

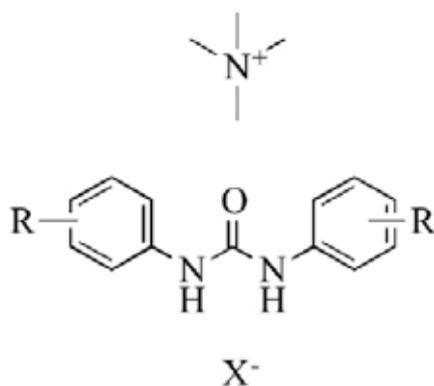
Oral Contributions

[MS13-04] Structural systematics of anion-receptor complexes: insights from electron density distributions

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The electron density distribution and hydrogen bonding interactions in a systematically varied series of five urea-based anion receptor complexes have been characterised. The family of receptors utilise the directional N–H bonds of the urea group in the 1,3- (diphenyl)urea receptor scaffold [1] to bind to an anion. Diversity has been introduced to the series in order to probe anion and substituent effects. Systematic changes, effected through a range of anions and substituent patterns in the receptor, are postulated to affect the hydrogen bonding between the anion and receptor.



- 1: R = *para*-NO₂ X⁻ = Cl⁻
- 2: R = *para*-NO₂ X⁻ = CH₃COO⁻
- 3: R = *para*-NO₂ X⁻ = F⁻
- 4: R = *meta*-NO₂ X⁻ = Cl⁻
- 5: R = 3,5-di-NO₂ X⁻ = CH₃COO⁻

Modelling of aspherical electron densities was performed on high resolution X-ray diffraction data from both home source diffractometers and the I19 beamline at Diamond Light Source [2] and using the Hansen-Coppens formalism [3]. This was complemented by neutron diffraction studies to accurately determine atomic positions for the hydrogen atoms in two of the structures.

Topological analysis using the Quantum Theory of Atoms In Molecules [4] quantified the nature of the various inter- and intramolecular interactions observed across the family of complexes. Our results suggest a trend of increasing hydrogen bond strength with increasing basicity of anion, supported by a corresponding increase in values of $\rho(r)$ and $\nabla^2\rho(r)$ at the N–H...anion bond critical points.

Modification of the receptor scaffold was also shown to affect both the electron density distribution and hydrogen bonding strength in the structures.

This work directly demonstrates how hydrogen bonding interactions depend on the nature of the donor and the acceptor and how these interactions can be modulated by varying the substituents

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