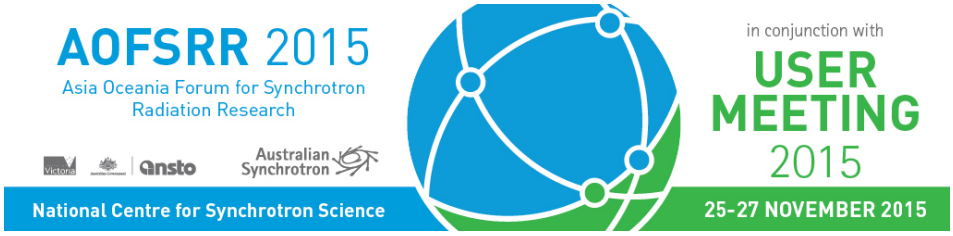

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Heteroleptic Iron(III) {Quinolylsalicylaldimine/Thiosemicarbazone-salicylaldimine} Complexes: Spin crossover, intermolecular structural and solvation features, magnetism and Mössbauer spectra

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The relationship between intermolecular interactions and spin-crossover features such as the abruptness of the spin transition and cooperativity, in crystalline complexes of iron(II) and iron(III), is of much current interest.1 We were particularly interested to make heteroleptic complexes of Hqsal and H2thsa ligands (where Hqsal = quinolylsalicylaldimine2 and H2thsa = thiosemicarbazone-salicylaldiminate3) for the first time, to explore the intermolecular interactions when two different ligands are present around each Fe(III) centre. A family of neutral, heteroleptic iron(III) complexes, [Fe(qsal)(thsa)]·solvent, is presented where solvent is 0.4BuOH, 0.5MeCN, 0.5THF, as well as two polymorphs of solvent free compounds i.e.[Fe(qsal)(thsa)]. We describe a fascinating array of intermolecular interactions occurring in the various crystals, all containing two distinct Fe sites, including similarities and differences and the importance of a void in the lattice structure wherein solvate molecules sit (or do not sit, in [Fe(qsal)(thsa)] polymorphs), and how these all relate to differences in spin states of neighbouring [Fe(qsal)(thsa)] molecules i.e. HS-HS and spin crossover HS-HS to HS-LS. Supporting information and insights are provided by TGA, PXRD and Mössbauer spectral data.

Keywords

Spin crossover, Fe(III), Single crystal X-ray diffraction

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