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Polymorphism, Hydration and Metal - Metal Contacts in a Luminescent Platinum Dicarbene. J.R. Stork, A.L. Balch, M.M. Olmstead, Dept. of Chemistry, Univ. of California Davis, Davis, CA 95616, USA.

We have prepared the dicarbene compound $\text{Pt}(\text{CN})_2(\text{C}_4\text{H}_{10}\text{N}_4)$ as a monohydrate, tetrahydrate, and two dimethyl formamide (DMF) solvates, and have elucidated the structures of the compounds by single crystal x-ray diffraction studies. The various solvates have very different physical properties and structures. Both hydrates form infinite, kinked chains linked through platinum atoms and stabilized by hydrogen bonding to lattice water. However, the monohydrate is yellow with a yellow luminescence while the tetrahydrate is orange and non-luminescent. The DMF solvate forms concomitant polymorphs: a colorless, non-luminescent morph, and a yellow morph with a green luminescence. The two morphs consist of dimers of the dicarbene molecules, capped at either end by DMF. We will also discuss the relationship between platinum-to-platinum distances and the optical properties of the compounds, along with DFT calculations of the relevant molecular orbital populations.

