Crystallographic, ¹H NMR and CD studies of sterically strained thiourea anion receptors possessing two stereogenic centres

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Electronic Supplementary Information

Figure 1. Comparison of the ¹H NMR (400 MHz, wet DMSO- d_6) spectra of thioureas 1-3. (* chemical shift of thiourea NH protons)



Figure 2. Hydrogen-bonding interaction between NH protons of the thiourea moiety within **1** and the O atom of a DMSO molecule





Figure 3. Packing diagram for compound 1. View along the c crystallographic axis.

Figure 4. Packing diagram for compound 2. View along the c crystallographic axis.





Figure 5. View along the c* crystallographic axis of structure of 3.

Figure 6. Relative cumulative changes in the chemical shift of NH proton at 7.7 ppm for sensor $1 (6 \times 10^3 \text{ M})$ against equivalents of putative anions in wet DMSO- d_6 .



Figure 7. Relative cumulative changes in the chemical shift of NH proton at 7.7 ppm for sensor $2 (6 \times 10^{-3} \text{ M})$ against equivalents of putative anions in DMSO- d_6 .



Figure 8. Relative cumulative changes in the chemical shift of NH proton at 7.7 ppm for sensor $3 (6 \times 10^{-3} \text{ M})$ against equivalents of putative anions in DMSO- d_6 .



Figure 9. WinEQNMR-generated graphs of the fit between the observed (points) and calculated (line) data for the binding of: (a) AcO– with **1** (ca. $6 \times 10-3$ M); (b) H2PO4– with **1** (ca. $6 \times 10-3$ M); (c) AcO– with **2** (ca. $6 \times 10-3$ M); (d) H2PO4– with **2** (ca. $6 \times 10-3$ M); (e) AcO– with **3** (ca. $6 \times 10-3$ M); (f) H2PO4– with **3** (ca. $6 \times 10-3$ M), carried out in DMSO-d6.





Figure 10. The CD Spectra of compounds 1 (top) and 2 (bottom)

Figure 11. Quantitative changes observed in the CD spectrum of 2 in DMSO in the presence of AcO-



Wavelength (nm)