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Supporting Information

Catalyst-free approach to a novel imidazo [4,5-f][1,10] phenanthroline ligand and its corresponding ruthenium(II) complex: insights into their applications in colorimetric anion sensing

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Figure S1. IR spectrum of 1-(3-Formyl-4-hydroxyphenylazo)-4-nitrobenzene



Figure S2. ¹H NMR spectrum of 1-(3-Formyl-4-hydroxyphenylazo)-4-nitrobenzene



Figure S3. IR spectrum of L



Figure S4. ¹H NMR spectrum of L



Figure S5. IR spectrum of 1



Figure S6. ¹H NMR spectrum of 1



Figure S7. MALDI-TOF mass spectrum of 1



Figure S8. UV-Vis absorption spectra of sensor **1** (2×10^{-5} mol L⁻¹) in dry DMSO upon addition of H₂PO₄ (0-5 equiv.).



Figure S9. Benesi–Hildebrand plots of sensor **1** with (A) F^- , (B) AcO⁻ and (C) $H_2PO_4^-$ anions associated with absorbance change at 560 nm in DMSO.



Figure S10. Job's plot for sensor **1** and anions with a total concentration of 2.0×10^{-5} M in DMSO at 560 nm.



Figure S11. UV-Vis absorption spectra of sensor **1** (2×10^{-5} mol L⁻¹) in 9:1, DMSO-water upon addition of (A) TBAF, (B) TBAOAc and (C) TBAH₂PO₄ (0-5 equiv.).



Figure S12. Benesi–Hildebrand plots of sensor **1** with (A) TBAF, (B) TBAOAc and (C) TBAH₂PO₄ associated with absorbance change at 560 nm in 9:1, DMSO-water.



(A)



(B)

Figure S13. UV-Vis absorption spectra of sensor L $(2 \times 10^{-5} \text{ mol } \text{L}^{-1})$ in DMSO upon addition of (A) TBAOAc and (B) TBAH₂PO₄ (0-5 equiv.).





(B)

Figure S14. Benesi–Hildebrand plots of sensor L with (A) TBAOAc and (B) TBAH₂PO₄ anions associated with absorbance change at 552 nm in DMSO.



Figure S15. Job's plot for sensor L and anions with a total concentration of 2.0×10^{-5} M in DMSO at 552 nm.

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Figure S16. UV-Vis absorption spectra of sensor L (2×10^{-5} mol L⁻¹) in 9:1, DMSO-water upon addition of (A) TBAF, (B) TBAOAc and (C) TBAH₂PO₄ (0-5 equiv.).



Figure S17. Benesi–Hildebrand plots of sensor L with (A) TBAF, (B) TBAOAc and (C) TBAH₂PO₄ associated with absorbance change at 529 nm in 9:1, DMSO-water.

Determination of the pK_a value:

To determine the pK_a values of L and 1, the spectrophotometric pH titrations were carried out in 9:1 DMSO-Water. The values were assigned as the maxima of the first derivative of the data shown in **Figure S18** (The inset shows the plot of the derivatives of the titrations).

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The p*K*a values were determined to be ~ 10.25 for L and 8.33 for 1 (on the basis of new band formed at 552 and 560 nm for L and 1, respectively) indicating that L and 1 likely are deprotonated with relatively basic anions.



Figure S18. (A) L and (B) 1



Figure S19. ¹H NMR spectra of L in DMSO- d_6 (2×10⁻² mol L⁻¹) in the absence and presence of TBAOAc and TBAH₂PO₄



Figure S20. ¹H NMR spectra of **1** in DMSO- d_6 (2×10⁻² mol L⁻¹) in the absence and presence of TBAOAc and TBAH₂PO₄



Figure S21. Fluorescence spectra of L (2×10^{-5} mol L⁻¹) in the presence of the different anions