

Supporting Information

for

Tetrathiafulvalene-based azine ligands for anion and metal cation coordination

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Additional analytical data

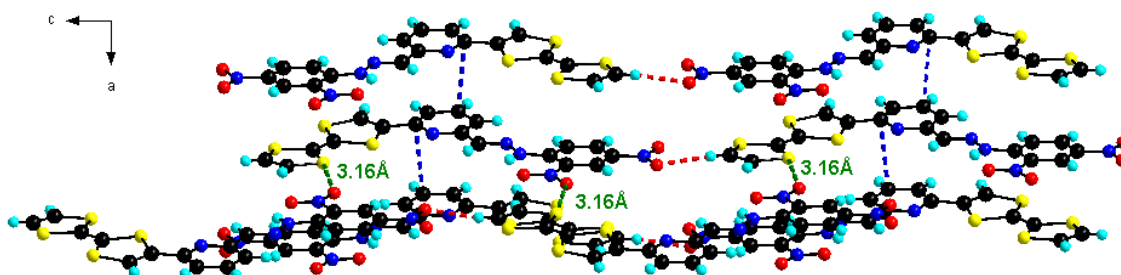


Figure S1: Partial crystal packing of ligand **L1** with columns of stacked head to tail molecules that are connected laterally through S...O heteroatom contacts.

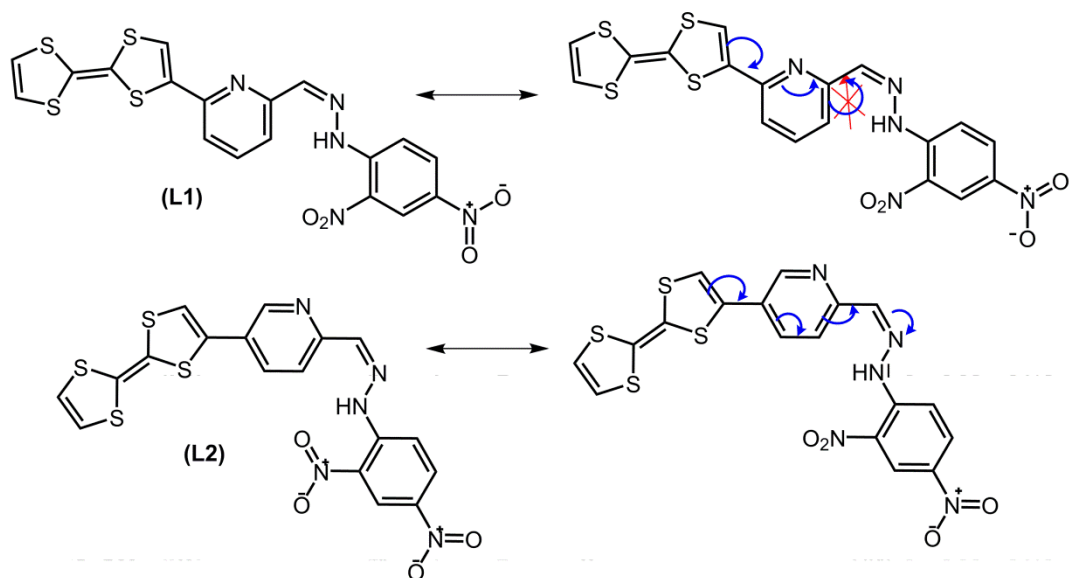


Figure S2: Electronic delocalization scheme for ligands **L1** and **L2**.

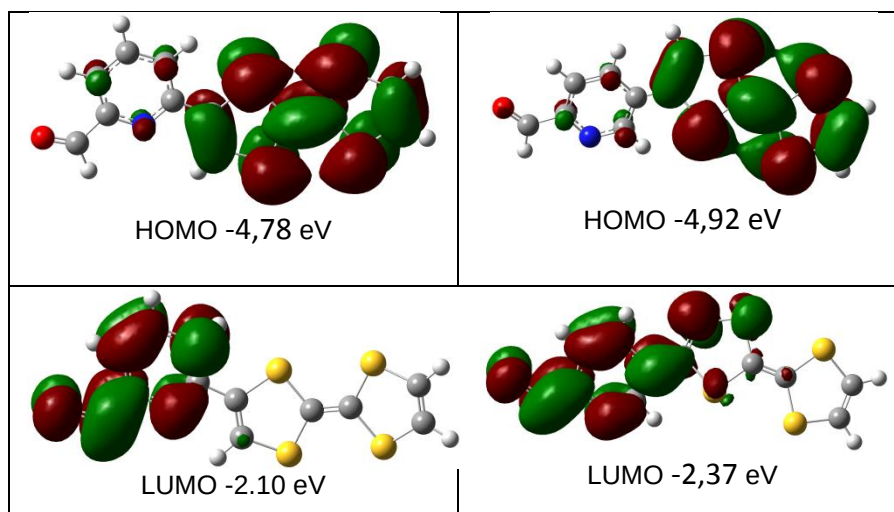


Figure S3: HOMO-LUMO Frontier orbitals representation for compounds **1** and **2**.

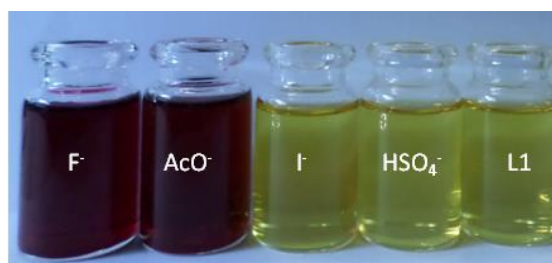


Figure S4: Color change of ligand **L1** upon addition of inorganic anions.



Figure S5: Color change of ligand **L2** upon addition of inorganic anions.

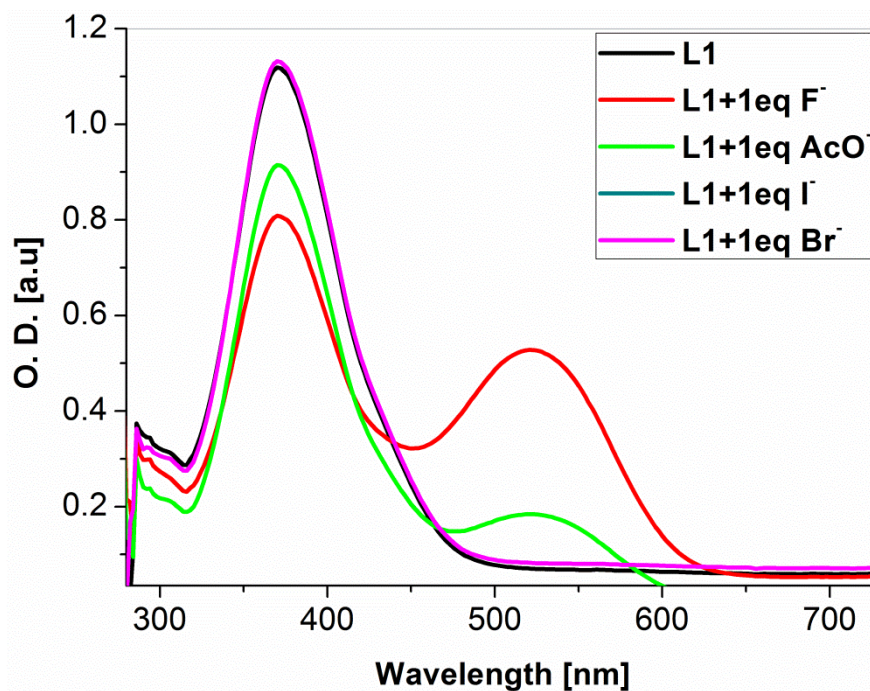


Figure S6: UV-visible absorption spectra of **L1** upon addition of 1 equiv of anion.

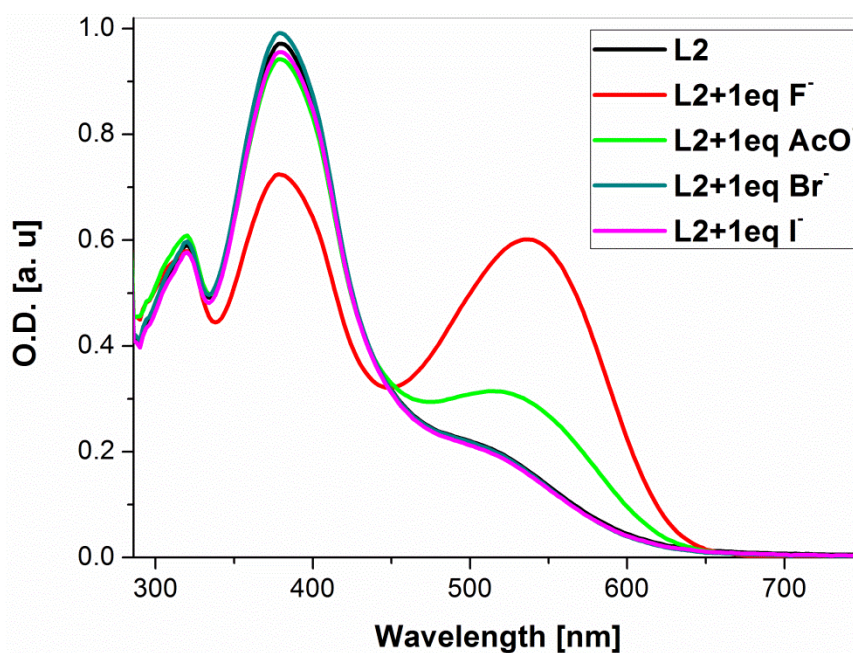


Figure S7: UV-visible absorption spectra of **L2** upon addition of 1 equiv of anion.

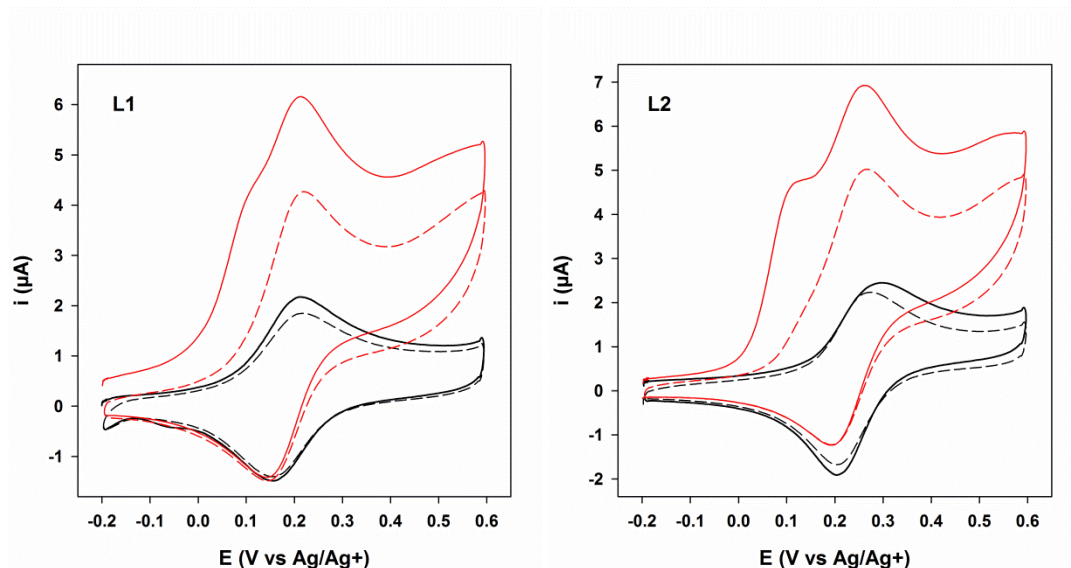


Figure S8: Cyclic voltammograms of ligands **L1** (left) and **L2** (right) (2×10^{-5} M) without (black, bold lines first cycle and dashed lines for second cycle) and with (red, bold lines first cycle and dashed lines for second cycle) 2 equiv of F^- . CVs recorded at $100 \text{ mV} \cdot \text{s}^{-1}$ on a glassy carbon electrode in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (9/1, v/v) with *n*- Bu_4NPF_6 (0.1 M).

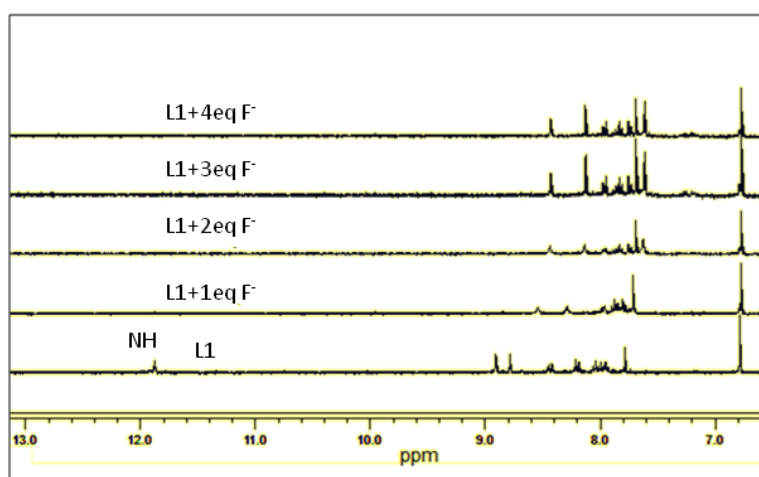


Figure S9: ^1H NMR spectra of ligand **L1** (4×10^{-3} M in $\text{DMSO}-d_6$) upon addition of successive aliquots of TBAF ($\text{DMSO}-d_6$).

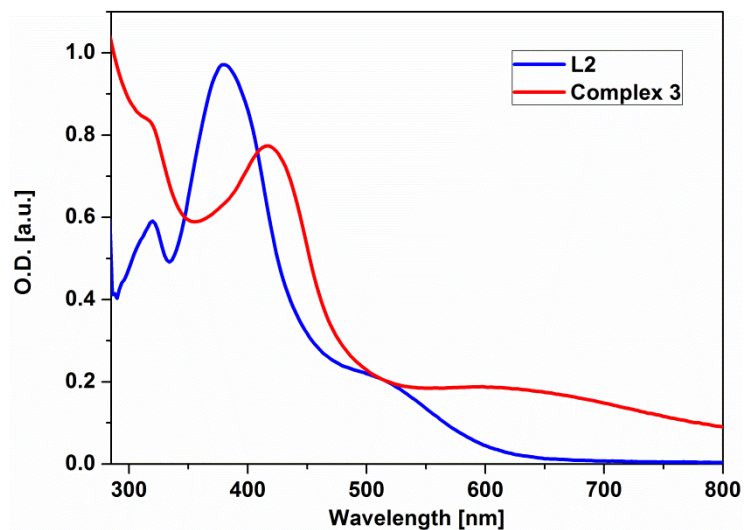


Figure S10: UV–visible absorption spectra of complex **3** ($c\ 1.1 \times 10^{-4}$ M in dichloromethane/acetonitrile, 9/1, (v/v)), room temperature. Ligand **L2** is added for comparison.

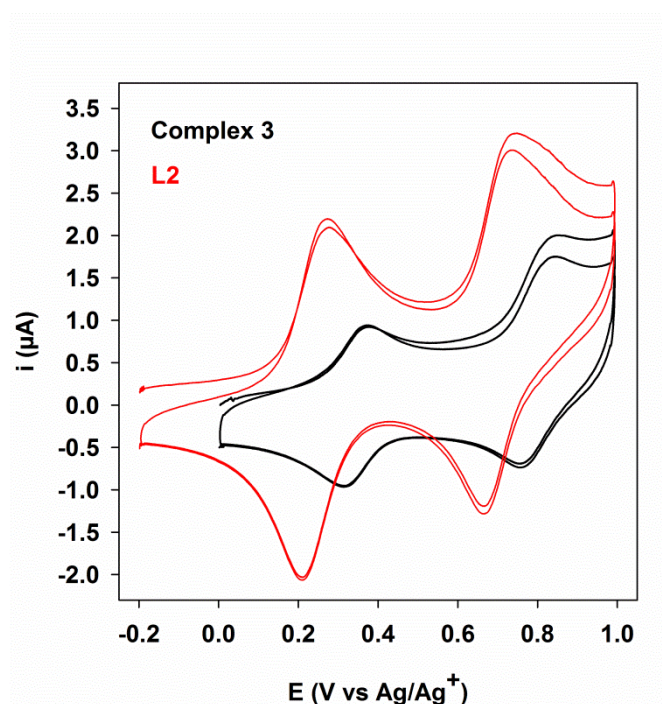


Figure S11: Cyclic voltammograms of **L2** (red, added for comparison) and complex **3** (black) (1.1×10^{-4} M) at $100\ \text{mVs}^{-1}$ on a glassy carbon electrode in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (9/1, v/v) with $n\text{-Bu}_4\text{NPF}_6$ (0.1 M).