Poster Presentation

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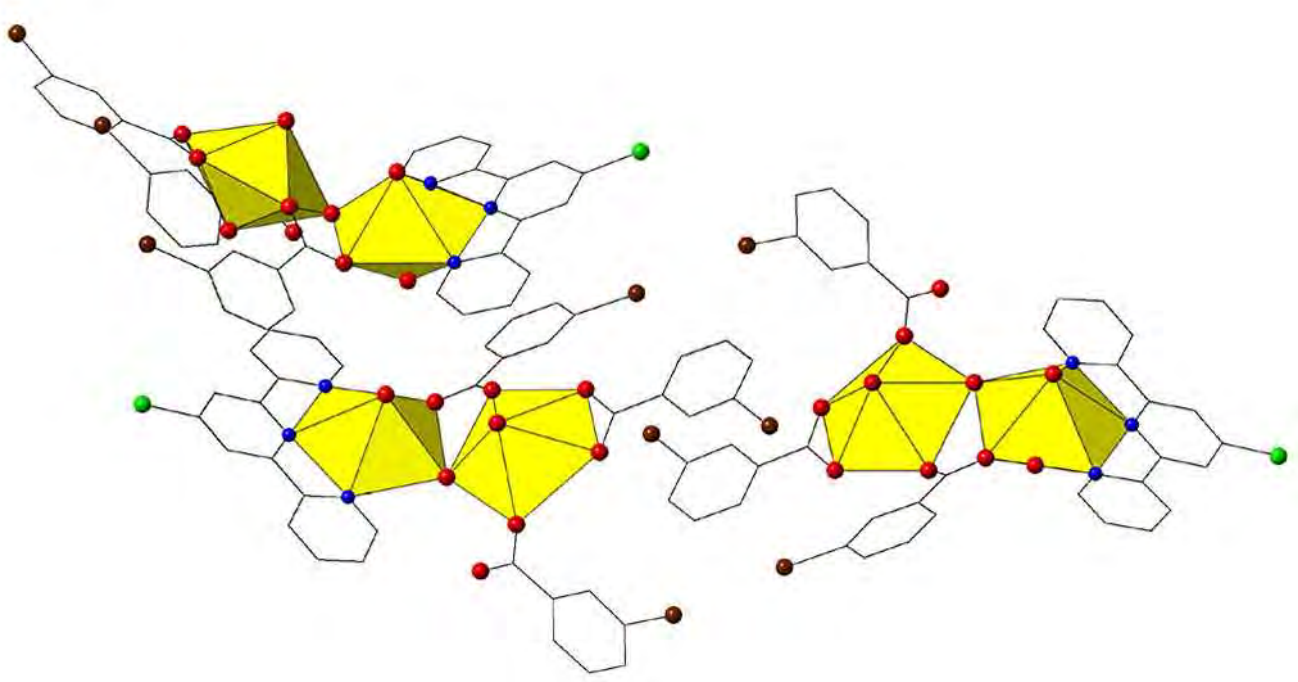
Exploration of supramolecular interactions in a series of UO22+ hybrid materials

K. Carter[1], S. Thangavelu[1], C. Cahill[1]

[1]*The George Washington University, Department of Chemistry, Washington, DC, USA*

Previous work from our group has focused on uranyl hybrid materials with para-substituted halogen benzoic acids.1 Applying a 'cap and link' strategy we have successfully controlled the nuclearity of UO22+ in a series of coordination polymers and Ln3+ in a family of molecular materials.2,3 Here we have expanded on this strategy and produced a series of 12 unique uranyl hybrid materials. The hydrothermally synthesized complexes all feature bromo-substituted benzoic acid linkers and the UO22+ metal centers are capped with a chelating N-donor. Single crystal X-ray diffraction analyses of these materials allowed for the exploration of the structural relationship between the benzoic acid group and the chelating N-donor as well as the influence of pH on uranyl speciation. At an unadjusted pH (~3) a mix of molecular monomers and dimers are observed while at higher pH (5-6) molecular uranyl dimers are exclusively produced. A systematic study of the supramolecular interactions that governed extended solid-state assembly was investigated by varying the bromine position on the benzoic acid groups along with the chelating N-donor with pH. Assembly via halogen-halogen, halogen-π, π-π, and halogen-oxygen interactions was observed and the influence of these interactions on uranyl emission was also investigated. Solid-state luminescence and lifetime measurements were used to explore the effects of speciation and chelating N-donor ligands on the spectroscopic properties of the uranyl cation.

[1] *N. P. Deifel and C. L. Cahill. Chem Comm. 2011, 47, 6114-6116.,* ***[2]*** *S. G. Thangavelu, S. J. A. Pope and C. L. Cahill. Inorg. Chem. 2013, 52, 2060-2069.,* ***[3]*** *K. P. Carter, S. J. A. Pope and C. L. Cahill. CrystEngComm. 2014, 16, 1873-1884.*



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