Polymorphism in coordination compounds

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Polymorphism is the appearance of the same substance in various forms or modifications. The form usually refers to the crystal packing, but a different molecule conformation is also possible. Polymorphs are chemically identical substances, but can differ in their physical, thermodynamic, spectroscopic, kinetic, surface, mechanical and chemical properties. Polymorphism is especially important in pharmaceutical industry and crystal engineering and is extensively studied in organic compounds. However, polymorphs of metal complexes have been much less studied, but start to gain more and more attention, especially in the fields of crystal engineering and solid-state chemistry (coordination polymers and metal-organic frameworks). Polymorphism is also important in development of new materials, since polymorphs offer an insight into potentially better properties. Unfortunately, a loss of control over a crystallization process results in inability to reproducibly obtain a desired polymorph in an industrial process.

This lecture will address the examples of polymorphs of metal complexes from own studies e. g. polymorphs of nickel(II) complexes with 6-hydroxypicolinate and pyridine, polymorphs of cobalt(II) complexes with 6-bromopicolinate and polymorphs of a 1D cadmium(II) coordination polymer with dipicolinate. The examples of pseudopolymorphs of metal complexes will be also presented e. g. pseudopolymorphs of nickel(II) complexes with 6-methylpicolinate, pseudopolymorphs of nickel(II) complexes with 6-bromopicolinate and pseudopolymorphs of iron(III) complexes with dipicolinate and 6-amino-2-picoline. The synthetic conditions to obtain these metal complexes, including the crystallization conditions needed for the said polymorphs, will be discussed in this lecture as well. A special attention will be given to the comparison of the crystal structures of polymorphs i. e. to the similarities and differences of their crystal packings, including the type and effect of weak intermolecular interactions (hydrogen bonds, π-π interactions) found in these crystal packings.

Graphical abstract