

Star molecule from IIT-M

Designer molecules can help drug delivery

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It is a marvel of synthetic chemistry that today we can build molecules pretty much like we make up structures with building blocks. Using this method for their science at Dillip Kumar Chand's lab at the Department of Chemistry, Indian Institute of Technology Madras, researchers have made a molecule that looks like a five-pointed star with its tips truncated.

All you have to do to build the molecule is to get together the component molecules and ligands and shake them with a solvent in a "one-pot." Of course, the hard work is in knowing what components you will add to the solvent and in what measure. Prof. Chand's team calculated the structures using the density functional theory, to work out the architecture of the molecule they were building.

Designer molecules

Such designer molecules with cavities in them can be used for drug delivery. Prof. Chand explains: "Molecules having a cavity are used for binding the guest [molecule] and transporting the guest to another site." For example, binding a drug and delivering the drug. In building this molecule, the researchers introduce more than one cavity in a single molecule. This makes it more interesting.

In order to build the desired molecule, the team uses three components: One is palladium (II) which can bind to molecules at four places 90 degrees apart. The second is the molecule 4-4'-bipyridine which is like a rod that can bind at its two ends. And the last is the molecule 1,4-phenylenebis(methylene) diisonicotinate which is like a stick bent twice



Dillip Kumar Chand

along its length and can bind to two molecules at its two ends. By throwing in five measures each of the three components, the team comes up with a star-shaped resultant molecule as shown in the picture.

The use of palladium(II) itself is unusual and new. Further, binding it to two different ligands has never been done before. Normally, using a rigid rod-like ligand would usually yield a square arrangement but in this case it yields a pentagonal star-like arrangement. "Since we anticipated a pentagonal architecture, it excited us to put our full effort on the project. In nature there are many pentagonal structures whereas among chemicals, the pentagonal structure is very rare," says Prof. Chand.

The team now aims to make different variations of this design and use the cavity for binding drug molecules and transport them to required sites. "Also, we want to utilise the related molecules in catalysis," he adds.