The Self-Assembly of a Supramolecular Cube

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A supramolecule is a structure of multiple molecules held together non-covalently. There are many known supramolecules with various shapes such as sticks, triangles, squares, spheres, tetrahedra, cubes, etc. that can be used for catalysis, ion exchange, molecular magnets, nano-electronics or nano-machines. Better understanding of how the molecular pieces assemble is crucial for enhancing applications.

For this particular project, the metal-ion directed self-assembling cube, created in Dr. Michael Ward’s lab, was assembled step-by-step by slowly adding a ligand called $L_{\text{naph}}$ (1,5-bis [3-(2-pyridyl)pyrazole] naphthalene) to nickel(II) cation in solution. At each step, the wavelength dependent color was measured on a UV-vis spectrometer. All of this measured data was modeled with Sivvu™, a special computer program for equilibrium-restricted factor analysis, to determine: 1) how many distinct chemical species are there in the series of solutions? 2) what is the unique color or the molar absorptivity curve of each distinct chemical species? and 3) what are the equilibrium constants for the reactions between these species? Also, to confirm the existence of the chemical species in the solution, the mass of each species was measured by a high resolution electro spray mass spectrometry.

Through Sivvu™, we could identify 2 possible models: one with 9 distinct species in the solution and another with 1 additional species. The molar absorptivity curves for each of the species and the equilibrium constants for the reactions between them were sensible for both models. Through mass spec, the existence of all the species was confirmed except for the extra one. Below is a schematic of the assembly and subsequent disassembly of the cube as the amount of ligand increases incrementally.

For future work, more UV-vis data should be obtained at different temperatures in order to work out the thermodynamic driving force of the assembly process. Also, more mass spec data should be obtained to identify the 1 unconfirmed species. Finally, based on the results, it may be possible to isolate at least one of the assemblages shown above apart from the cube itself.

The summer research project at Calvin College was a great opportunity to broaden my experience in the research field. First of all, I learned that a number of laboratory techniques, instrumental procedures and computational analysis, which will be helpful for my future laboratory work. Also, I noticed that information exchange between researchers are crucial to accelerate the research projects forward; the active communications between the researchers brought out many creative suggestions and valuable ideas. Along with these, it was a great chance for me to build up relationships with faculty and students. Secondly, I learned what to expect in the future as a researcher. Now, I have a better mindset for a project even when experiments do not work as expected.