

Unit Cellmates: the *Cis* and *Trans* Isomers of an Iron(II) Complex Co-crystallize

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The crystal structure of dichloro-bis(2-picolylamine)-iron(II) contains a 1:1 ratio of the *cis* and *trans* isomers. The former lies on a two-fold axis whereas the latter lies on an inversion centre. The equatorial chlorine and NH₂ ligands of the two isomers lie in the same crystal planes exhibiting an intricate 2D hydrogen bond network with four eight-membered rings around each iron constructing a tiling pattern throughout the layer. These hydrogen bonded layers are interconnected through extended π - π interaction between the axial pyridine ligands.

The number of crystal structures with co-crystallized isomers found in the CSD is very limited. In fact only one analogous, ordered example with *similar* ligand atoms (MN₄Cl₂) seems to exist [1].

The rare occurrence of this phenomenon may be understood intuitively from the facts that firstly, both isomers, which are expected to have different energies and most probably also different synthesis conditions, must happen to be present during crystallization, and that secondly, the formation of the co-crystal must be more favourable in thermodynamic and/or kinetic terms than the formation of crystals containing the individual isomers only.

[1] Zhu D., Xu Y., Yu Z., Guo Z., Sang H., Liu T., You X, *Chem. Mater.*, 2002, **14**, 838.

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