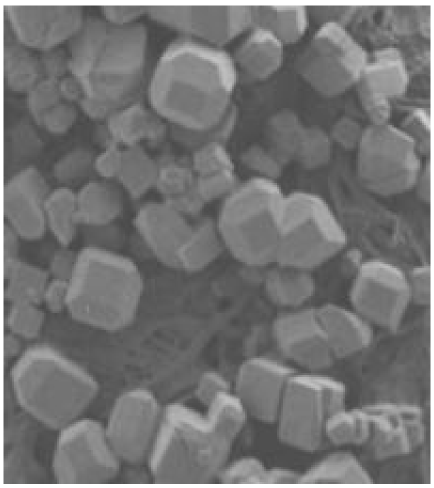
Chemists create molecular polyhedron

July 21 2011



This is a scanning electron microscope image of a new material that self-assembles into a polyhedron using the attractive interactions associated with hydrogen bonds. The shapes then further organize into a crystal lattice that resembles a porous structure called zeolite, an absorbent material with many industrial uses. Credit: Michael D. Ward, New York University

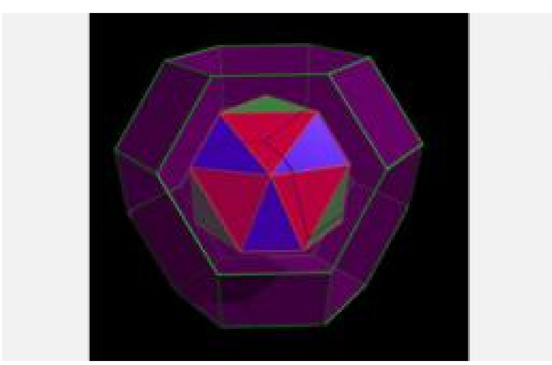
Chemists have created a molecular polyhedron, a ground-breaking assembly that has the potential to impact a range of industrial and consumer products, including magnetic and optical materials.

The work, reported in the latest issue of the journal *Science*, was conducted by researchers at New York University's Department of Chemistry and its Molecular Design Institute and the University of Milan's Department of Materials Science.

Researchers have sought to coerce molecules to form regular polyhedra—three-dimensional objects in which each side, or face, is a polygon—but without sustained success. Archimedean solids, discovered by the ancient Greek mathematician Archimedes, have attracted considerable attention in this regard. These 13 solids are those in which each face is a regular polygon and in which around every vertex—the corner at which its geometric shapes meet—the same polygons appear in the same sequences. For instance, in a truncated tetrahedron, the pattern forming at every vertex is hexagon-hexagon-triangle. The synthesis of such structures from molecules is an intellectual challenge.

The work by the NYU and University of Milan chemists forms a quasi-truncated octahedron, which also constitutes one of the 13 Archimedean solids. Moreover, as a polyhedron, the structure has the potential to serve as a cage-like framework to trap other molecular species, which can jointly serve as building blocks for new and enhanced materials.

"We've demonstrated how to coerce molecules to assemble into a polyhedron by design," explained Michael Ward, chair of NYU's Department of Chemistry and one of the study's co-authors. "The next step will be to expand on the work by making other polyhedra using similar design principles, which can lead to new materials with unusual properties."



This image is a simplified representation of a compound (red, blue and green) nesting inside a single truncated octahedron (purple). Credit: Michael D. Ward, New York University

The research team's creation relies on a remarkably high number of hydrogen bonds—72—to assemble two kinds of hexagonal molecular tiles, four each, into a truncated octahedron, which consists of eight molecular tiles. Although chemists often use hydrogen bonds because of their versatility in building complex structures, these bonds are weaker than those holding atoms together within the molecules themselves, which often makes larger scale structures constructed with hydrogen bonds less predictable and less sustainable. The truncated octahedron discovered by the NYU team proved to be remarkably stable, however, because the hydrogen bonds are stabilized by the ionic nature of the molecules and because no other outcomes are possible. In fact, the truncated octahedra assemble further into crystals that have nanoscale pores, resembling a class of well-known compounds called zeolites, which are made from inorganic components.

Because the structure also serves as a molecular cage, it can house, or encapsulate, other molecular components, giving future chemists a vehicle for developing a range of new compounds.

Provided by New York University