

Crystals Of New Bis-2ampy Ni(II) Compounds With TCNQ Or TCNQF₄. Unexpected Structural Differences.

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Crystallographic characterization of coordination complexes of TCNQ or TCNQF₄ is often hindered by difficulty in preparing crystals for X-ray analysis. Conventional wisdom has it that the crystallization process has to be slow enough to favor substantial crystal growth in order to obtain a sample adequate for X-ray diffraction. However, compounds of TCNQ and its derivatives famously undergo changes in solution, leading to decomposition of their coordination complexes before sufficient crystal growth has occurred. At the other end of the time line, if the target compound is a polymer, the insolubility and rapid formation of the resulting solid limit the experimenter's ability to vary the crystallization conditions in order to obtain samples of optimum size. We present the preparation of crystals of [*trans*-Ni(2ampy)₂(TCNQ)₂] (**1**) and [*cis*-Ni(2ampy)₂TCNQF₄] (**2**) using as starting material in both cases [*trans*-Ni(2ampy)₂(NO₃)₂] (2ampy = 2-aminomethylpyridine). Among the differences between these two nickel compounds are that compound **1** is a discrete molecule with the 2ampy ligands *trans*- to each other, as in the starting material, while compound **2** is a 1D polymer with the two 2ampy ligands *cis*- to each other. In the polymer the TCNQF₄ group bridges successive nickel centers, coordinated through only the two CN groups *syn*- to each other at the C7 and C8 positions -- which is a new coordination mode for this group. Other chemical and structural differences will be presented together with the horizontal diffusion crystallization process used to prepare crystals for X-ray analysis.

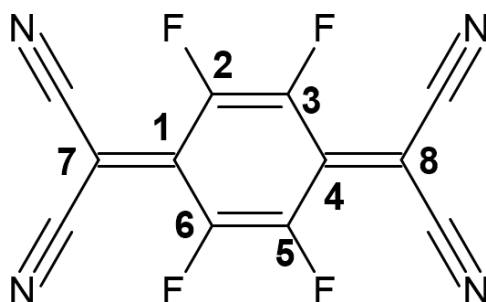


Figure 1