Can Crystallography Help Us Design Successful Organocatalysts

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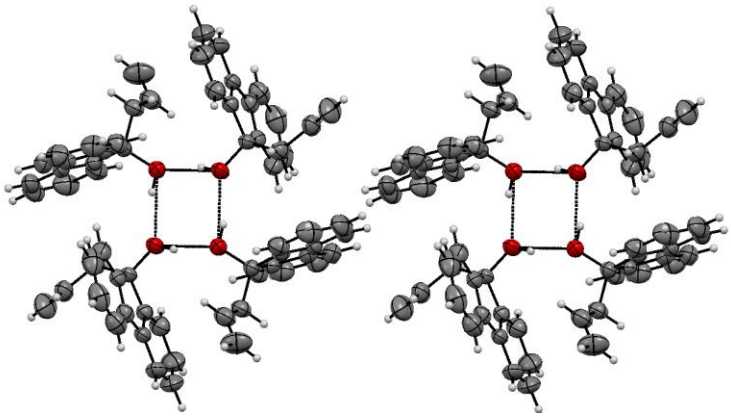
Organocatalysts are small organic molecules that activate other organic molecules, increasing their reactivity.[1] This often involves specific non-covalent interactions that allow the catalyst to bind to the substrate and alter its reactivity. These organocatalysts can be designed to have a shape that, when bound to the substrate, directs the approach of a second reagent. It therefore controls the stereoselectivity of the reaction. In order to create new organocatalysts, we need to have a good understanding of the non-covalent intermolecular forces that allow for the association of the catalyst to the substrate

X-ray crystallography is an analytical technique in which a single crystal of a compound is irradiated with an x-ray beam. Since a crystal is an ordered matrix of atoms, the crystal will diffract the x-rays into a pattern that contains information about the precise coordinates of the atoms in the crystal.

Small organic molecules in a crystal align themselves into a matrix because of the presence of favorable non-covalent interactions. X-ray crystallography can let us see specific non-covalent interactions. For example, shown below is a view of the crystal structure of 9-allylflourenol.[2] The molecule organizes itself into ordered tetramers using a combination of hydrogen-bonding and aromatic T-stacking interactions.



We hope to build molecules that are designed to be potential new organocatalysts and study them using x-ray crystallography, and to use that crystallographic information to help guide further designs. Ideally, this will involve co-crystallization of the catalyst and the desired substrate. We also hope to see if they actually work as organocatalysts by using them to promote chemical reactions.

1. List, B., Organocatalysis. *Beilstein J. Org. Chem.* **2012,** *8*, 1358-1359, No. 156.
2. Knight, K. S.; Wood, H. B., 9-Allyl-9H-fluoren-9-ol. *Acta Crystallogr., Sect. E: Struct. Rep. Online* **2014,** *70*, o677.