

Supplementary Material (ESI) for New Journal of Chemistry

Luminescent sensing, DFT, extraction and monitoring of Cr³⁺ and Al³⁺ via the application of first derivative fluorescence spectroscopy

Soma Mukherjee ^{a*}, Soumi Betal ^a, Asoke Prasun Chattopadhyay ^b

^a Department of Environmental Science, University of Kalyani

^b Department of Chemistry, University of Kalyani

Kalyani, Nadia – 741235, West Bengal, India

Email: somam580@gmail.com

Fax: 033-25828282; Phone: 033-25828750 Ext. 291, 292

Contents

1. ¹H NMR spectra of L in DMSO-*d*₆.
2. ¹³C NMR spectra of L in DMSO-*d*₆.
3. IR spectra of L.
4. Mass Spectra of L.
5. IR spectra of L-Cr³⁺.
6. Mass Spectra of L-Cr³⁺.
7. IR spectra of L-Al³⁺.
8. Mass Spectra of L-Al³⁺.
9. Job's plot of (a) L-Al³⁺ (b) L-Cr³⁺.
10. Effect of emission L upon addition of water (0.0-50.0% in DMSO).
11. Solvent effects (DCM, DMSO, CH₃OH, DMSO/H₂O (1:1)) of L.
12. Fluorescence titration (λ_{ex} , 340.0 nm) of L (1.0×10^{-7} M) upon addition of various amounts of (a) Fe³⁺ ions (0.5 equiv.) in DMSO.
13. FTIR spectra of (a) L, (b) L-Al³⁺, (c) L-Cr³⁺.
14. Optimized structure of L.
15. Frontier molecular orbitals of L.
16. Optimised structure of (a) L-Al³⁺ and (b) L-Cr³⁺.
17. Frontier molecular orbitals of L-Al³⁺.
18. Frontier molecular orbitals of L-Cr³⁺.
19. pH effects on absorbance values of (a) L-Al³⁺ and (b) L-Cr³⁺.

Fig. S1 ^1H NMR spectra of L in $\text{DMSO-}d_6$.

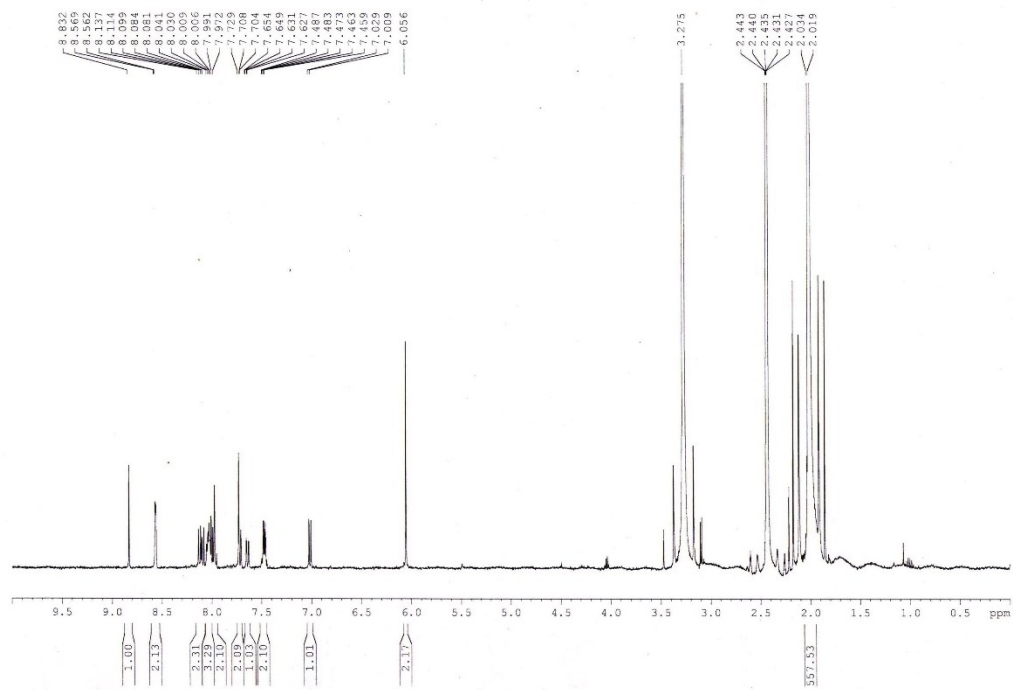


Fig. S2 ^{13}C NMR spectra of L in $\text{DMSO-}d_6$.

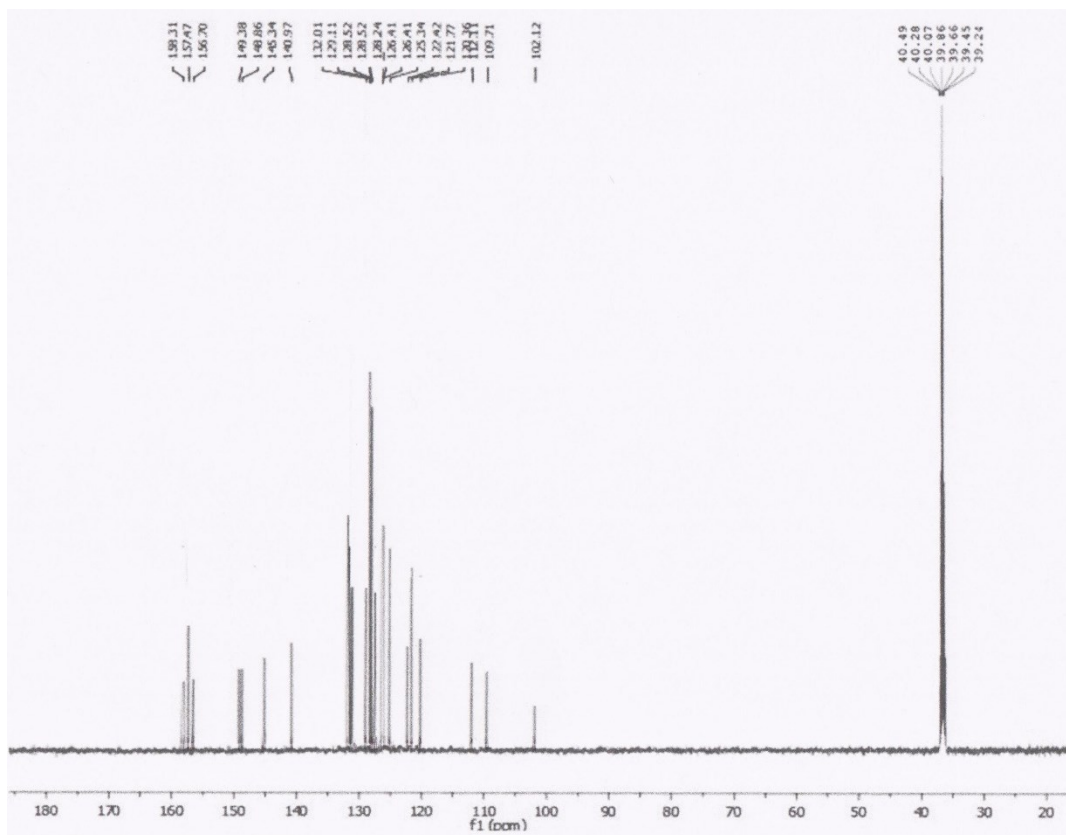


Fig. S3 IR spectra of L.

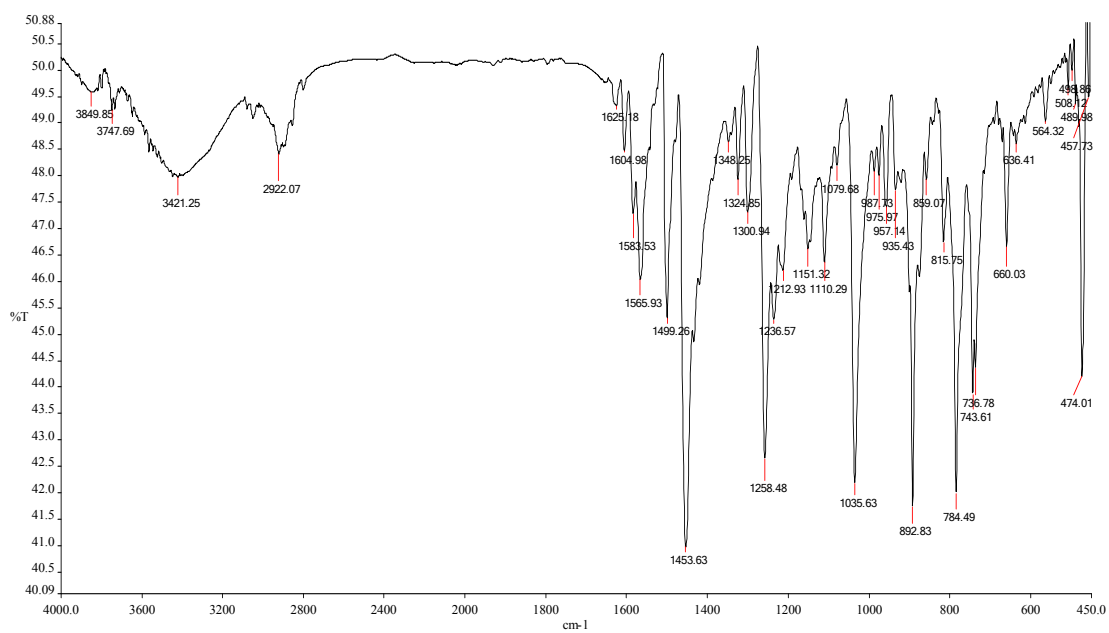


Fig. S4 Mass Spectra of L.

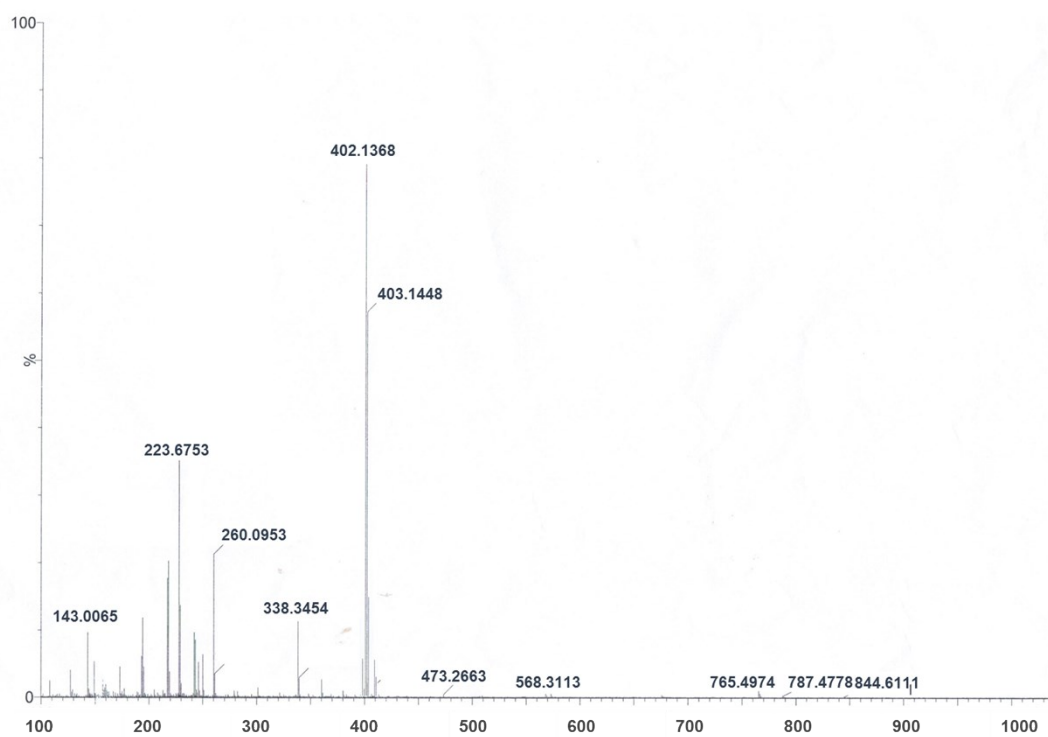


Fig. S5 IR spectra of L-Cr³⁺.

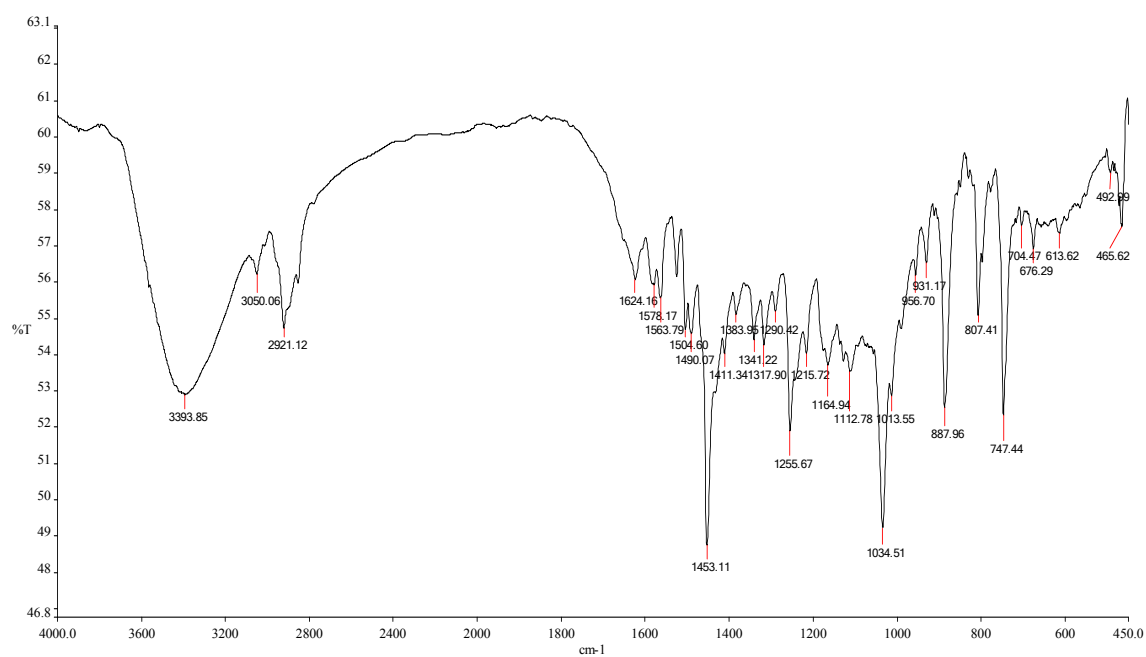


Fig. S6 Mass Spectra of L-Cr³⁺.

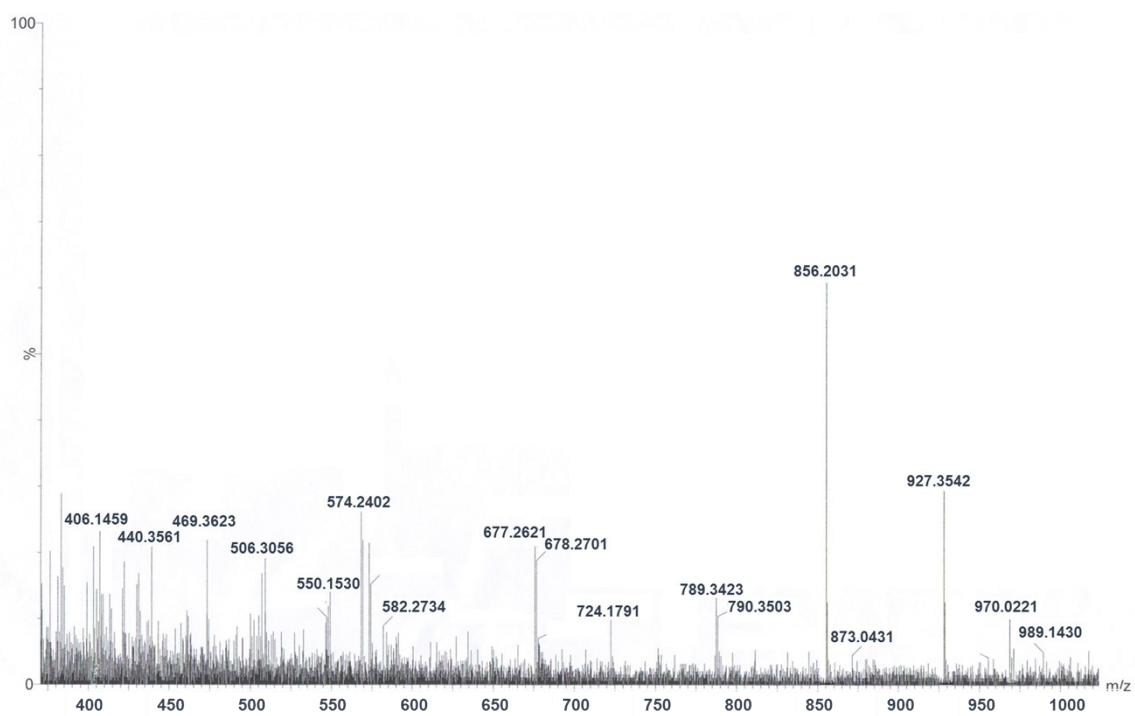


Fig. S7 IR spectra of L-Al³⁺.

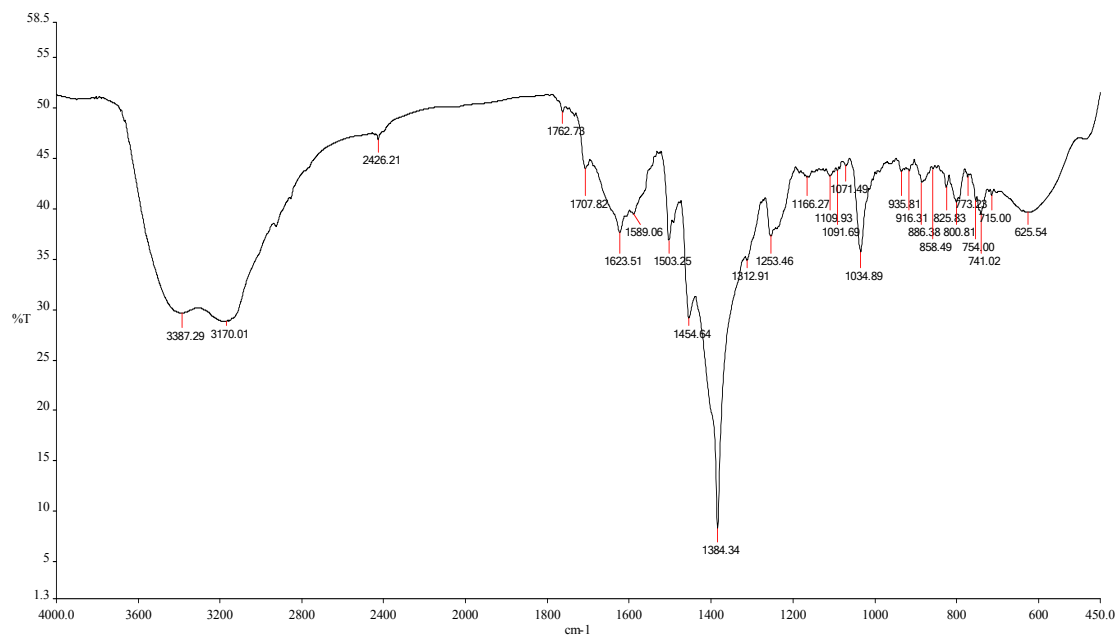
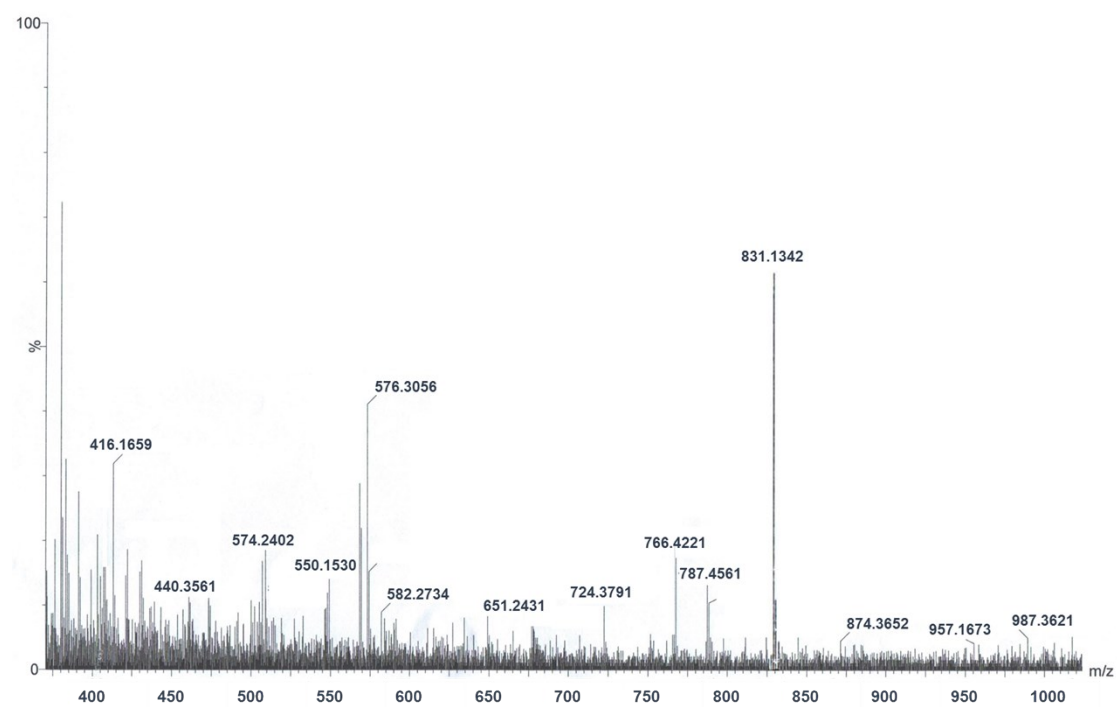


Fig. S8 Mass Spectra of L-Al³⁺.



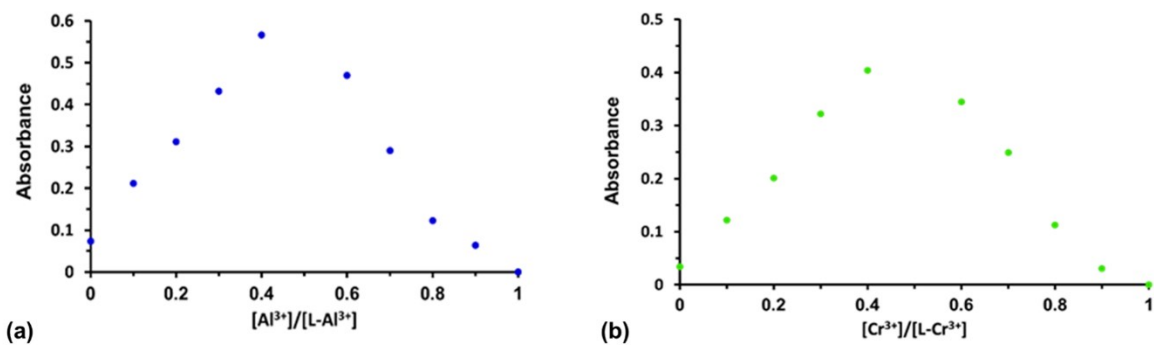


Fig. S9 Job's plot of (a) L-Al³⁺ (b) L-Cr³⁺.

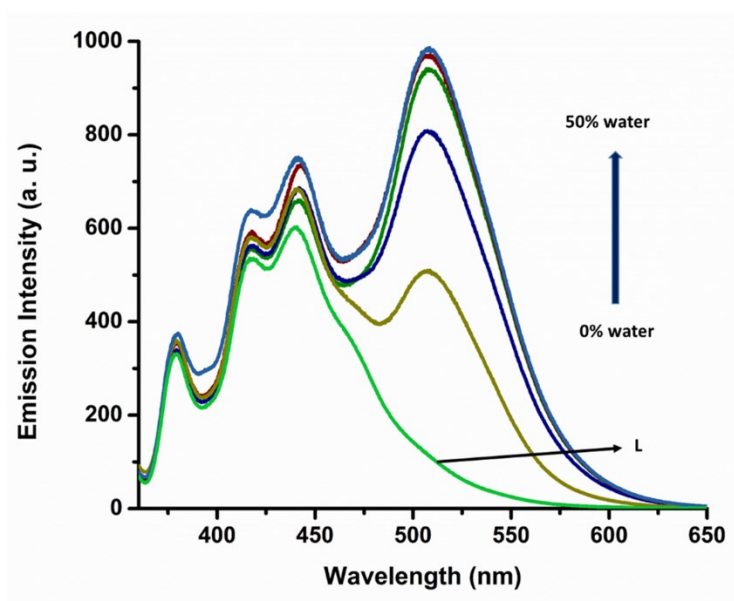


Fig. S10 Effect of emission L upon addition of water (0.0-50.0% in DMSO).

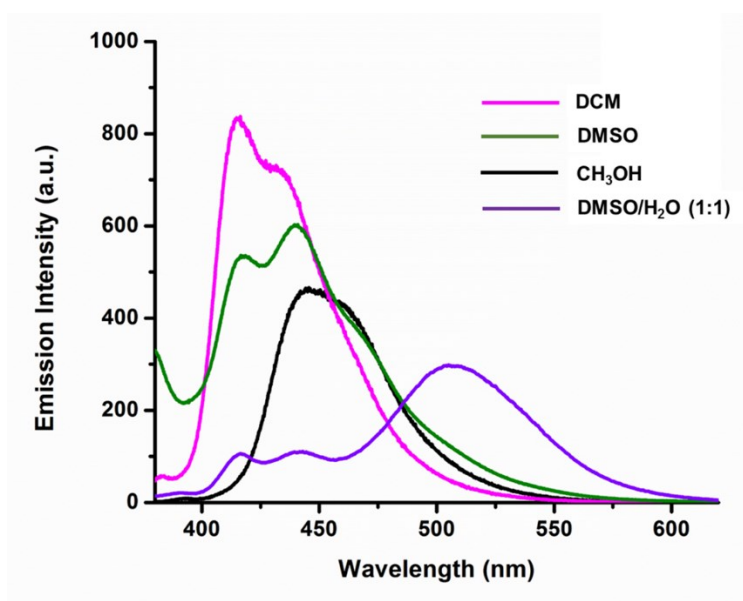


Fig. S11 Solvent effects (DCM, DMSO, CH₃OH, DMSO/H₂O (1:1)) of L.

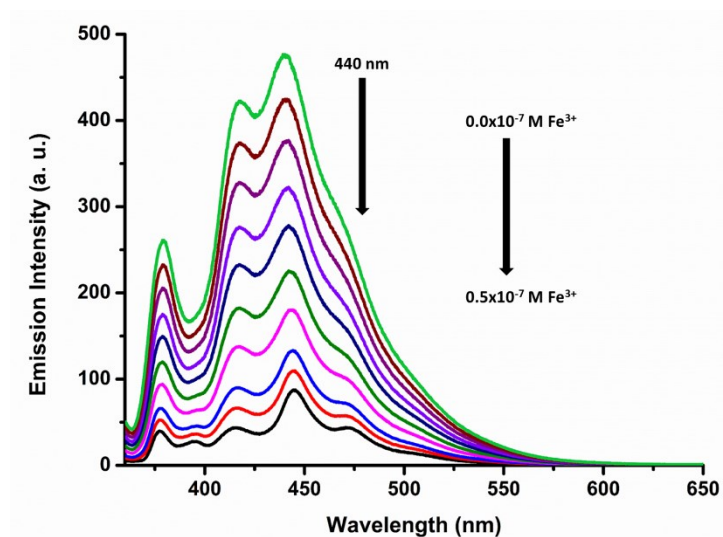


Fig. S12 Fluorescence titration (λ_{ex} , 340.0 nm) of L (1.0×10^{-7} M) upon addition of various amounts of (a) Fe^{3+} ions (0.5 equiv.) in DMSO.

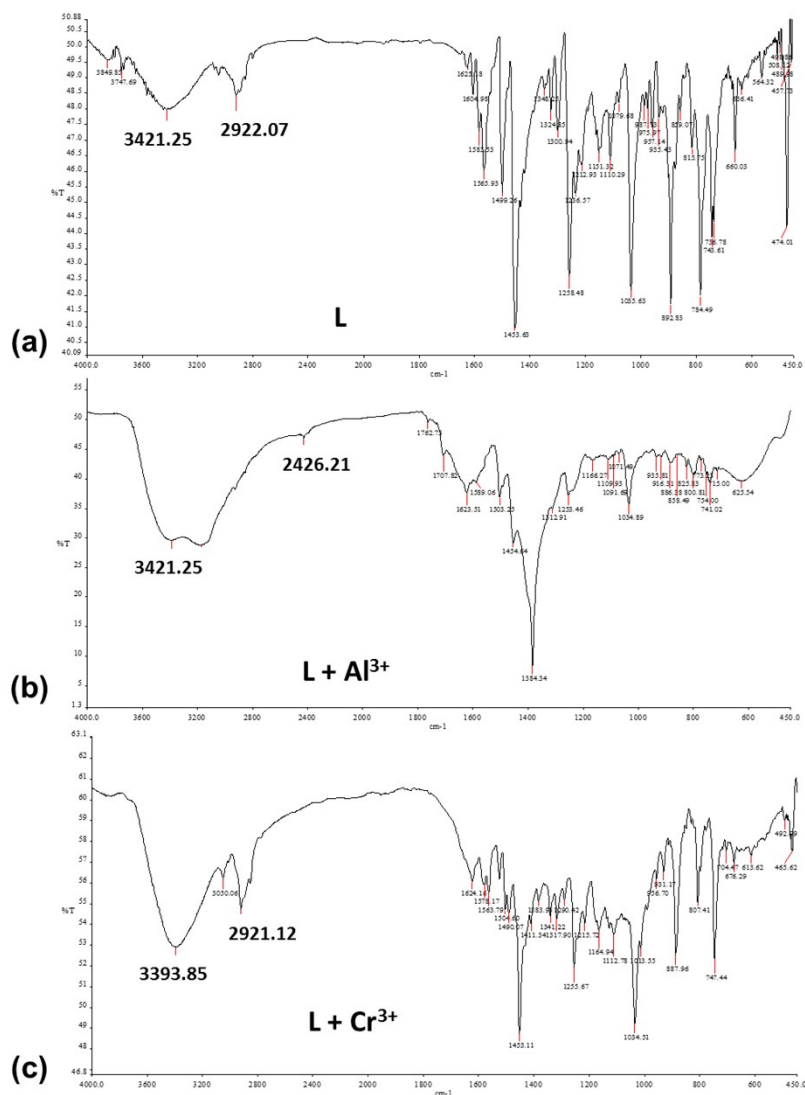


Fig. S13 FTIR spectra of (a) L, (b) L-Al^{3+} , (c) L-Cr^{3+} .

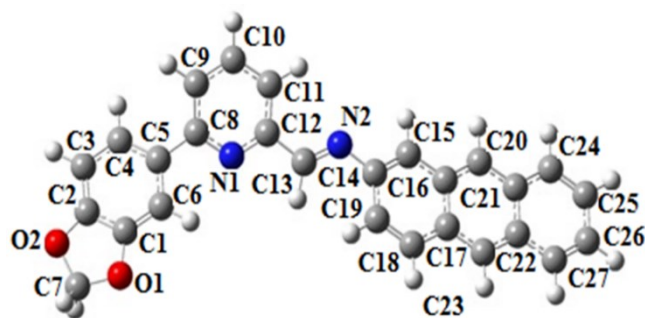


Fig. S14 Optimized structure of L.

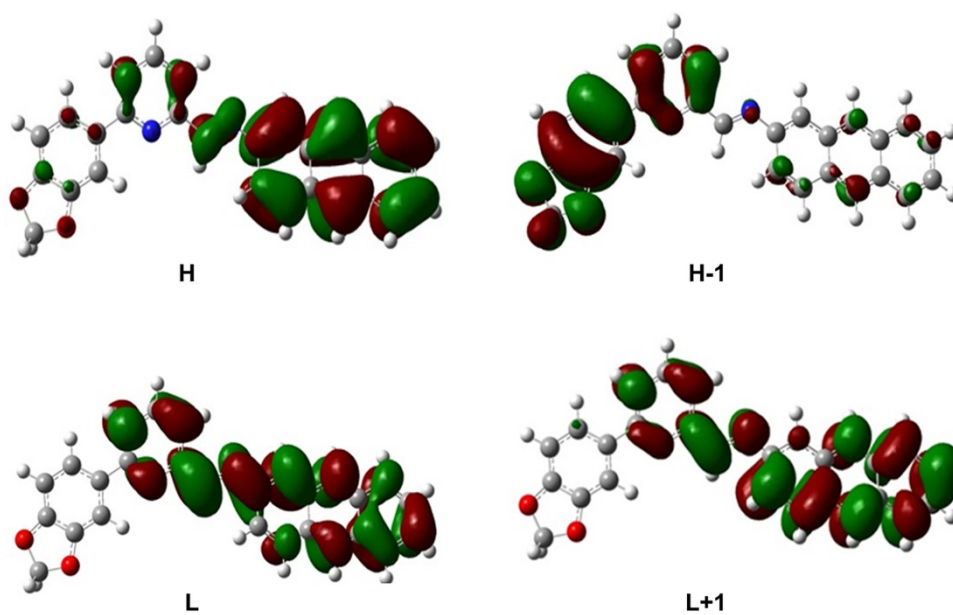


Fig. S15 Frontier molecular orbitals of L.

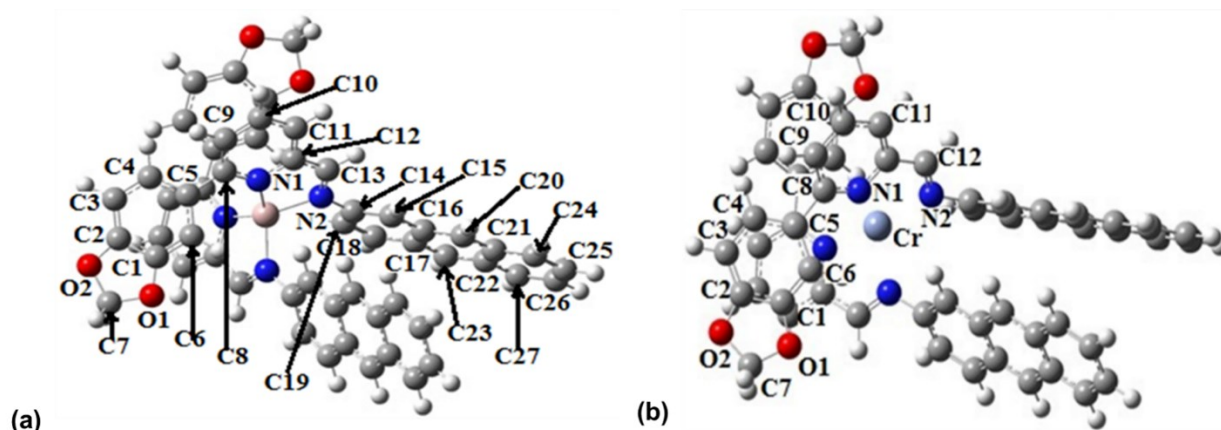


Fig. S16 Optimised structure of (a) L-Al³⁺ and (b) L-Cr³⁺.

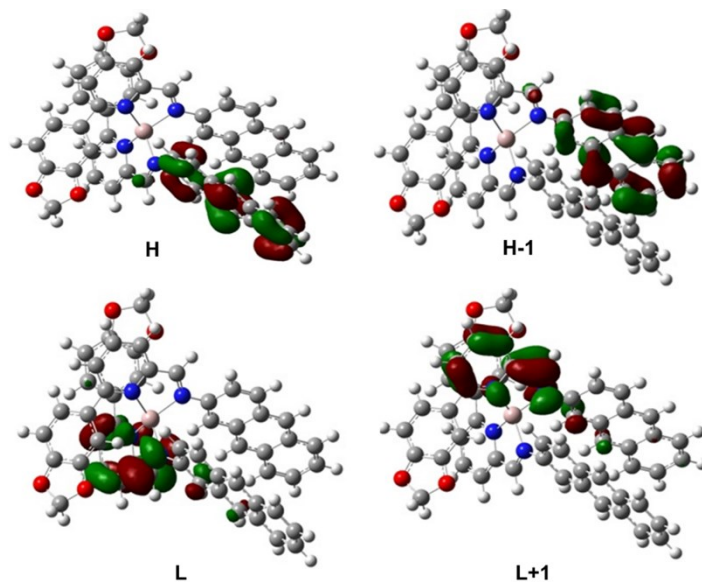


Fig. S17 Frontier molecular orbitals of L-Al³⁺.

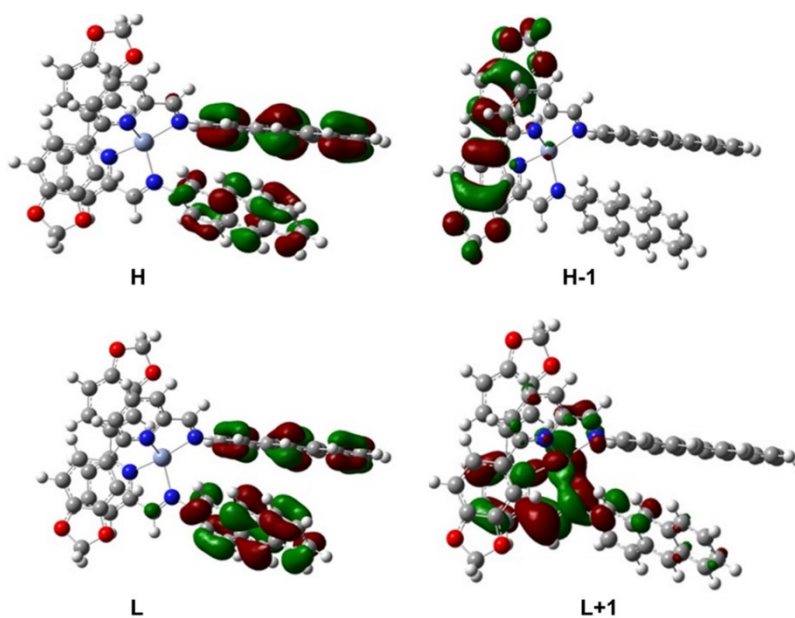


Fig. S18 Frontier molecular orbitals of L-Cr³⁺.

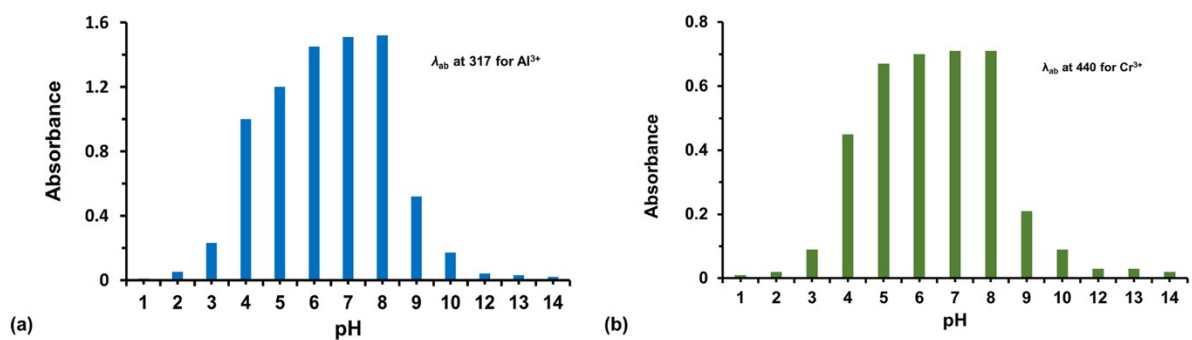


Fig. S19 pH effects on absorbance values of (a) L-Al³⁺ and (b) L-Cr³⁺.