# Development of Solvatochromic (color-changing) “Molecular Grid” Materials

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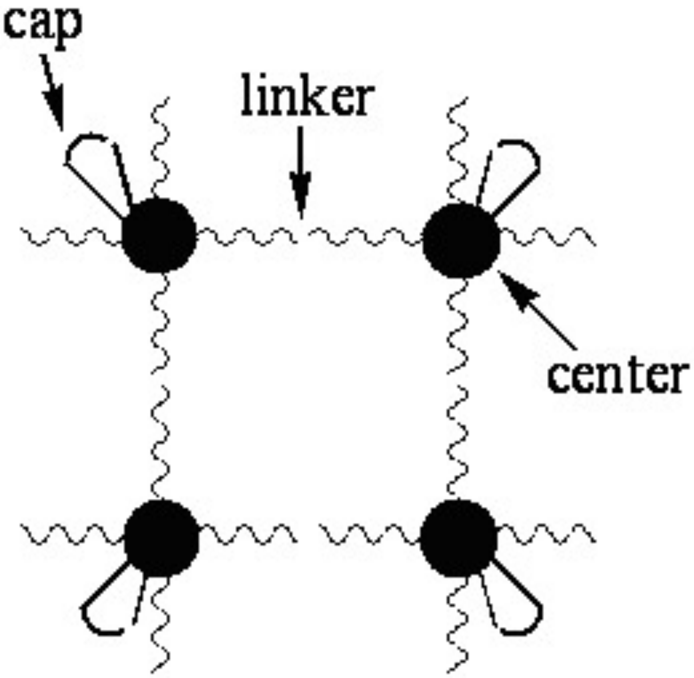
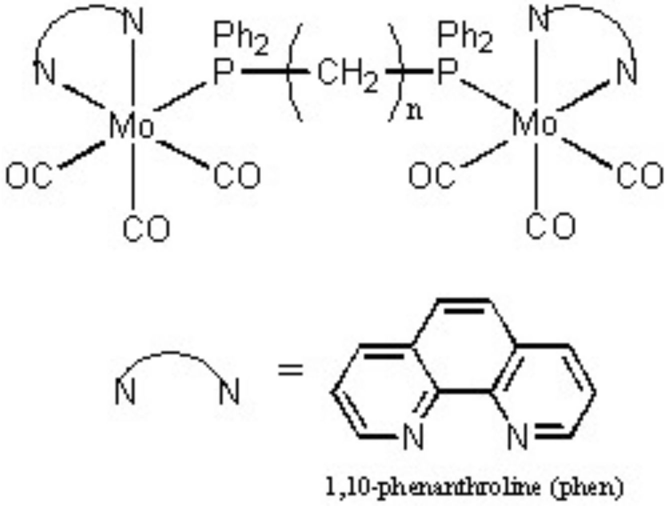
Structure engineering is a research process in which the molecular structure of a target compound is designed for a specific application.[1] In environmental sensor development, structure engineering has been employed to create materials with built-in molecular cavities designed to absorb specific contaminant molecules. Several inorganic complexes containing two- and three-dimensional molecular cavities have since been reported.[2] However, their responses upon absorbing guest contaminant molecules are limited to observation by NMR spectroscopy and X-ray diffraction. Adding a **visual** response to this type of material would greatly facilitate sensor development and open up numerous research avenues in multiphase intermolecular interactions. In this work, we are taking steps to develop “molecular grid” materials based on solvatochromic (color-changing) chemical systems.

A schematic diagram of our proposed molecular grid materials is shown below. The grid consists of three components: “center” atoms, “cap” ligands, and “linker” ligands. Using diimine “cap” ligands on Mo “centers” create solvatochromic metal-to-ligand-charge-transfer (MLCT) transitions as reported for numerous Mo(diimine)$(CO)_4$ systems. Out of the several bidentate diamines, dipyridines, diisocyanides, and diphosphines with potential to serve as “linker” ligands, the last are of greatest interest as phosphorous coordination may be observed by $^{31}$P NMR spectroscopy.



The initial phase in development of such a grid material is the connection of two Mo centers that contain “cap” ligands.



**2:** n = 4
**3:** n = 2

In reactions of $Mo(CO)_4(phen)$ and diphosphines using 2:1 or 1:1 mole ratios, we have prepared the novel bridged dppb and dppe complexes **2** and **3**, respectively. UV-vis, IR, and NMR ($^1H$ and $^{31}P$) spectroscopy confirm the stoichiometry and the nature of diphosphine coordination in these complexes. Work on expanding this type of structure to a "square" as well as utilizing diisocyanides as bridging ligands is underway.

**Notes and References**

1. (a) Braga, D.; Grepioni, F.; Orpen, A.G. *Crystal Engineering: From Molecules and Crystals to Materials*; NATO Science Series, Mathematical and Physical Sciences, Vol. 538; Kluwer Academic Publishers: Dordrecht, The Netherlands, 1999 and references therein. (b) Lehn, J.M. *Supramolecular Chemistry – Concepts and Perspectives*; VCH: Weinheim, Germany, 1995 and references therein. (c) Leininger, S.; Olenyuk, B.; Stang, P.J. *Chem. Rev.* **2000**, *100*, 853.
2. Dozens of references are found pertaining to molecular cavity materials and their formation. An excellent review of literature that is pertinent to our reported work is given by Fujita, M.; Tominaga, M.; Hori, A.; Therrien, B. *Acc. Chem. Res.* **2005**, *38*, 371-380.