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Synthesis, characterization, and coordination of benzothiadiazines

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Abstract:

Metal complexes have many important roles in chemical and biological processes. The organic ligands bound to the metal influence their properties and reactivity. Redox-active ligands which can gain or lose electrons are particularly important in many chemical and biological processes involving electron transfer, i.e. the shuttling of electrons between molecular species. The development of new redox-active ligands provides opportunities to explore these important electron transfer processes. The Rawson group has previously investigated the synthesis of a family of polydentate *N*-donor ligands known as thiadiazines. These molecules are known to bind to metals and undergo both single and two electron oxidation. My project focuses on the synthesis, purification, and characterization of the bis(btda)H₂ ligand (**1**), shown in Fig. 1, and its reactivity with transition metal and lanthanide ions. I will characterize the structures of the complexes through single crystal X-ray diffraction, UV/visible and NMR spectroscopy and examine their redox chemistry through cyclic voltammetry.

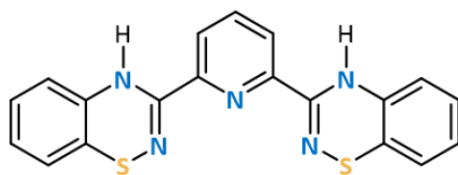


Fig. 1 Molecular structure of the bis(btda)H₂ ligand (**1**).

The synthesis and purification of ligand **1** is described and its structure determined using 1-D and 2-D NMR experiments, elemental analysis (CHN), IR spectroscopy, mass spectrometry, melting point determination, and single crystal X-ray diffraction studies. Recent progress towards the identification of coordination complexes of bis(btda)H₂ with various first-row transition metals and lanthanides are underway. Initial studies indicate selective oxidation of one of the two redox-active rings on each ligand, suggesting some degree of cooperative response between the two heterocycles.

Long term objectives are to study (i) the biological properties of ligand **1** which is structurally related to a range of thiazide drugs utilised to treat hypertension and (ii) to utilise the ligand field associated with **1** to develop new spin crossover materials which have potential applications in data storage and thermal imaging.