

10.1071/CH14414_AC

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Australian Journal of Chemistry 2014, 67(12), 1871-1877

Supplementary Material

Coordination polymers constructed from TCNQ²⁻ anions and chelating ligands

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Modelling of disordered 1,10-phenanthroline groups in $M^{II}(\text{TCNQ}^{II})(\text{phen})\cdot\text{DMF}$ (M = Mn or Cd)

Inspection of the Fourier difference map revealed that the 1,10-phenanthroline (phen) ligand in $M^{II}(\text{TCNQ}^{II})(\text{phen})\cdot\text{DMF}$ (M = Mn, Cd) is disordered over two closely separated, almost co-planar, symmetry related sites. In both the Cd and Mn structures, one C atom from each phen ligand, which is located on a crystallographic 2-fold axis, is common to both orientations of the phen ligand; the 2-fold axis also passes through the metal centre to which the phen is coordinated. Accordingly, all phen atoms, except for the C atom common to each orientation, were refined with 50% site occupation.

Modelling of disordered 1,10-phenanthroline groups in $\text{Co}^{II}(\text{TCNQ}^{II})(\text{phen})$

Inspection of the Fourier difference map revealed that the phen ligands bound to either Co1 or Co2 are disordered over two closely separated, symmetry related sites. The two orientations of the phen in each case are inclined at an angle of approximately 20° to each other. In each case the two orientations are related by a mirror plane that passes through the cobalt centre to which the phen is coordinated. Accordingly all phen atoms were refined with 50% site occupation.