

Poster Presentation

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Thiourea based-ligands: intergrown polymorphism, and a new route to benzothiazoles

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A suite of urea and thiourea based-ligands have been synthesized and characterized spectroscopically, and by small molecule X-ray crystallography. A mismatch between ligand donor capabilities and metal coordination preference leads to inclusion of labile ligands (i.e. water) upon complexation, which can be readily replaced by stronger donor ligands. Design principles were employed to facilitate surface attachment, as well as coordination, and detection, of co-ligands implied in environmental contamination. On route to these research goals, characterization of one thiourea ligand showed it to be a rare example of an intergrown polymorph (with only one other reported example [1]), while upon copper(II) coordination to a structurally analogous ligand, a new route to the synthesis of benzothiazole-derivatives was revealed. These results will be presented, with an emphasis on the methodology employed to characterize two different phases contained within a single crystal of the intergrown polymorph.

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