Supplementary Information

Combined experimental and theoretical studies on Phenyl thiadiazole based novel *turn-on* fluorescent colorimetric Schiff base chemosensor for the selective and sensitive detection of Al^{3+}

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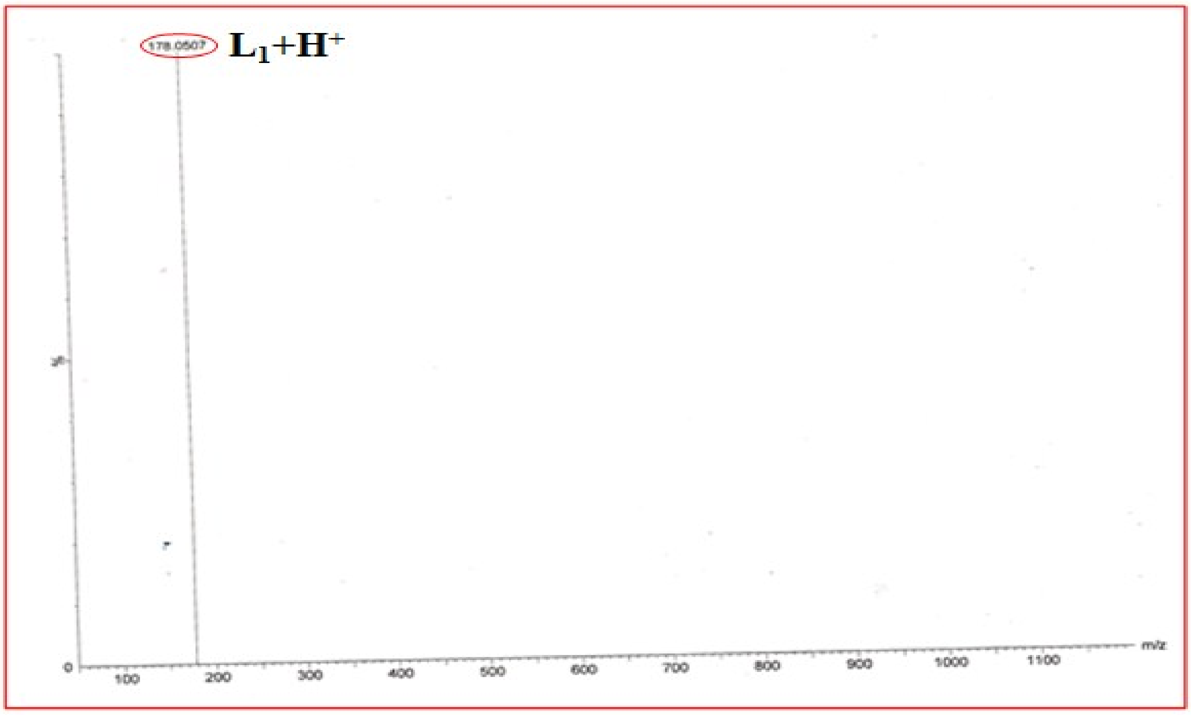

Fig. S1. Mass spectra of **1**.

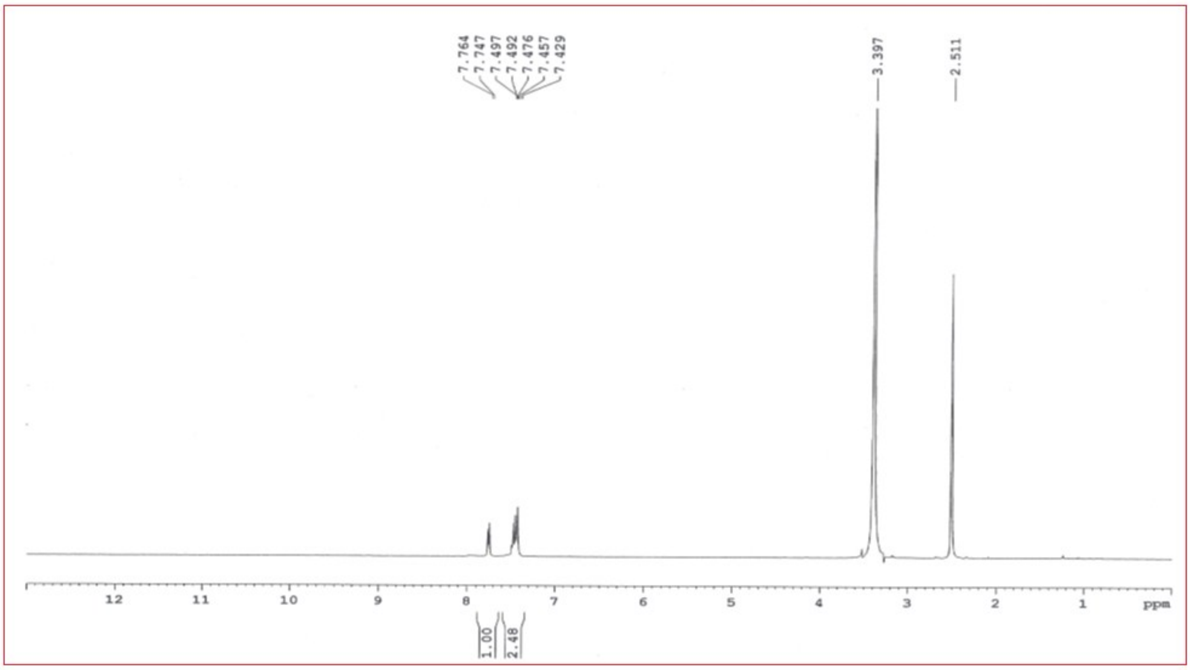

Fig. S2. ^{1}H-NMR spectra of **1**.

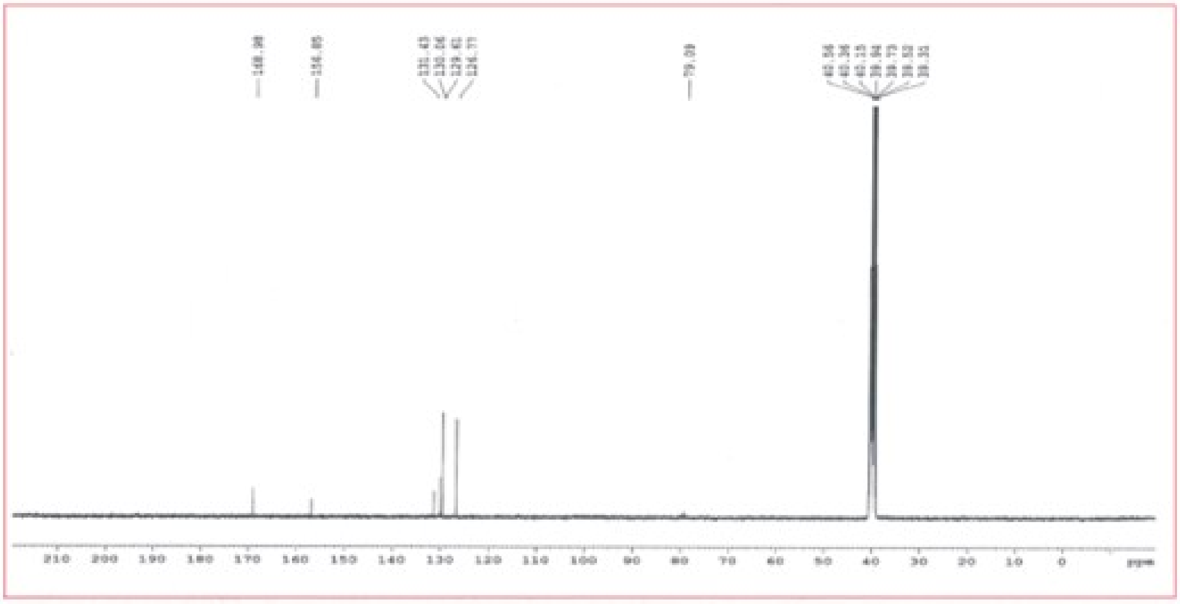

Fig. S3. ^{13}C-NMR spectra of **1**.

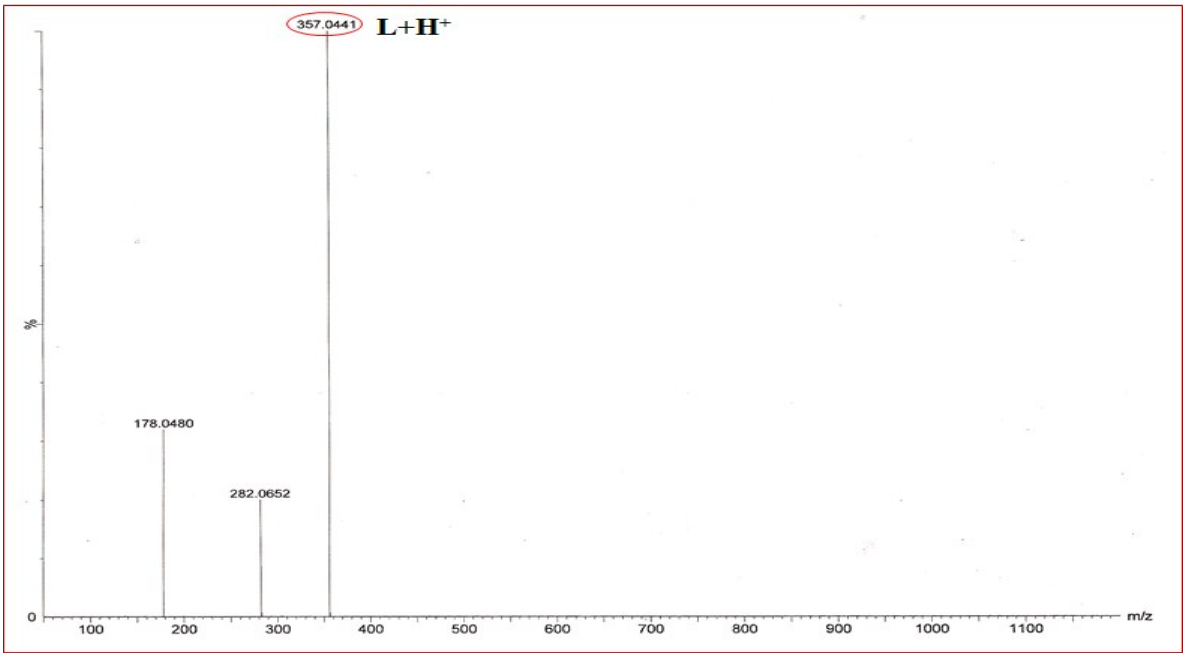

Fig. S4. Mass spectra of **L**.

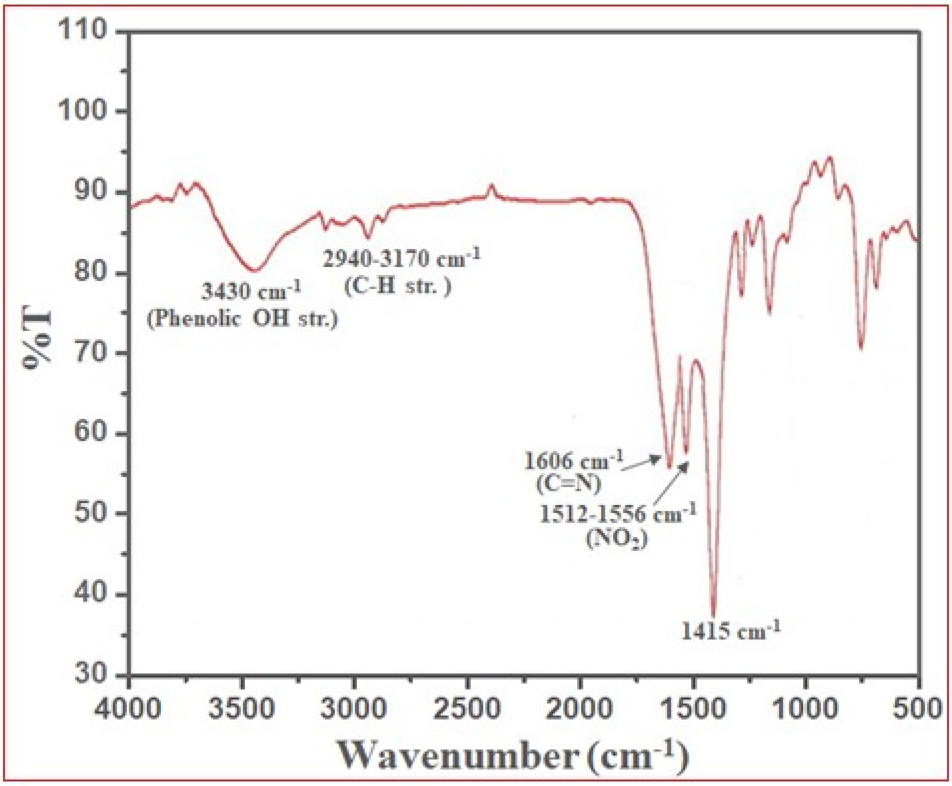

Fig. S5. FT-IR spectra of **L**.

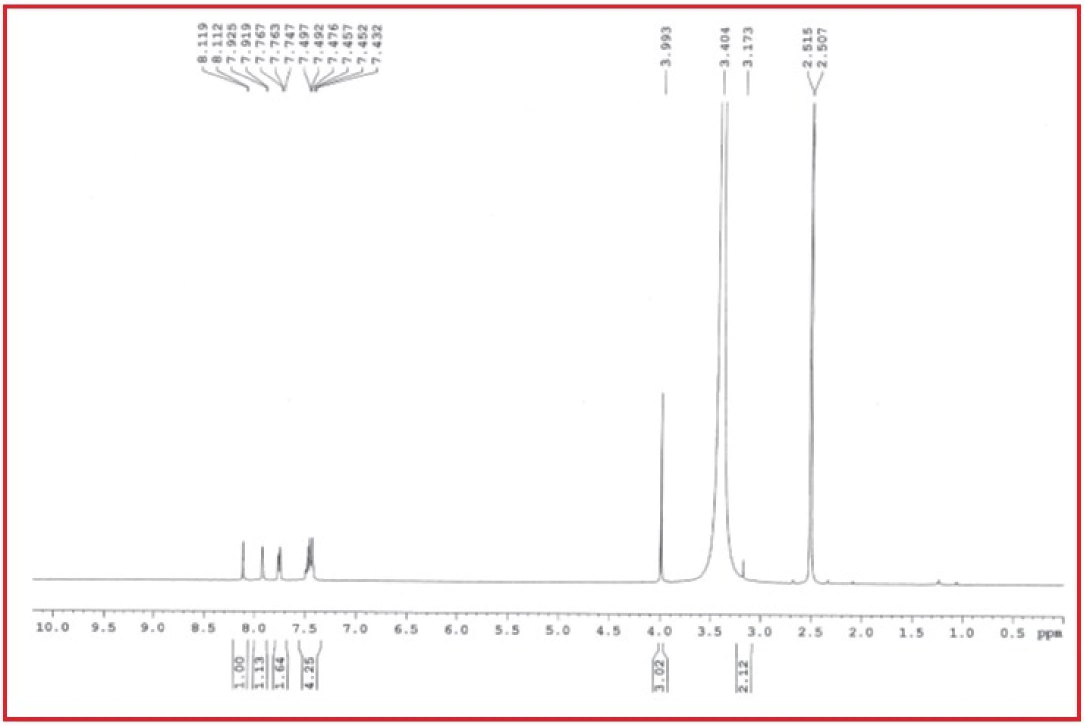

Fig. S6. ^{1}H-NMR spectra of **L**.

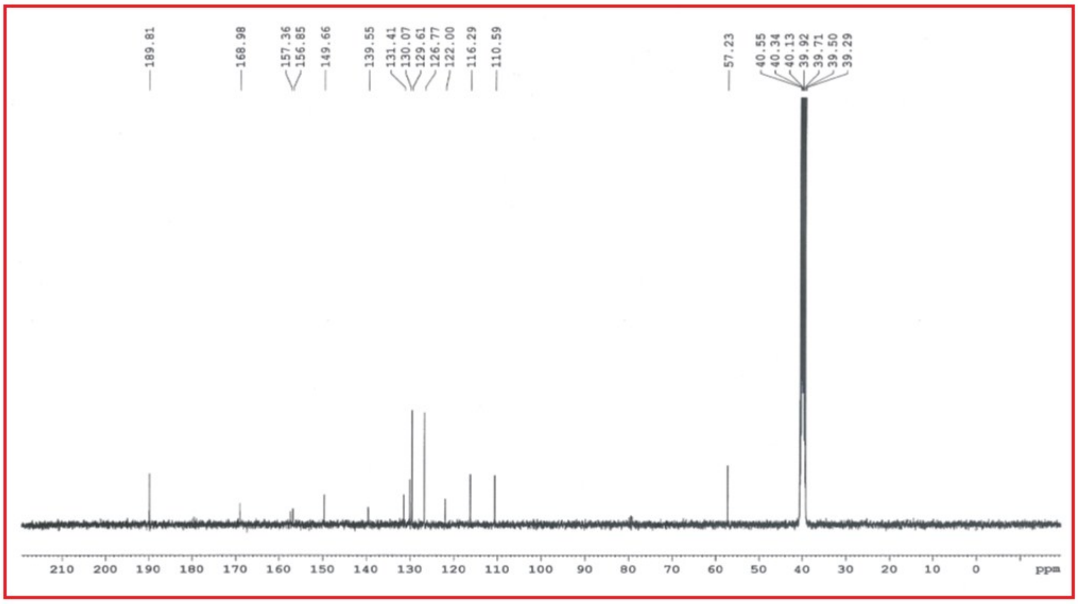

Fig. S7. ^{13}C-NMR spectra of **L**.

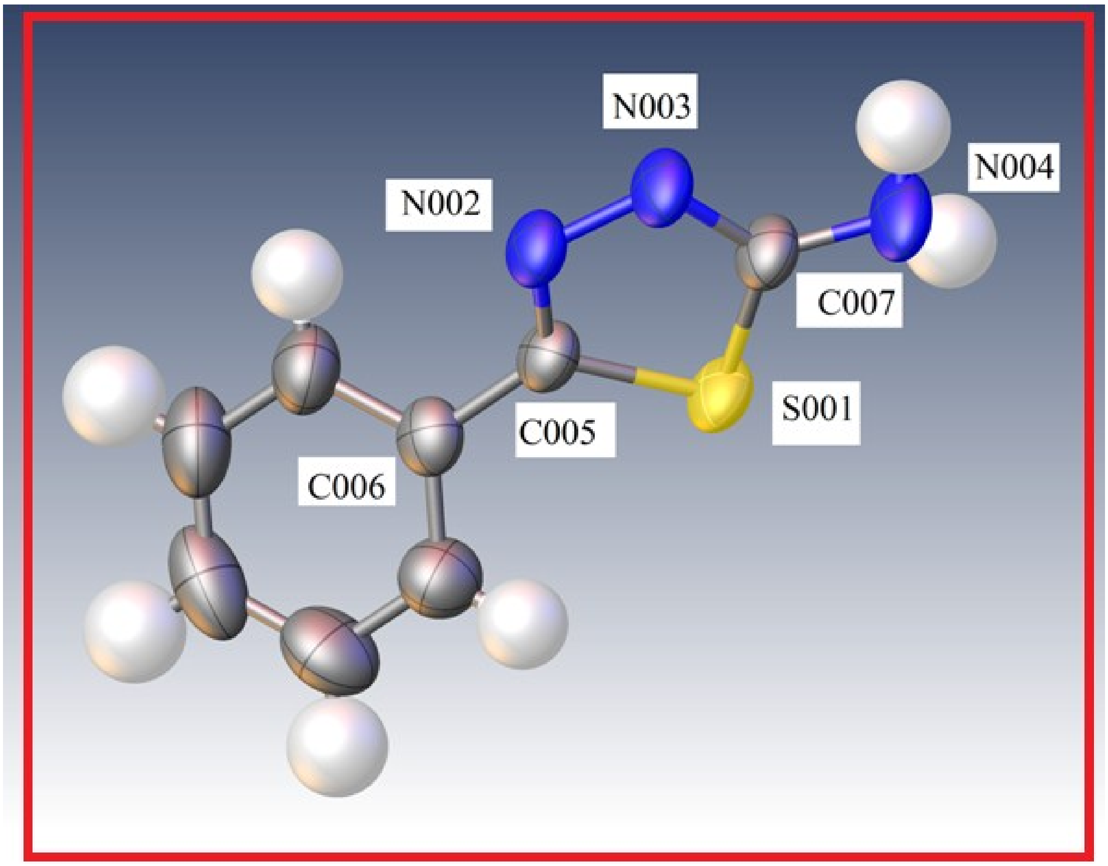

Fig. S8. Crystal structure of **1** with 40% ellipsoid.

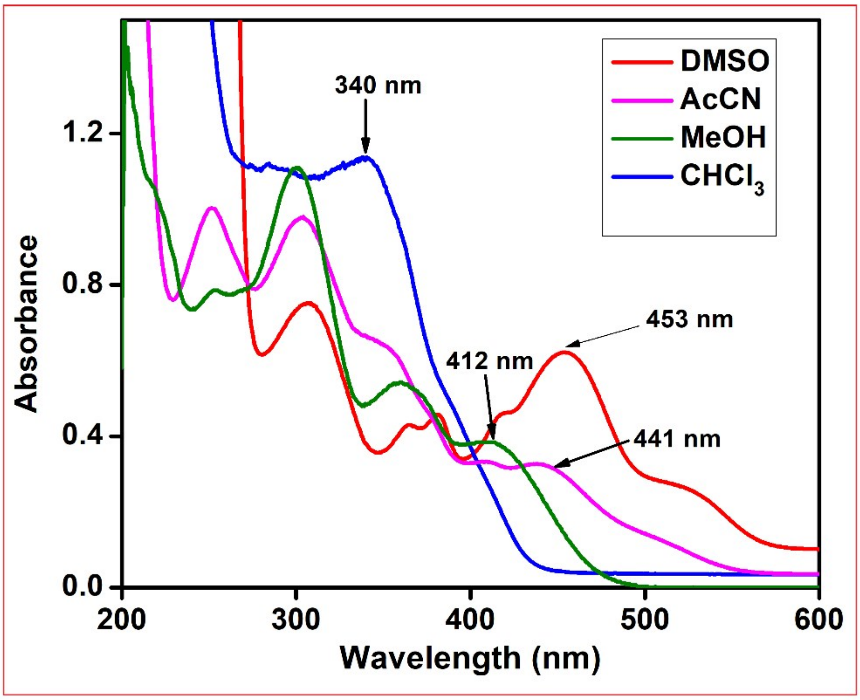

Fig. S9. UV-Vis spectra of **L** in different solvents.

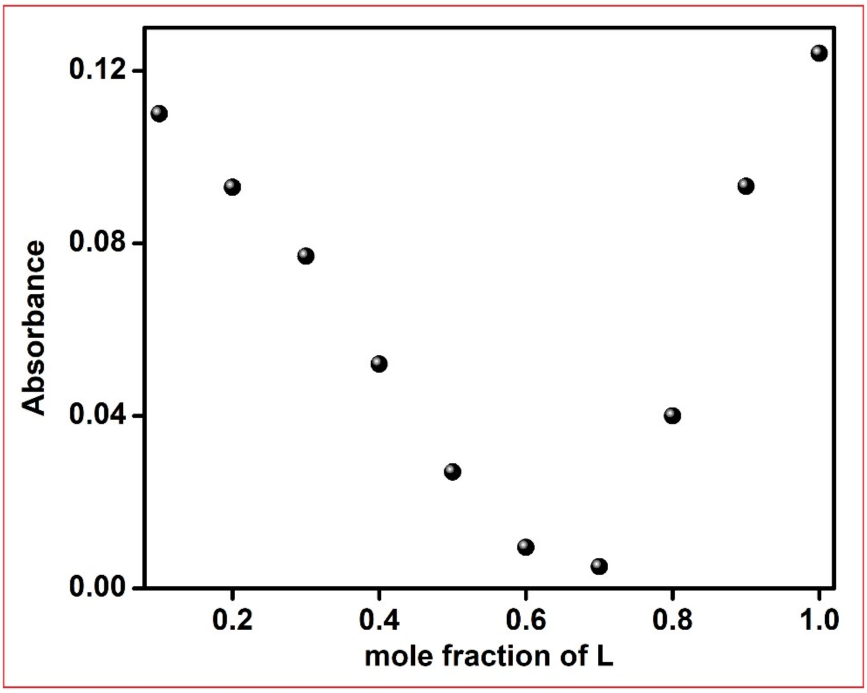

Fig. S10. Job's plot of **L** from absorption spectra.

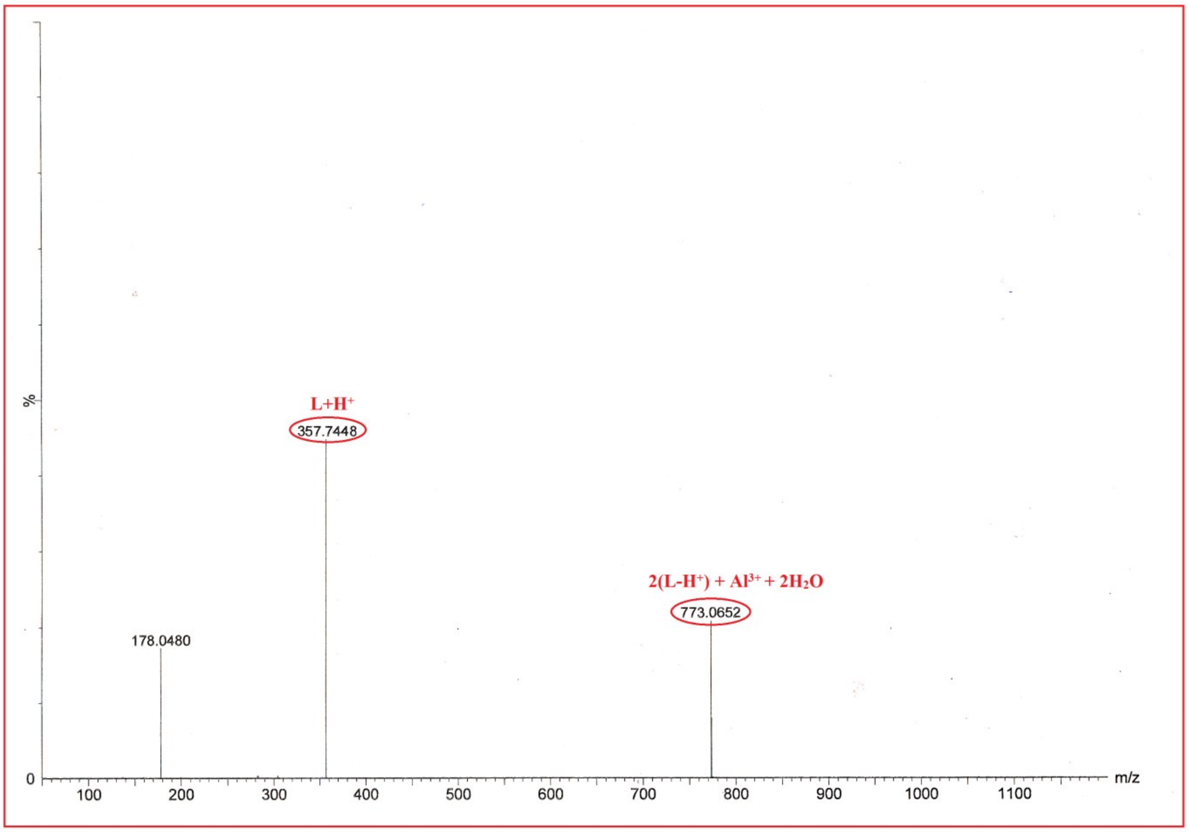

Fig. S11. Mass spectra of **L-**Al^{3+}adduct.

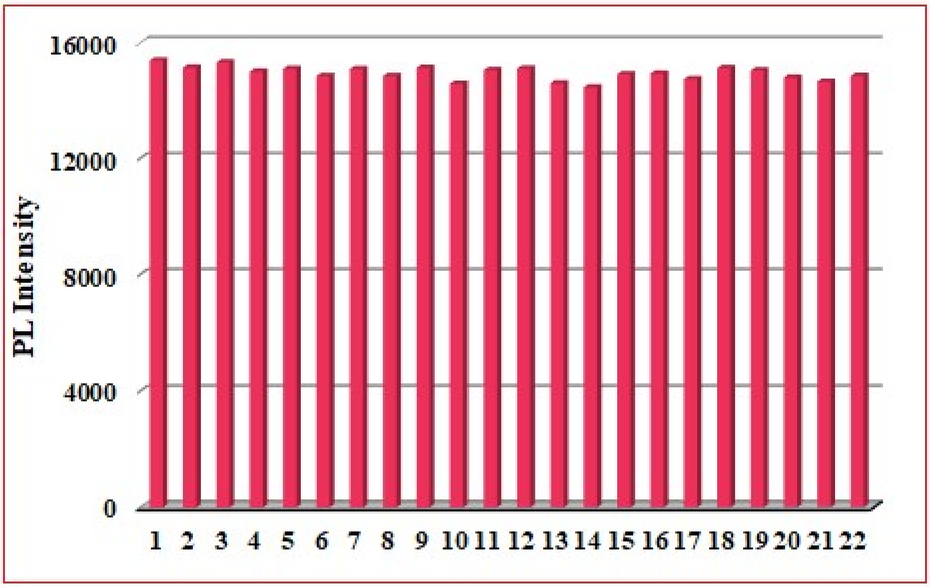

Fig. S12. Competitive experiment in presence of **L** and other metal ions (where 1 = **L**, 2 = Na^{+}, 3 = K^{+}, 4 = Mg^{2+}, 5 = Fe^{3+}, 6 = Ni^{2+}, 7 = Co^{2+}, 8 = Cd^{2+}, 9 = Hg^{2+}, 10 = Pb^{2+}, 11 = Cu^{2+}, 12 = Ag^{+} , 13 = Zn^{2+}, 14 = Mn^{2+} 15 = Al^{3+},16 = Cr^{3+}, 17=Mn^{7+}, 18=Cr^{6+}, 19=Mo^{6+}, 20 =Ga^{3+}, 21=Fe^{2+} and 22= Pd^{2+})in methanol-*tris*-HCl buffer (10 mM, pH 7.2) solution (1:1 v/v)..

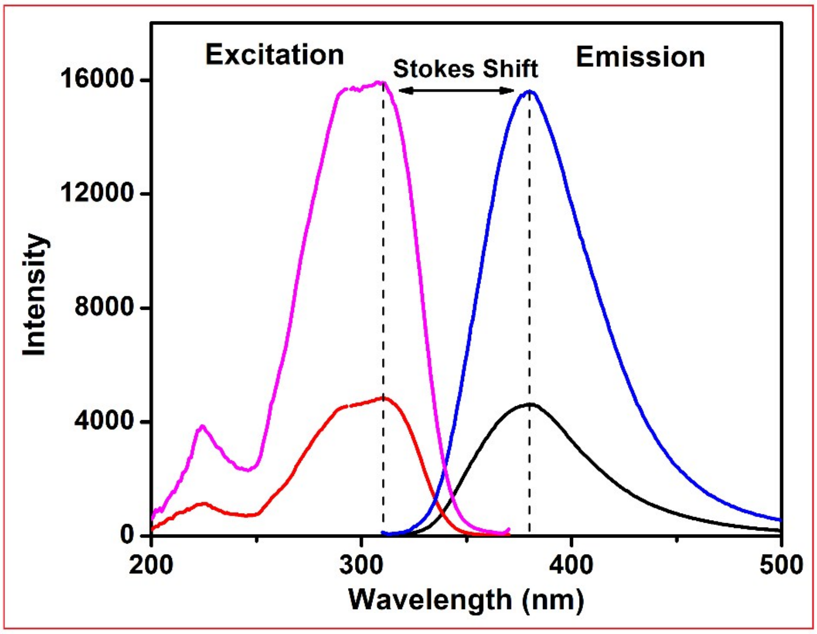

Fig. S13. Excitation and emission spectra of **L** and **L-**Al^{3+} adduct.

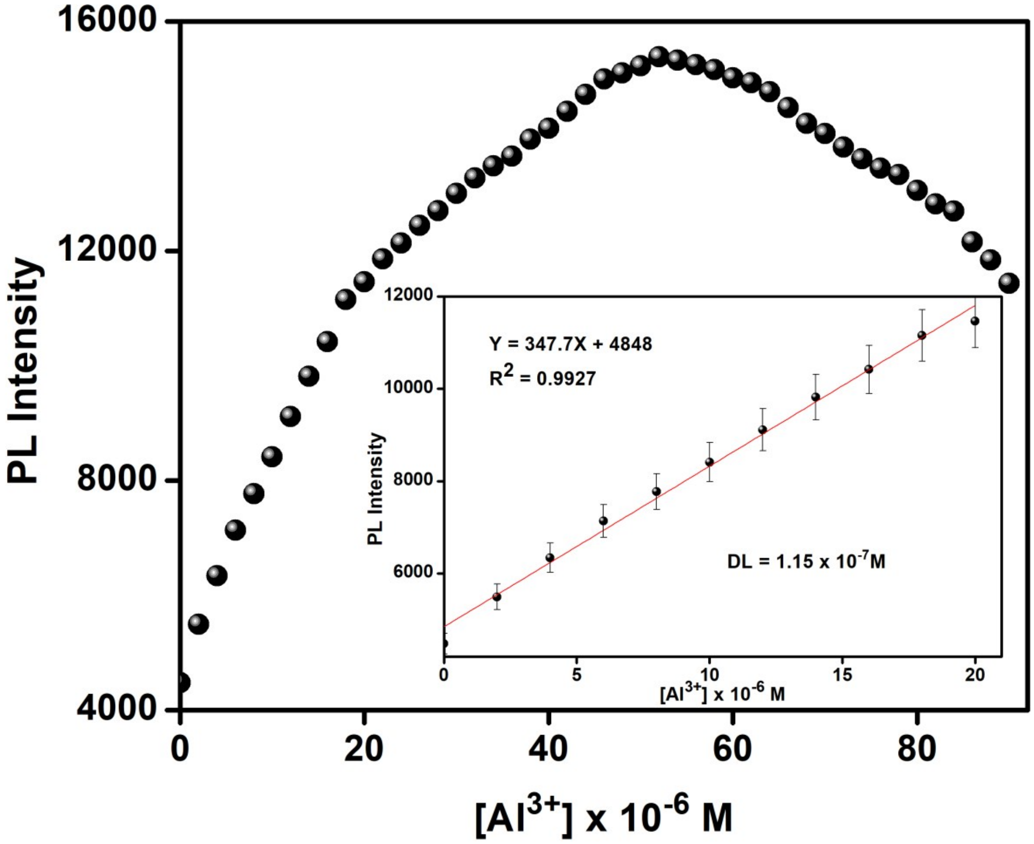

Fig. S14. Emission intensity change of **L** with slow addition of **Al**$^{3+}$ion (inset: detection limit)

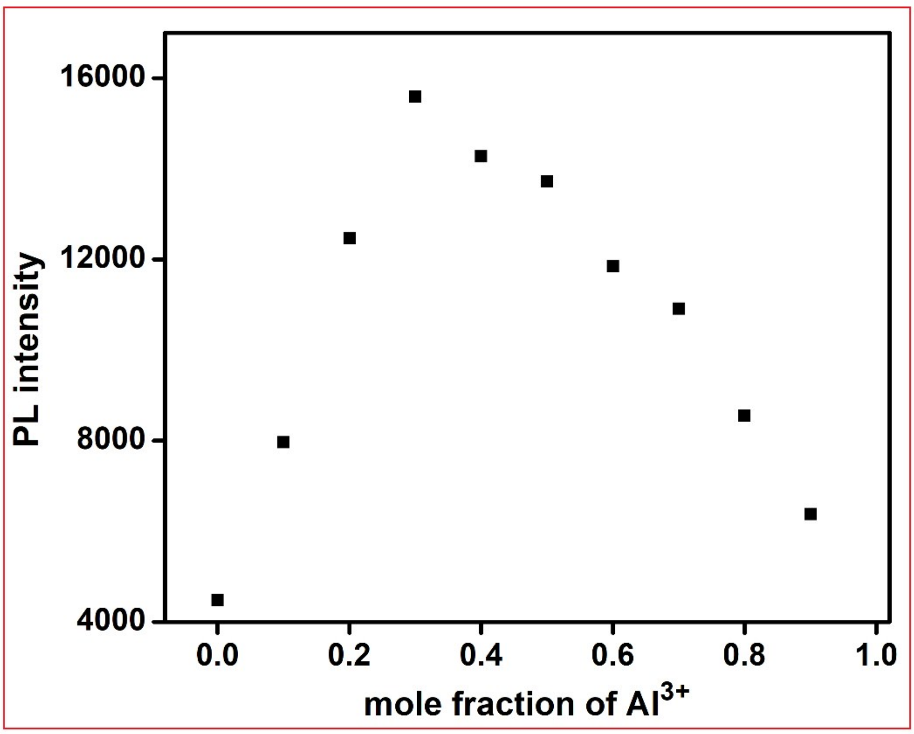

Fig. S15. Job's plot from emission spectra.

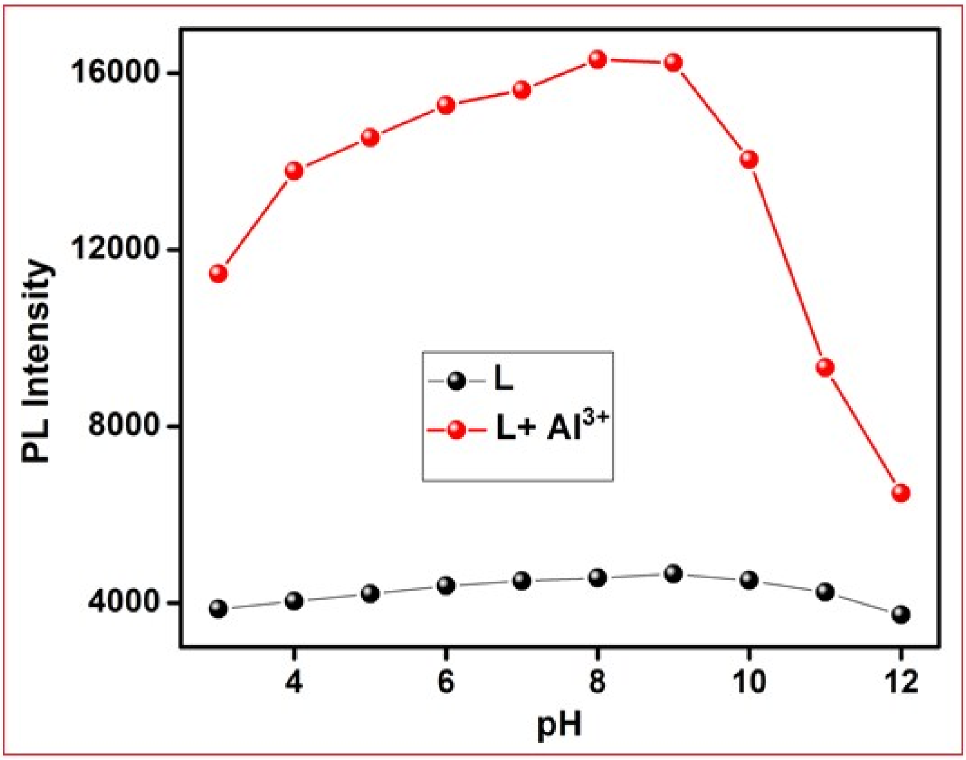

Fig. S16. pH effect of **L** and **L**–Al^{3+}complex by fluorescence studies.

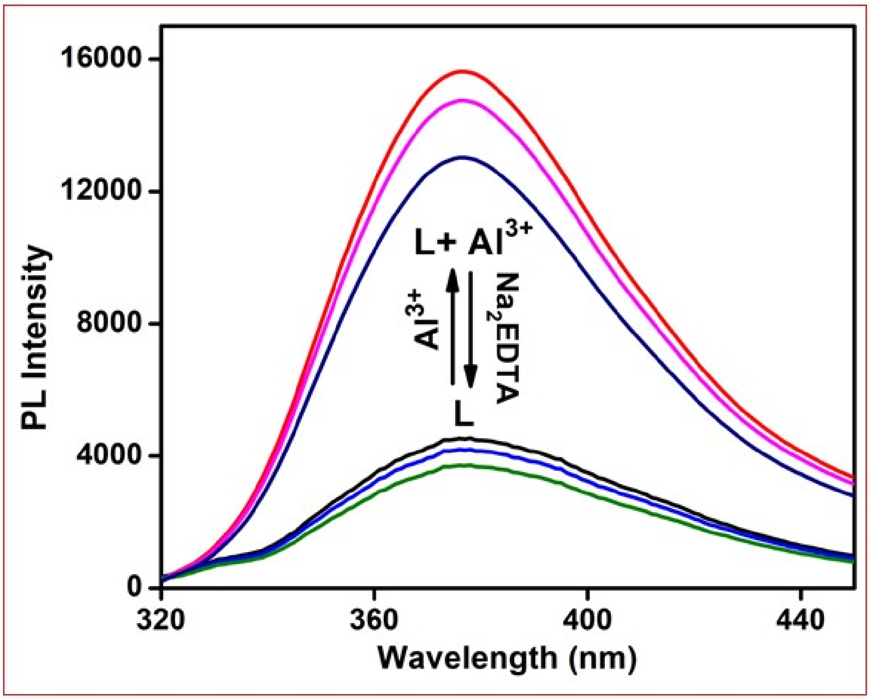

Fig. S17. Fluorometric reversibility study of **L** with Al^{3+} and Na_2EDTA

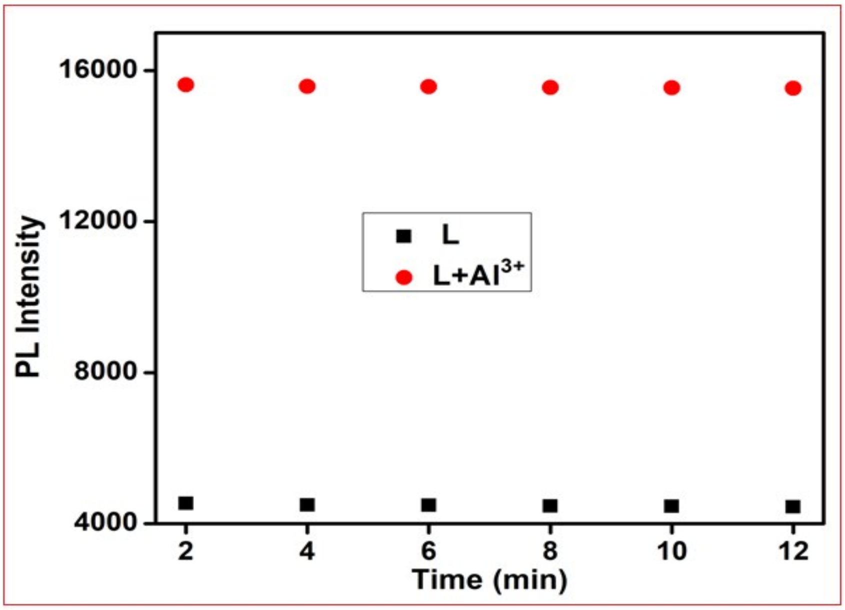

Fig. S18. Fluorometic time dependence.

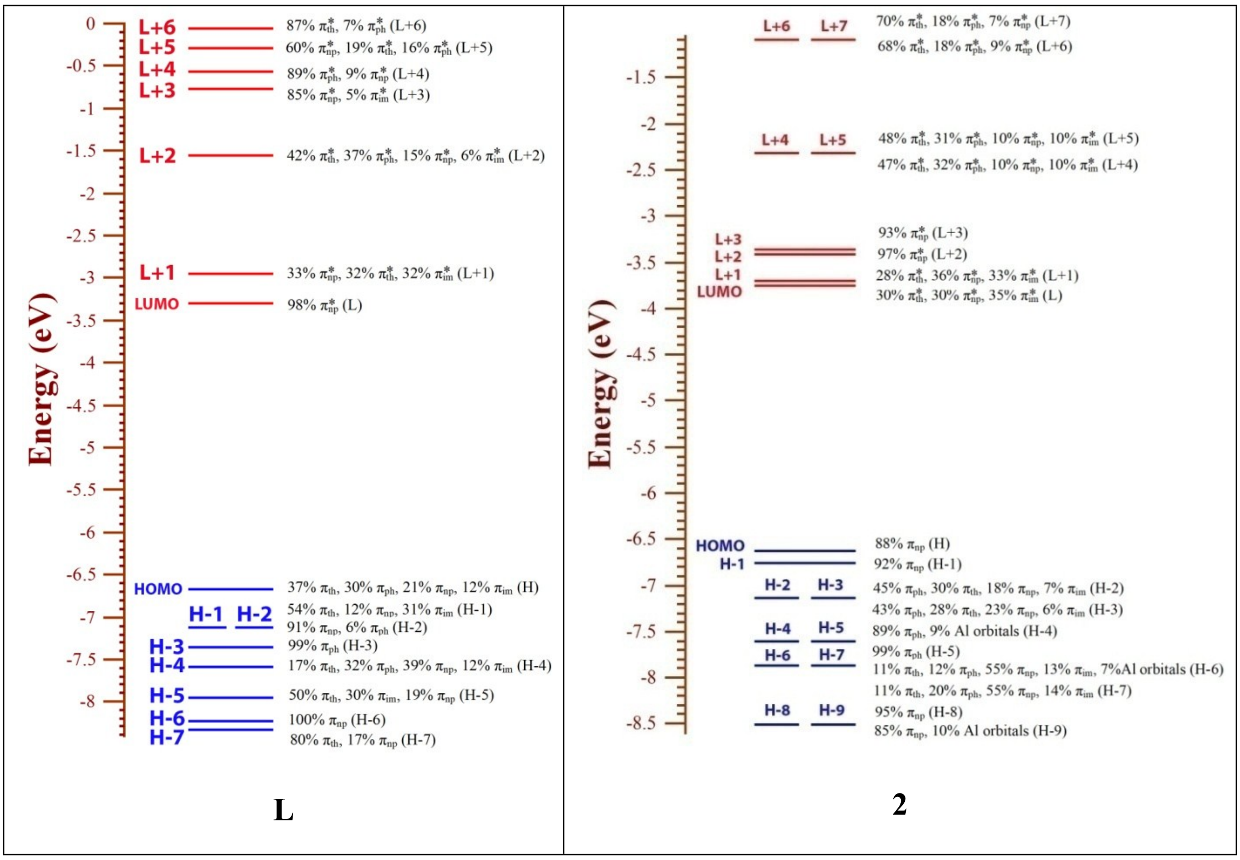

Fig. S19. The MO diagram of **L** and **2** are showing the character and energy (eV) (th = thiadiazole moiety, np = methoxy nitrophenol moiety, im= iminomethyl moiety, ph = phenyl moiety).

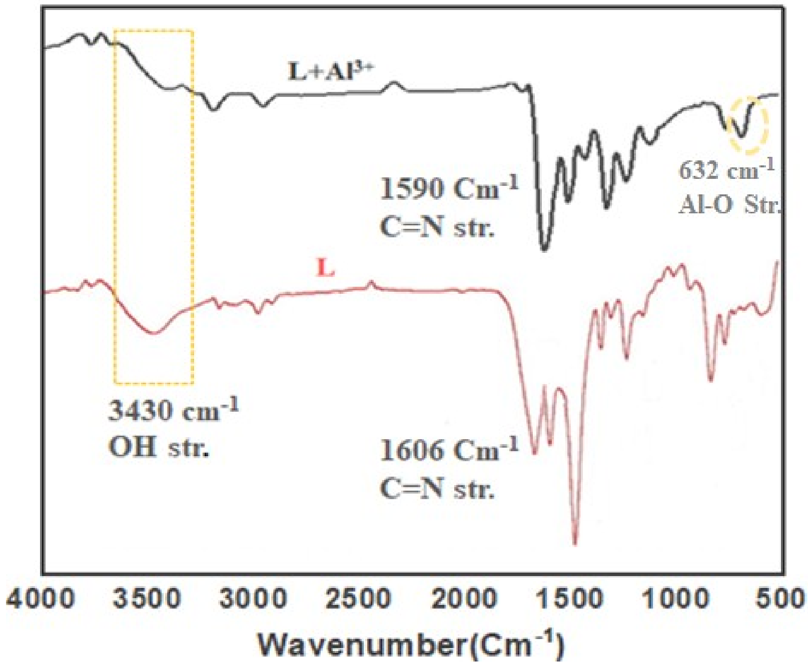

Fig. S20. IR spectra of **L** and **L**+Al^{3+}

Table S1. Selected optimized bond lengths (Å) and angles (º) for **L** and **2**.

L		**2**	
Bond lengths (Å)			
C1-N1	1.3056	Al1-O1	1.8605
N1-C9	1.3853	Al1-O6	1.9112
C1-C2	1.4639	Al1-O′1	1.8603
C2-C3	1.4182	Al1-O5	1.9113
C3-C4	1.3946	Al1-N1	2.1255
C4-C5	1.4125	Al1-N′1	2.1260
C5-C6	1.3892	N1-C1	1.3462
C6-C7	1.4291	C1-C2	1.4210
C7-O1	1.3676	C2-C7	1.4465
C9-N2	1.3314	C7-O1	1.3041
N2-N3	1.3980	N′1-C′1	1.3462
N3-C10	1.3239	C′1-C′2	1.4210
C6-O2	1.3957	C′2-C′7	1.4465
O2-C8	1.4620	C′7-O′1	1.3041
C4-N4	1.4677		
N4-O3	1.2830		
N4-O4	1.2800		
C9-S1	1.8320		
S1-C10	1.7994		
C10-C11	1.5400		
C11-12	1.3948		

Bond angle (º)			
C10-S1-C9	84.80	N1-Al1-O1	88.38
C10-N3-N2	112.81	N′1-Al1-O′1	88.38
N3-N2-C9	113.82	O5-Al1-O6	88.78
C9-N1-C1	120.29	N1-Al1-O6	91.72
N1-C1-C2	124.21	N′1-Al1-O6	93.37
C2-C3-C4	120.57	O1-Al1-O5	88.42
C3-C4-N4	119.50	O1-Al1-O′1	94.36
C5-C6-O2	125.98	N1-Al1-N′1	172.89
C6-C7-O1	117.98	O5-Al1-N1	93.33
C6-O2-C8	119.08	O5-Al1-N′1	91.73
N3-C10-C11	122.56	O1-Al1-O6	177.20
C12-C11-C16	119.99	O′1-Al1-O5	177.22

Table S2. Electronic transitions of **L** and **2** calculated in methanol using the TD-DFT method.

Most important orbital excitations	*λ*	*f*	Experimental λ
L			
H→L, H-2→L	408.92	0.08125	410
H→L+1, H-2→L+1	369.03	0.16202	360
H-4→L, H-2→L, H→L	355.96	0.12405	
H-2→L+1, H-4→L, H→L+1	337.50	0.04786	
H-4→L, H-2→L, H-2→L+1	316.40	0.08765	
H-3→L+1, H-3→L	312.11	0.00255	300
H-4→L+1, H→L+2	289.39	0.26459	
H-8→L, H-8→L+1, H-1→L+2	270.55	0.00117	
H-7→L, H→L+2, H-10→L, H-7→L+1	269.06	0.02430	
H-8→L+1, H-1→L+2, H-8→L	264.06	0.00286	
H-7→L, H-7→L+1, H→L+2	262.77	0.02271	
H-10→L, H-9→L, H-9→L+1, H-7→L	253.87	0.08143	252
H-7→L+1, H→L+2, H-9→L	249.73	0.01125	
H-3→L+2, H→L+4	246.70	0.00637	
H-10→L, H-9→L+1	245.06	0.02122	
H-10→L+1, H-2→L+2, H→L+3	240.06	0.03555	
H-10→L+1, H-2→L+2, , H→L+5	237.92	0.00138	
H-4→L+2, H→L+3, H-10→L+1	227.17	0.01008	
H-4→L+2, H→L+3, H-9→L	222.29	0.10166	
H-10→L, H-9→L, H-9→L+1, H-4→L+2	221.07	0.09582	
H-1→L+3, H→L+6	218.24	0.00159	
H-3→L+2, H→L+4	215.21	0.04022	218sh
H-13→L, H-2→L+3, H→L+5	210.87	0.05242	
H-13→L, H→L+5, H-16→L	209.08	0.02101	
H-13→L, H-7→L+2, H-2→L+3	205.84	0.27067	

2			
H→L, H-4→L	390.18	0.01165	
H-1→L+1, H-4→L+1	377.94	0.06551	350sh
H→L+2, H-6→L	328.22	0.12722	
H→L+3, H-1→L+2	316.84	0.00503	
H-3→L+1, H-2→L, H-1→L+2	310.55	0.00722	
H-2→L, H-1→L+2, H-3→L+1	310.39	0.11908	
H-3→L, H-2→L+1, H-6→L	308.45	0.36716	302
H-1→L+3, H-3→L+2	305.52	0.05434	
H-3→L+1, H-2→L, H-2→L+1	300.72	0.05792	
H-3→L+1, H-2→L+1, H-3→L	300.54	0.14357	
H-3→L+2, H-2→L+3, H-1→L+3	265.56	0.06692	
H-3→L+3, H-2→L+2, H-2→L+3	256.99	0.08235	250
H-5→L, H-5→L+1	255.84	0.00251	
H-4→L, H-5→L	255.80	0.00265	
H-6→L, H-2→L+1	231.58	0.13284	
H-7→L, H-6→L+1	229.94	0.0738	
H-7→L+1, H-6→L+2	224.46	0.1858	
H-9→L, H-11→L+1	214.90	0.65342	206
H→L+5, H-1→L+4	213.70	0.00867	
H-10→L, H-8→L, H-6→L+2	207.18	0.01311	
H-7→L+3, H-6→L+2, H-10→L	206.71	0.0505	
H-6→L+2, H-1→L+4, H→L+5	200.31	0.05037	

λ –wavelength (nm); *f* – oscillator strength; H – highest occupied molecular orbital; L – lowest unoccupied molecular orbital.