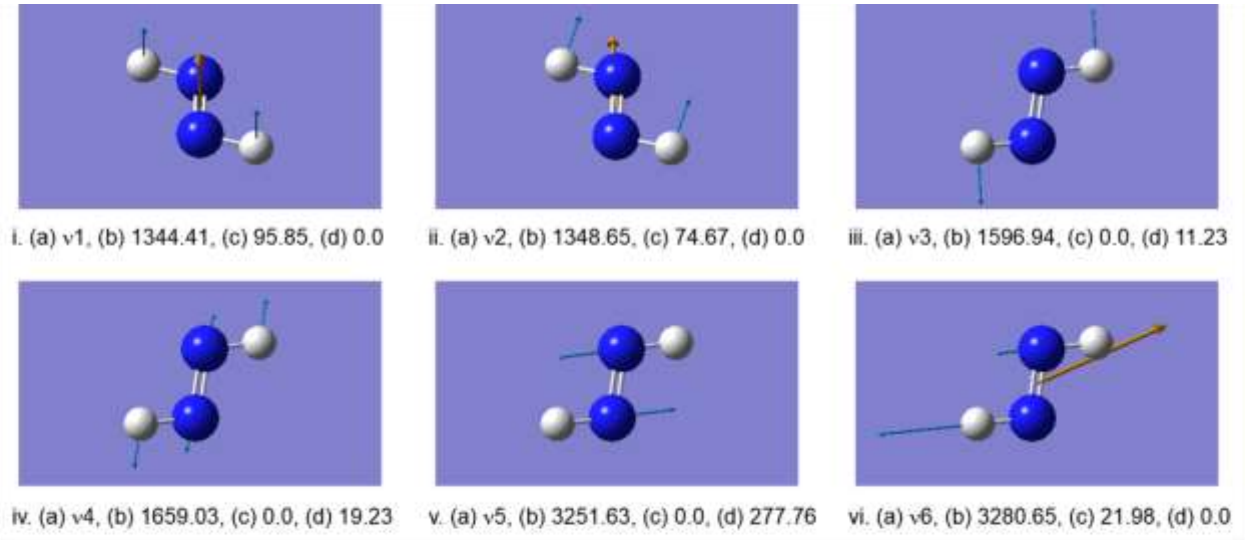


Figure S2. A comparison of UV-Vis spectra for (a) *trans*- and (b) *cis*-isomers of AzoFL (red line); DZ (blue line); DFDZ (green line); FL (black line) calculated by TD-DFT/B3LYP/6-31+G(d,p) method (All the starting geometries are obtained from DFT/B3LYP/6-31+G(d,p) method). The calculated UV-Vis spectra are represented with a Gaussian UV-Vis peak half-width at half height 0.333 eV.



i. (a) ν1, (b) 1344.41, (c) 95.85, (d) 0.0

ii. (a) ν2, (b) 1348.65, (c) 74.67, (d) 0.0

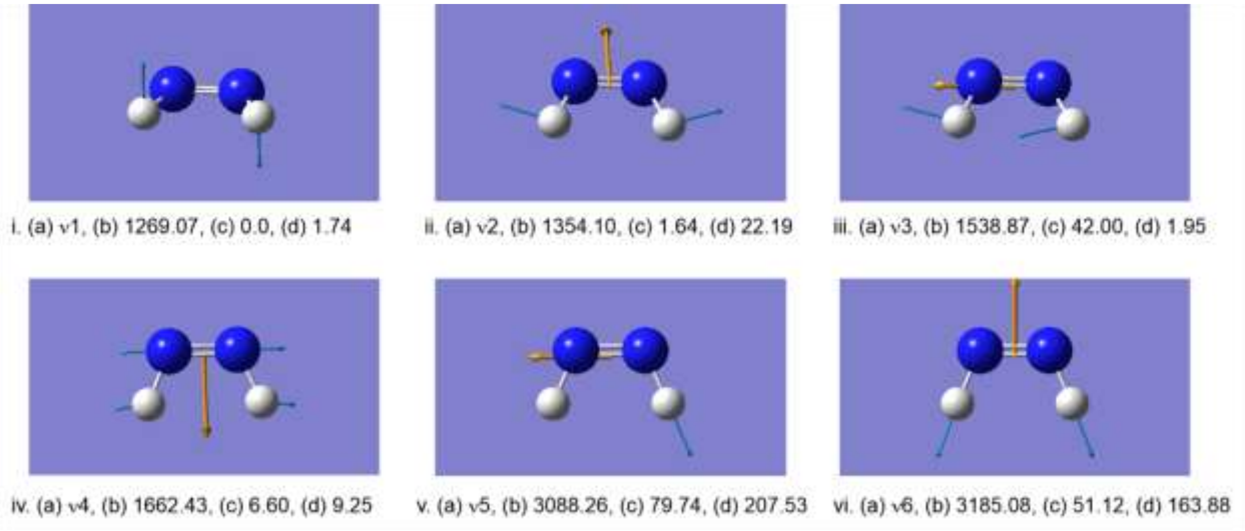
iii. (a) ν3, (b) 1596.94, (c) 0.0, (d) 11.23

iv. (a) ν4, (b) 1659.03, (c) 0.0, (d) 19.23

v. (a) ν5, (b) 3251.63, (c) 0.0, (d) 277.76

vi. (a) ν6, (b) 3280.65, (c) 21.98, (d) 0.0

Figure S3. (a) vibrational mode (b) frequency (c) IR intensity (d) Raman scattering activities of *trans*-DZ; (i) out-of-plane vibration of HNN (ii) in-plane vibration of HNN (iii) in-plane vibration of HNNH; (iv) stretching vibration of N=N (v) symmetric stretching vibration of N-H (vi) asymmetric stretching vibration of N-H. Displacement vector and dipole derivative unit vector are shown in each figure.



i. (a) ν1, (b) 1269.07, (c) 0.0, (d) 1.74

ii. (a) ν2, (b) 1354.10, (c) 1.64, (d) 22.19

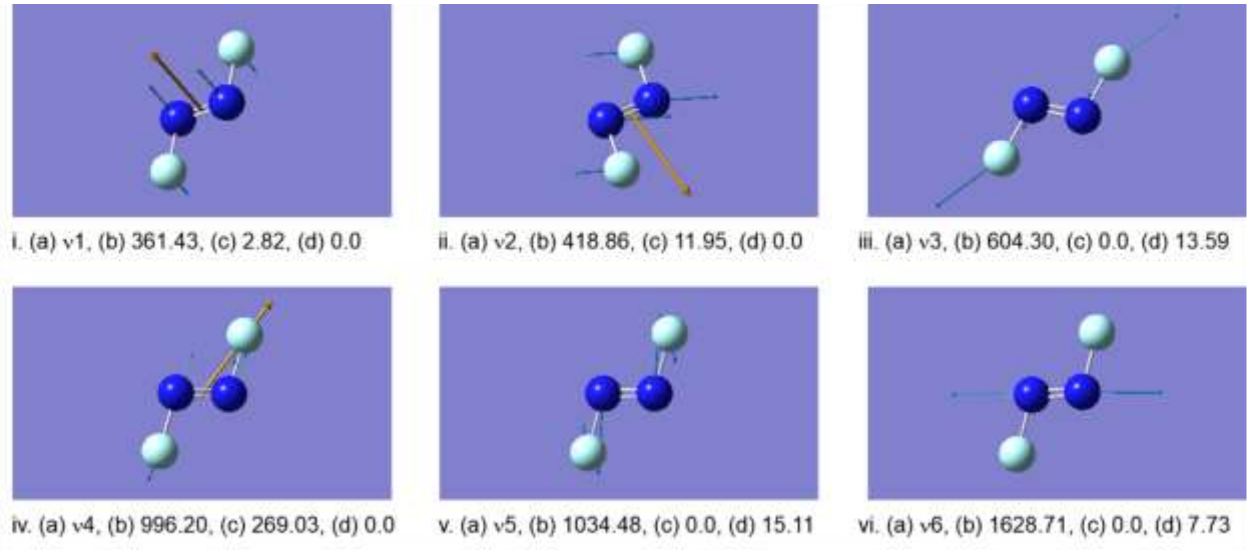
iii. (a) ν3, (b) 1538.87, (c) 42.00, (d) 1.95

iv. (a) ν4, (b) 1662.43, (c) 6.60, (d) 9.25

v. (a) ν5, (b) 3088.26, (c) 79.74, (d) 207.53

vi. (a) ν6, (b) 3185.08, (c) 51.12, (d) 163.88

Figure S4. (a) vibrational mode (b) frequency (c) IR intensity (d) Raman scattering activities of *cis*-DZ; Top left to right, (i) out-of-plane vibration of HNN (ii) in-plane vibration of HNNH (sci) (iii) in-plane vibration of HNNH (roc); Bottom left to right (iv) stretching vibration of N=N (v) asymmetric stretching vibration of N-H (vi) symmetric stretching vibration of N-H. Displacement vector and dipole derivative unit vector are shown in each figure.



i. (a) ν1, (b) 361.43, (c) 2.82, (d) 0.0

ii. (a) ν2, (b) 418.86, (c) 11.95, (d) 0.0

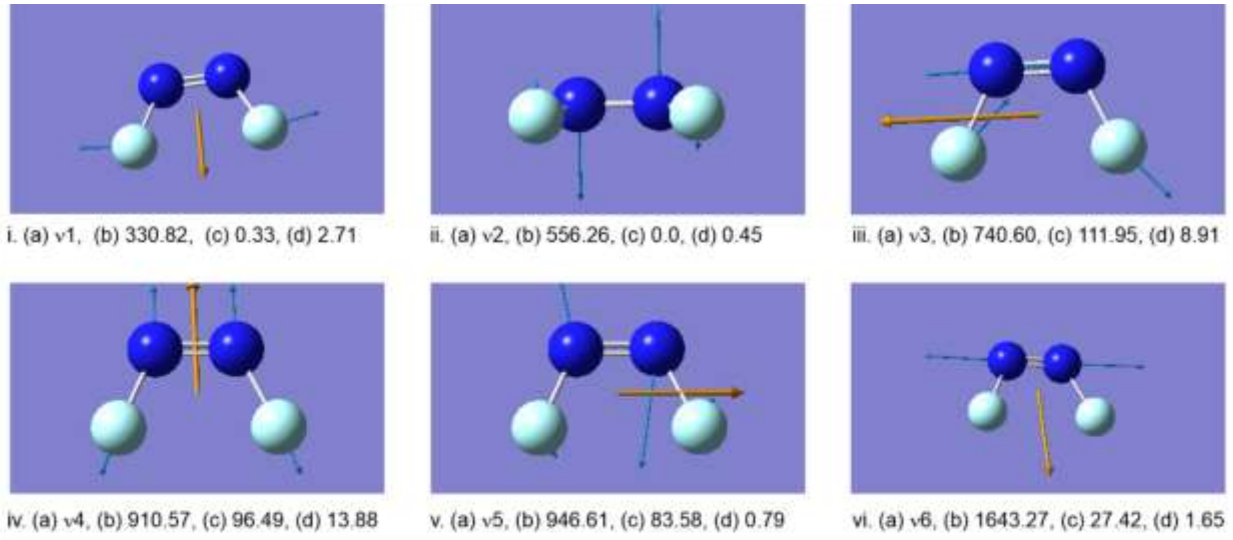
iii. (a) ν3, (b) 604.30, (c) 0.0, (d) 13.59

iv. (a) ν4, (b) 996.20, (c) 269.03, (d) 0.0

v. (a) ν5, (b) 1034.48, (c) 0.0, (d) 15.11

vi. (a) ν6, (b) 1628.71, (c) 0.0, (d) 7.73

Figure S5. (a) vibrational mode (b) frequency (c) IR intensity (d) Raman scattering activities of *trans*-DFDZ; (i) out-of-plane vibration of FNN, (ii) in-plane vibration of FNN, (iii) defm. FNNF, (iv) asymmetric stretching vibration of N-F + ip NN, (v) symmetric stretching vibration of N-F + defm FNN, (vi) stretching vibration of N=N.



i. (a) ν1, (b) 330.82, (c) 0.33, (d) 2.71

ii. (a) ν2, (b) 556.26, (c) 0.0, (d) 0.45

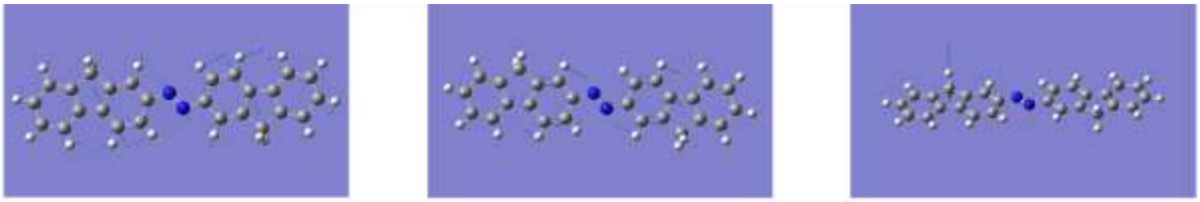
iii. (a) ν3, (b) 740.60, (c) 111.95, (d) 8.91

iv. (a) ν4, (b) 910.57, (c) 96.49, (d) 13.88

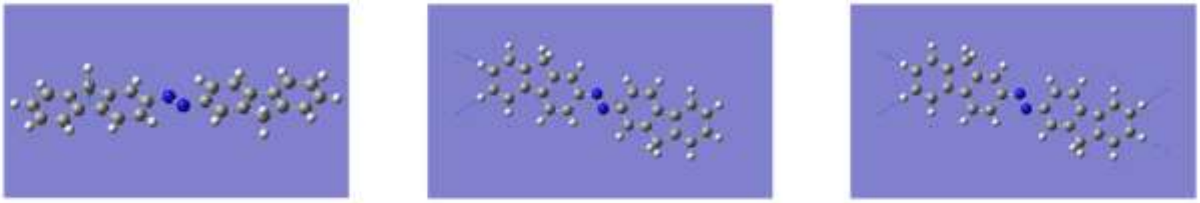
v. (a) ν5, (b) 946.61, (c) 83.58, (d) 0.79

vi. (a) ν6, (b) 1643.27, (c) 27.42, (d) 1.65

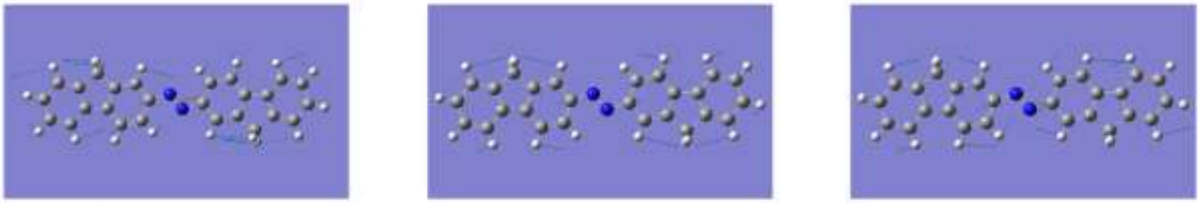
Figure S6. (a) vibrational mode (b) frequency (c) IR intensity (d) Raman scattering activities of *cis*-DFDZ; (i) in-plane vibration (sci) of FNNF (ii) out-of-plane vibration of FNF (iii) in-plane vibration (defm) of FNN; Bottom left to right (iv) symmetric stretching vibration of N-F + ip (NN) (v) asymmetric stretching vibration of N-F + ip (NN) (vi) stretching vibration of N=N. Displacement vector and dipole derivative unit vector are shown in each figure.



i. (a) ν108, (b) 1613.87, (c) 0.0, (d) 141.78 ii. (a) ν114, (b) 1658.61, (c) 0.0, (d) 7430.50 iii. (a) ν115, (b) 3033.36, (c) 25.84, (d) 0.0001

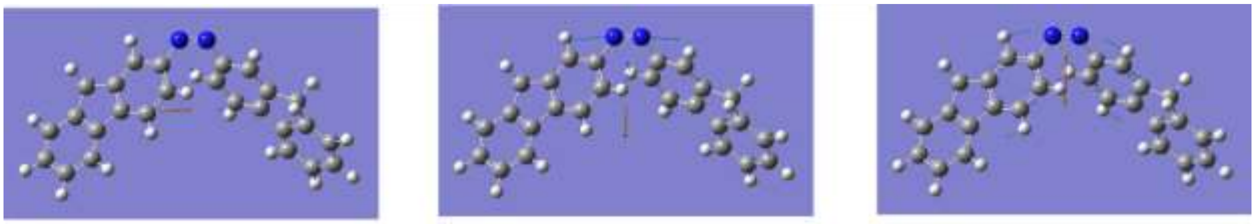


iv. (a) ν116, (b) 3033.37, (c) 0.0, (d) 387.48 v. (a) ν129, (b) 3204.19, (c) 82.78, (d) 0.0 vi. (a) ν130, (b) 3204.26, (c) 0.0, (d) 925.64



vii. (a) ν85, (b) 1231.20, (c) 54.51, (d) 0.0 viii. (a) ν86, (b) 1264.60, (c) 0.0, (d) 12036.59 ix. (a) ν87, (b) 1289.01, (c) 75.35, (d) 0.0

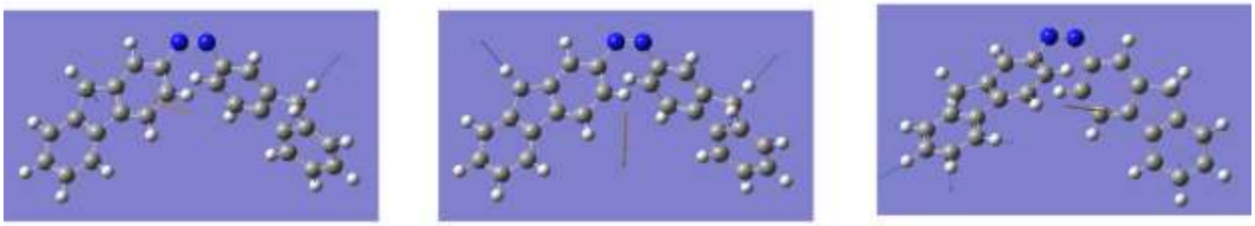
Figure S7. (a) vibrational mode (b) frequency (c) IR intensity (d) Raman scattering activities of *trans*-AzoFL; Top left to right, stretching vibration of (i) N=N (ii) C=C (iii) C_9-H. Middle left to right, stretching vibration of (iv) C_9-H (v) + (vi) C-H. Bottom left to right (vii) - (ix) stretching vibration of C-N. Displacement vector and dipole derivative unit vector are shown in each figure.



i. (a) ν 92, (b) 1345.36, (c) 33.93, (d) 100.73

ii. (a) ν 106, (b) 1581.21, (c) 77.54, (d) 6875.28

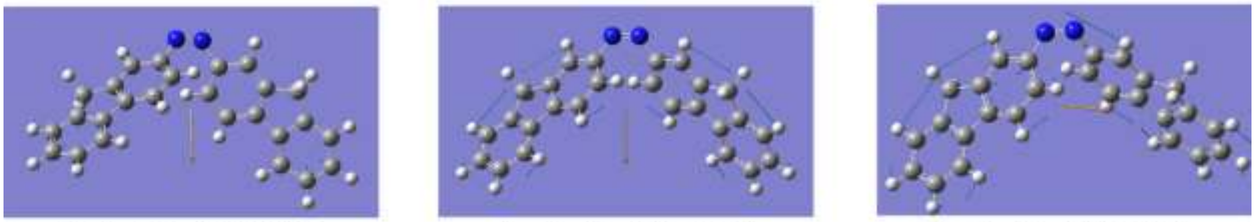
iii. (a) ν 114, (b) 1657.49, (c) 0.66, (d) 981.40



iv. (a) ν 115, (b) 3033.87, (c) 21.80, (d) 64.73

v. (a) ν 116, (b) 3033.89, (c) 7.32, (d) 388.42

vi. (a) ν 129, (b) 3204.14, (c) 32.26, (d) 178.34



vii. (a) ν 130, (b) 3204.20, (c) 30.13, (d) 552.09

viii. (a) ν 86, (b) 1260.81, (c) 0.56, (d) 1171.35

ix. (a) ν 87, (b) 1261.24, (c) 0.35, (d) 368.23

Figure S8. (a) vibrational mode (b) frequency (c) IR intensity (d) Raman scattering activities of *cis*-AzoFL; Top left to right, stretching vibration of (i) C=C (ii) N=N (iii) C=C. Middle left to right, stretching vibration of (iv) C_9-H (v) C_9-H (vi) C-H. Bottom left to right, stretching vibration of (vii) C-H (viii) - (ix) C-N. Displacement vector and dipole derivative unit vector are shown in each figure.

Tables (from DFT-B3LYP//6-31+G(d,p) calculation)

Table S1. Absorption wavelengths λ_{max} (nm), excitation energies, E_{ex} (eV), and oscillator strengths (f) obtained by TD/DFT-B3LYP/6-31+G(d,p) calculation for *trans*- and *cis*-DFDZ.

compound	electronic transition	λ_{max}	f	E_x	MO[a]	MO[b]	sym[c]	wave function[d,e]
trans-DFDZ[f]	$S_0 \rightarrow S_1$	219.74	0.0000	5.6423	16→17	0.70627	BG	H→L (99%)
	$S_0 \rightarrow S_2$	172.36	0.0067	7.1931	15→17 16→18	0.39596 0.58059	BU	H-1→L (31%) H→L+1 (67%)
	$S_0 \rightarrow S_3$	161.62	0.0092	7.6712	14→17	0.70553	AU	H-2→L (99%)
cis-DFDZ[f]	$S_0 \rightarrow S_1$	185.82	0.0181	6.6722	15→18 16→17	0.12561 0.69511	B1	H-1→L +1 (3%) H→L (96%)
	$S_0 \rightarrow S_2$	185.81	0.0000	6.6725	14→17	0.70646	A2	H-2→L (99%)
	$S_0 \rightarrow S_3$	166.23	0.0001	7.4585	15→17 16→18	0.45034 0.53729	B2	H-1→L (40%) H→L+1 (57%)

[a]molecular orbitals involved in the transition: [b]molecular orbital coefficients; [c]sym, orbital symmetry-singlet, [d]the wave functions based on the eigenvectors predicted by TD-DFT. H and L are used to denote the HOMO and LUMO. [e]percentage of contribution obtained by (100×c×c×2), where c is the co-efficient. [f]calculated by TD/DFT-B3LYP/6-31+G(d,p) from initial optimized geometry of HF/6-31+G(d,p).

Table S2. Absorption wavelengths λ_{max} (nm), excitation energies, E_{ex} (eV), and oscillator strengths (f) obtained by Zindo calculation for all the *trans*-compounds.

compound	electronic transition	λ_{max}	f	Ex	MO[a]	MO[b]	sym[c]	wave functions[d, e]
trans-DZ	$S_0 \rightarrow S_1$	516.76	0.00	2.187	6→7	0.70682	BG	H→L (99%)
	$S_0 \rightarrow S_2$	149.71	0.0678	8.2816	4→7	0.70641	AU	H-2→L (99%)
	$S_0 \rightarrow S_3$	140.80	0.4735	8.8057	5→7	0.61645	BU	H-1→L (76%)
					6→8	-0.31624		H→L+1 (20%)
trans-DFDZ	$S_0 \rightarrow S_1$	299.65	0.00	4.1464	11→13	0.70255	BG	H-1→L (99%)
	$S_0 \rightarrow S_2$	175.65	0.4028	7.0586	11→14	0.10889	BU	H-1→L+1 (2%)
					12→13	0.68740		H→L (94%)
	$S_0 \rightarrow S_3$	163.06	0.0524	7.6037	6→13	-0.12114	AU	H-6→L (2%)
					10→13	0.69654		H-2→L (97%)
trans-AzoFL	$S_0 \rightarrow S_1$	562.02	0.0105	2.2060	59→67	0.54484	B	H-7→L (59%)
					59→69	-0.22990		H-7→L+2 (10%)
					59→75	-0.17517		H-7→L+8 (6%)
					60→67	-0.25208		H-6→L (12%)
					60→69	0.10699		H-6→L+2 (2%)
	$S_0 \rightarrow S_2$	387.20	1.5678	3.2021	59→67	-0.12483	B	H-7→L (3%)
					65→68	-0.17920		H-1→L+1 (6%)
					66→67	0.65144		H→L (84%)
	$S_0 \rightarrow S_3$	315.04	0.0001	3.9355	61→67	-0.16091	A	H-5→L (5%)
					63→67	-0.20113		H-5→L (8%)
					65→67	0.50612		H-1→L (5%)
					65→69	0.12328		H-1→L +2 (3%)
					66→68	-0.29902		H→L +1 (17%)
					66→72	-0.10089		H→L +5 (3%)
FL	$S_0 \rightarrow S_1$	296.84	0.4446	4.1767	29→32	-0.12494	B2	H-2→L (3%)
					29→34	0.10311		H-2→L+2 (2%)
					30→35	0.10860		H-1→L+3 (2%)
					31→32	0.64994		H→L (84%)
	$S_0 \rightarrow S_2$	289.59	0.0001	4.2814	28→34	0.17669	A1	H-3→L+2 (6%)
					29→35	-0.19150		H-2→L+3(7%)
					30→32	0.43639		H-1→L (38%)
					31→33	0.48450		H→L+1 (46%)
	$S_0 \rightarrow S_3$	281.39	0.0170	3.9355	28→33	-0.17851	B2	H-3→L+1 (6%)
					29→32	-0.31462		H-2→L (19%)
					30→35	0.18954		H-1→L+3 (7%)
					31→32	0.15709		H→L (4%)
					31→34	-0.54432		H→L+2 (59%)

[a] molecular orbitals involved in the transition: [b]molecular orbital coefficients; [c]symmetry, singlet, [d]the wave functions based on the eigenvectors predicted by ZIndo. H and L are used to denote the HOMO and LUMO. [e]percentage of contribution obtained by (100×c×c×2), where c is the co-efficient.

Table S3. Absorption wavelengths λ_{max} (nm), excitation energies, E_{ex} (eV), and oscillator strengths (f) obtained by Zindo calculation for all the *cis*-compounds.

compound	electronic transition	λ_{max}	f	Ex	MO[a]	MO[b]	sym[c]	wave functions[d, e]
cis-DZ	$S_0 \rightarrow S_1$	524.24	0.0114	2.365	6→7	0.70705	B1	H→L (99%)
	$S_0 \rightarrow S_2$	191.59	0.00	6.4715	4→7	0.70692	A2	H-2→L (100%)
	$S_0 \rightarrow S_3$	135.98	0.5269	9.1177	4→8 5→7 6→9	0.17997 0.65437 0.16893	B2	H-2→L+1 (6%) H-1→L (85%) H→L+2 (5%)
cis-DFDZ	$S_0 \rightarrow S_1$	238.90	0.00	5.1899	6→13 10→13	0.12831 0.69519	A2	H-6→L (3%) H-2→L (96%)
	$S_0 \rightarrow S_2$	233.92	0.0543	5.3002	11→13	0.70441	B1	H-1→L (99%)
	$S_0 \rightarrow S_3$	169.51	0.3671	7.3142	10→14 12→13	-0.16009 0.68023	B2	H-2→L+1 (5%) H→L (92%)
cis-AzoFL	$S_0 \rightarrow S_1$	545.64	0.0252	2.2723	59→67 59→69 60→67 60→69 60→75 62→67 66→67	0.24310 0.13732 0.47247 0.26253 0.13889 -0.11113 0.22933	B	H-7→L (11%) H-7→ L+2 (3%) H-6→L (44%) H-6→ L+2 (13%) H-6→ L+8 (3%) H-4→ L (2%) H→ L (10%)
	$S_0 \rightarrow S_2$	355.21	0.7533	3.4905	59→67 59→69 65→68 66→67	-0.18188 -0.10053 -0.21342 0.60186	B	H-7→ L (6%) H-7→ L+2 (2%) H-7→ L+1 (9%) H→ L (72%)
	$S_0 \rightarrow S_3$	316.74	0.2766	3.9144	58→67 58→69 65→67 66→68	-0.19128 -0.10813 0.57314 -0.24780	A	H-8→ L+2 (7%) H-8→ L+2 (2) H-1→ L (65%) H→ L+1 (12%)

[a]molecular orbitals involved in the transition: [b]molecular orbital coefficients; [c]symmetry, singlet, [d]the wave functions based on the eigenvectors predicted by TD-DFT. H and L are used to denote the HOMO and LUMO. [e]percentage of contribution obtained by (100×c×c×2), where c is the co-efficient.

Table S4. Calculated vibrational frequencies of FL with B3LYP/6-31+G(d,p) in the ground state

mode no.	sym[a]	freq[b]	I_{IR}[c]	I_{Raman}[d]	k[e]	approximate description of mode[f]
1	B1	99.79	0.6106	0.1252	0.0249	butterfly mode
2	A2	138.13	0.0000	0.0073	0.0415	twist FL ring
3	A1	216.71	0.2216	0.4608	0.1211	ip FL ring
4	B1	243.42	7.4453	0.6364	0.0745	oop C_9Hs
5	A2	279.12	0.0000	4.8240	0.2023	twist (ring A, ring C) + twist C_9Hs
6	A1	419.18	0.4243	7.3573	0.6694	tor FL ring
7	B1	425.03	6.3887	0.0015	0.3031	twist (ring A CHs + ring C CHs)
8	A2	443.20	0.0000	0.8933	0.3315	roc CHs + wag C_9Hs
9	B1	482.23	0.8224	0.0241	0.4080	twist (ring A + ring C) + wag C_9Hs
10	B2	497.06	0.3277	0.1978	0.5996	defm FL ring
11	B2	551.51	0.1584	10.5162	1.0167	defm CCC + defm C_9H
12	A2	577.61	0.0000	0.0709	0.6784	wag CHs
13	B2	634.11	7.6790	0.3109	1.6397	defm CCC
14	A1	642.18	0.2985	0.3431	1.4907	wag all CHs
15	B1	708.01	5.0470	0.0123	0.9303	wag (CHs ring A, C) + wag C_9Hs
16	A2	739.75	0.0000	1.9170	0.5129	twist (CHs ring A, C) + twist C_9Hs
17	B1	754.23	134.9046	0.1000	0.4216	wag CHs
18	A1	754.67	0.0327	31.7300	1.7922	breathing FL ring
19	A2	795.98	0.0000	4.5570	0.8247	twist (CHs ring A, CHs ring C) + defm C_9Hs + twist CC
20	B2	813.37	0.4222	0.1359	1.4850	ip CCC + ip C_9Hs
21	A1	851.15	0.0780	36.5986	2.2582	ip CCC + ip C_9Hs
22	B1	871.81	0.5936	1.0956	0.5780	twist (CHs ring A + CHs ring C) + defm C_9Hs
23	A2	881.31	0.0000	0.0337	0.6488	twist (CHs ring A + CHs ring C) + oop C_9Hs
24	B1	932.16	0.0054	0.0742	0.8039	twist (CHs ring A + CHs ring C) + oop C_9Hs
25	A2	952.17	0.0000	0.0886	0.7536	twist (CHs ring A + CHs ring C) + twist C_9Hs
26	B1	975.51	3.8353	0.1005	1.0424	twist (CHs ring A + CHs ring C) + oop C_9Hs
27	A2	989.66	0.0000	0.6224	0.7474	twist (CHs ring A + CHs ring C)
28	B1	991.17	0.0500	0.0569	0.7444	twist (CHs ring A + CHs ring C) + twist CC
29	B2	1021.77	3.7746	0.4091	4.2253	asym (breathing ring A, ring C) + ip C_{11}-C_{12} + ip CCC
30	A1	1047.15	0.8604	82.3985	1.4502	sym (Breathing ring A, ring C) + ip CCC + defm CHs
31	B2	1052.43	6.5428	0.1496	1.3279	breathing (ring A, ring C) + roc CHs
32	A1	1117.24	3.0875	11.9926	1.5366	roc CHs + sci CHs
33	B2	1131.19	0.1197	0.0289	1.2637	roc CHs + sci CHs
34	A2	1155.58	0.0000	3.0002	0.8965	twist C_9Hs
35	B2	1177.41	0.0377	6.8809	1.0490	sci CHs + wag C_9Hs
36	A1	1181.55	0.0038	24.8983	0.9303	sci CHs
37	B2	1192.54	2.8540	1.8082	1.2297	sci CHs + C_9Hs
38	A1	1207.66	2.9012	16.8263	2.1703	sci CHs
39	B2	1223.69	3.3013	21.6854	1.6194	roc (C_4H, C_5H)

40	A1	1257.30	3.1240	139.6773	2.2601	sci (C_1H, C_8H)
41	A1	1323.95	0.4659	178.8203	1.9643	roc CHs
42	B2	1333.51	0.3893	1.0205	1.7467	roc CHs
43	B2	1357.03	10.2519	5.2452	4.9852	str Ar (C=C)+ sci CHs
44	A1	1386.23	0.1349	42.7804	5.1304	breathing B ring + str Ar (C=C)
45	A1	1454.09	9.6680	27.3033	1.4122	sci C_9Hs
46	A1	1481.63	9.0249	11.0564	3.1120	roc (ring A + ring C)+ sci (ring A + ring C)
47	B2	1487.48	17.4768	1.2401	2.9181	roc (ring A + ring C)+ sci (ring A + ring C)
48	A1	1513.66	0.1243	134.7581	3.9939	roc (ring A + ring C)+ sci (ring A + ring C) + sci C_9Hs
49	B2	1514.29	7.4190	8.9593	3.5263	roc (ring A + ring C)
50	A1	1623.76	1.1380	41.3439	8.6135	str Ar (C=C)
51	B2	1628.97	0.8982	0.3711	10.0846	str Ar (C=C)
52	A1	1654.80	0.0234	549.3156	10.2798	str Ar (C=C)
53	B2	1654.87	4.2392	13.0053	10.8983	str Ar (C=C)
54	A1	3032.08	15.2969	190.8769	5.7423	sym str (C_9Hs)
55	B1	3060.75	7.4160	88.2854	6.0833	asym str C_9Hs
56	B2	3173.37	2.5548	0.0949	6.4459	asym str (CH ring A + CH ring C)
57	A1	3173.71	10.0959	89.5906	6.4483	sym str + asym str (CH ring A + CH ring C)
58	B2	3179.55	2.3614	133.3531	6.4824	asym str (CH ring A + CH ring C)
59	A1	3181.13	4.4774	77.4502	6.4889	asym str (CH ring A + CH ring C)
60	B2	3190.85	7.2431	92.4392	6.5554	asym str (CH ring A + CH ring C)
61	A1	3192.06	41.4633	101.8711	6.5598	asym str (CH ring A + CH ring C)
62	B2	3203.15	48.7240	7.5319	6.6325	asym str (CH ring A, CH ring C)
63	A1	3203.80	5.9494	626.8632	6.6347	sym str (all CH ring C, CH ring A)

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[a]Sym, symmetry. [b]Vibrational frequencies in cm^{-1}. [c]Infrared intensities in KM/Mol. [d]Raman scattering activities in A^4/AMU. [e]k, Force constants in mDyne/A. [f]defm, deformation; tor, torsion; str, stretching; sym, symmetric; asym, asymmetric; oop, out-of-plane; ip, in-plane; sci, scissoring; roc, rocking; wag, waging.

Table S5. Cartesian co-ordinates for the ground state geometry of *trans*-AzoFL at DFT-B3LYP//6-31+G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.473594	0.416715	0.000076
2	7	0	-0.473594	-0.416715	0.000076
3	6	0	0.086498	1.776909	0.000154
4	6	0	1.147193	2.701284	-0.000177
5	6	0	-1.250770	2.229093	0.000485
6	6	0	0.864637	4.060200	-0.000173
7	1	0	2.165118	2.321819	-0.000416
8	6	0	-1.531069	3.590475	0.000529
9	1	0	-2.048044	1.495038	0.000721
10	6	0	1.812088	5.242917	-0.000480
11	6	0	-0.472545	4.511834	0.000181
12	1	0	-2.562706	3.931638	0.000811
13	1	0	2.467727	5.241866	-0.881428
14	6	0	0.866861	6.427600	-0.000345
15	1	0	2.468042	5.242041	0.880241
16	6	0	-0.472545	5.978432	0.000056
17	6	0	1.153252	7.789435	-0.000498
18	6	0	-1.528598	6.896078	0.000308
19	6	0	0.094288	8.706825	-0.000244
20	1	0	2.181560	8.142115	-0.000821
21	6	0	-1.234777	8.262047	0.000159

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   22          1           0       -2.561152    6.558176    0.000623
   23          1           0        0.304779    9.772381   -0.000363
   24          1           0       -2.043748    8.986872    0.000363
   25          6           0       -0.086498   -1.776909    0.000154
   26          6           0       -1.147193   -2.701284   -0.000177
   27          6           0        1.250770   -2.229093    0.000485
   28          6           0       -0.864637   -4.060200   -0.000173
   29          1           0       -2.165118   -2.321819   -0.000416
   30          6           0        1.531069   -3.590475    0.000529
   31          1           0        2.048044   -1.495038    0.000721
   32          6           0       -1.812088   -5.242917   -0.000480
   33          6           0        0.472545   -4.511834    0.000181
   34          1           0        2.562706   -3.931638    0.000811
   35          1           0       -2.467727   -5.241866   -0.881428
   36          6           0       -0.866861   -6.427600   -0.000345
   37          1           0       -2.468042   -5.242041    0.880241
   38          6           0        0.472545   -5.978432    0.000056
   39          6           0       -1.153252   -7.789435   -0.000498
   40          6           0        1.528598   -6.896078    0.000308
   41          6           0       -0.094288   -8.706825   -0.000244
   42          1           0       -2.181560   -8.142115   -0.000821
   43          6           0        1.234777   -8.262047    0.000159
   44          1           0        2.561152   -6.558176    0.000623
   45          1           0       -0.304779   -9.772381   -0.000363
   46          1           0        2.043748   -8.986872    0.000363
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Table S6. Cartesian co-ordinates for the ground state geometry of *cis*-AzoFL at DFT-B3LYP//6-31+G(d,p) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.082658	0.620291	-3.279123
2	7	0	0.082658	-0.620291	-3.279123
3	6	0	-0.077704	1.437061	-2.102050
4	6	0	-1.013112	2.486252	-2.074498
5	6	0	0.920161	1.348788	-1.112948
6	6	0	-0.990898	3.383159	-1.015622
7	1	0	-1.735776	2.566989	-2.881911
8	6	0	0.965413	2.276258	-0.073834
9	1	0	1.665110	0.563014	-1.170084
10	6	0	-1.895851	4.567168	-0.739083
11	6	0	-0.001497	3.286304	-0.012134
12	1	0	1.748680	2.207445	0.675784
13	1	0	-2.943194	4.261700	-0.614300
14	6	0	-1.316110	5.139369	0.539356
15	1	0	-1.876255	5.295581	-1.560625
16	6	0	-0.202466	4.374837	0.951501
17	6	0	-1.728290	6.241547	1.282243
18	6	0	0.501331	4.715383	2.111250
19	6	0	-1.022596	6.580875	2.444148
20	1	0	-2.584316	6.834603	0.970264
21	6	0	0.082658	5.822961	2.853505

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    22          1           0        1.359370    4.132595    2.434624
    23          1           0       -1.334362    7.438916    3.032559
    24          1           0        0.619096    6.099678    3.756546
    25          6           0        0.077704   -1.437061   -2.102050
    26          6           0        1.013112   -2.486252   -2.074498
    27          6           0       -0.920161   -1.348788   -1.112948
    28          6           0        0.990898   -3.383159   -1.015622
    29          1           0        1.735776   -2.566989   -2.881911
    30          6           0       -0.965413   -2.276258   -0.073834
    31          1           0       -1.665110   -0.563014   -1.170084
    32          6           0        1.895851   -4.567168   -0.739083
    33          6           0        0.001497   -3.286304   -0.012134
    34          1           0       -1.748680   -2.207445    0.675784
    35          1           0        2.943194   -4.261700   -0.614300
    36          6           0        1.316110   -5.139369    0.539356
    37          1           0        1.876255   -5.295581   -1.560625
    38          6           0        0.202466   -4.374837    0.951501
    39          6           0        1.728290   -6.241547    1.282243
    40          6           0       -0.501331   -4.715383    2.111250
    41          6           0        1.022596   -6.580875    2.444148
    42          1           0        2.584316   -6.834603    0.970264
    43          6           0       -0.082658   -5.822961    2.853505
    44          1           0       -1.359370   -4.132595    2.434624
    45          1           0        1.334362   -7.438916    3.032559
    46          1           0       -0.619096   -6.099678    3.756546
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Table S7. Cartesian co-ordinates for the ground state geometry of *trans*-DFDZ at DFT-B3LYP//6-31+G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	0.591248	1.554890	0.000000
2	7	0	0.591248	0.159907	0.000000
3	7	0	-0.591248	-0.159907	0.000000
4	9	0	-0.591248	-1.554890	0.000000

Table S8. Cartesian co-ordinates for the ground state geometry of *cis*-DFDZ at DFT-B3LYP//6-31+G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	0.000000	1.198097	-0.555025
2	7	0	0.000000	0.608341	0.713603
3	7	0	0.000000	-0.608341	0.713603
4	9	0	0.000000	-1.198097	-0.555025

Table S9. Cartesian co-ordinates for the ground state geometry of *trans*-DZ at DFT-B3LYP//6-31+G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.992451	0.920407	0.000000
2	7	0	0.000000	0.622151	0.000000
3	7	0	0.000000	-0.622151	0.000000
4	1	0	0.992451	-0.920407	0.000000

Table S10. Cartesian co-ordinates for the ground state geometry of *cis*-DZ at DFT-B3LYP//6-31+G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.028268	0.840028
2	7	0	0.000000	0.620857	-0.120004
3	7	0	0.000000	-0.620857	-0.120004
4	1	0	0.000000	-1.028268	0.840028

Table S11. Cartesian co-ordinates for the ground state geometry of FL at DFT-B3LYP//6-31+G(d,p) level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.880530	0.000000	2.489546
2	6	0	0.000000	3.019587	-1.212779
3	6	0	0.000000	3.465051	0.115426
4	6	0	0.000000	2.546664	1.173849
5	6	0	0.000000	1.184758	0.887221
6	6	0	0.000000	0.735210	-0.450760
7	6	0	0.000000	1.652504	-1.505774
8	1	0	0.000000	3.743218	-2.022880
9	1	0	0.000000	4.530406	0.326880
10	1	0	0.000000	2.899475	2.202209
11	1	0	0.000000	1.315207	-2.538586
12	6	0	0.000000	0.000000	1.833244
13	1	0	0.880530	0.000000	2.489546
14	6	0	0.000000	-1.184758	0.887221
15	6	0	0.000000	-2.546664	1.173849
16	6	0	0.000000	-3.465051	0.115426
17	6	0	0.000000	-3.019587	-1.212779
18	6	0	0.000000	-1.652504	-1.505774
19	6	0	0.000000	-0.735210	-0.450760
20	1	0	0.000000	-2.899475	2.202209
21	1	0	0.000000	-4.530406	0.326880
22	1	0	0.000000	-3.743218	-2.022880
23	1	0	0.000000	-1.315207	-2.538586