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Supporting Information

A Case of Oxoanions Recognition Based on Combined Cationic and Neutral C–H Hydrogen Bond Interactions.

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PART I: ¹H-NMR and ¹³C-NMR Spectra

1-[(pyren-1-yl)methyl]-1H-benzo[d]imidazole 3.







Bis-(benzoimidazolium) receptor as hexafluorophosphate salt 5²⁺·2PF₆⁻.



Part II ESI mass spectrum of receptor 5²⁺·2PF₆-



PART II: UV-vis Anion Binding Studies.



Figure SI1: Changes in the absorption spectra of receptor $5^{2+} \cdot 2PF_6^-$ in DMSO (2.5× 10⁻⁵ M) upon addition of HP₂O₇³⁻ anions at 20 °C. Arrows indicate the absorptions that increase or decrease during the titration.



Figure SI2: Changes in the absorption spectra of receptor $5^{2+} \cdot 2PF_6^-$ in DMSO (2.5× 10⁻⁵ M) upon addition of SO₄²⁻ anions at 20 °C. Arrows indicate the absorptions that increase or decrease during the titration.



Figure SI3: Changes in the absorption spectra of receptor $5^{2+}\cdot 2PF_6^-$ in DMSO/H2O 9:1 (2.5× 10⁻⁵ M) upon addition of SO₄²⁻ anions at 20 °C. Arrows indicate the absorptions that increase or decrease during the titration.

PART III: Fluorescence Anion Binding Studies.



Figure SI4. Fluorescence spectra of receptor $5^{2+} \cdot 2PF_6^-$ (2.5 × 10⁻⁵ M) in DMSO and upon addition of the anions tested at 20 °C, $\lambda_{exc} = 360$ nm.



Figure SI5. Changes in the fluorescence spectra of receptor $5^{2+} \cdot 2PF_6^-$ (2.5 × 10⁻⁵ M) in DMSO upon addition of HP₂O₇³⁻ anions at 20 °C, $\lambda_{exc} = 360$ nm.



Figure SI6. Changes in the fluorescence spectra of receptor $5^{2+} \cdot 2PF_6^-$ (2.5 × 10⁻⁵ M) in DMSO upon addition of SO₄²⁻ anions at 20 °C, $\lambda_{exc} = 360$ nm.



Figure SI7. Changes in the fluorescence spectra of receptor $5^{2+} \cdot 2PF_6^-$ (2.5 × 10⁻⁵ M) in DMSO/H₂O 9:1 upon addition of HP₂O₇³⁻ anions at 20 °C, $\lambda_{exc} = 360$ nm.

PART IV: ¹H-NMR Anion Binding Studies



Figure SI8. ¹H-NMR spectral changes observed in receptor $5^{2+} \cdot 2PF_6^-$ (c = 2.5 × 10⁻³ M in DMSO-d₆) during the addition of up to 1.2 equiv of HP₂O₇³⁻ anions.



Figure SI9. Job Plot experiment indicating 1:1 stoichiometry for the receptor $5^{2+}\cdot 2PF_6^$ and $HP_2O_7^{3-}$ in DMSO-d₆.



Figure SI10. ¹H-NMR spectral changes observed in receptor $5^{2+} \cdot 2PF_6^-$ (c = 2.5 × 10⁻³ M in DMSO-d₆) during the addition of up to 3 equiv of ATP anions.



Figure SI11. ¹H-NMR spectral changes observed in receptor $5^{2+} \cdot 2PF_6^-$ (c = 2.5 × 10⁻³ M in DMSO-d₆) during the addition of up to 4 equiv of ADP anions.



Figure SI12. ¹H-NMR spectral changes observed in receptor $5^{2+} \cdot 2PF_6^-$ (c = 2.5 × 10⁻³ M in DMSO-d₆) during the addition of up to 4 equiv of AMP anions.



Figure SI13. ¹H-NMR spectral changes observed in receptor $5^{2+} \cdot 2PF_6^-$ (c = 2.5 × 10⁻³ M in DMSO-d₆) during the addition of up to 4 equiv of H₂PO₄⁻ anions.



Figure SI14. ¹H-NMR spectral changes observed in receptor $5^{2+} \cdot 2PF_6^-$ (c = 2.5 x 10⁻³ M in DMSO-d₆/D₂O 9:1) during the addition of up to 2 equiv of HP₂O₇³⁻ anions.



Figure SI15. Job Plot experiment indicating 1:1 stoichiometry for the receptor $5^{2+} \cdot 2PF_6^-$ and $HP_2O_7^{3-}$ in DMSO-d₆/D₂O.



Figure SI16. ¹H NMR spectral changes observed in receptor $5^{2+} \cdot 2PF_6^-$ (c = 1 x 10⁻³ M in DMSO- d_6/D_2O 9:1) during the addition of up to 2 equiv of SO₄²⁻ anions.



Figure SI17. Job Plot experiment indicating 1:1 stoichiometry for the receptor $5^{2+} \cdot 2PF_6^-$ and SO_4^{2-} in DMSO-d₆.