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Project 1: Surface-catalyzed reactions in space

The Universe was long considered to be a vast mostly empty expanse, apart from the odd comet, asteroid, planet or star dotted here and there. It was also generally accepted that not a lot of interesting chemistry happened out there. In the last few decades, however, astronomers have discovered that the Universe is anything, but empty and that certain regions show extremely interesting chemistry initiated by starlight and fast-moving particles. In fact, approximately 120 different molecules have already been detected. They vary from familiar molecules like H_2, CO, and H_2O to exotic ones, like $HC_{11}N$, a large linear unsaturated molecule.

Most interesting chemistry occurs in so-called interstellar clouds (see Illustration 1), where small dust particles block the harsh UV light of stars, allowing molecules to be formed both in the gas-phase and on the surface of the dust particles. The temperatures in these clouds are low (10K-100K) and the gas is very tenuous (~10^{-13} Torr). As a result, experimental data on reactions forming these molecules is difficult to obtain, which makes calculations on these reactions imperative to explain the reactions in interstellar space.

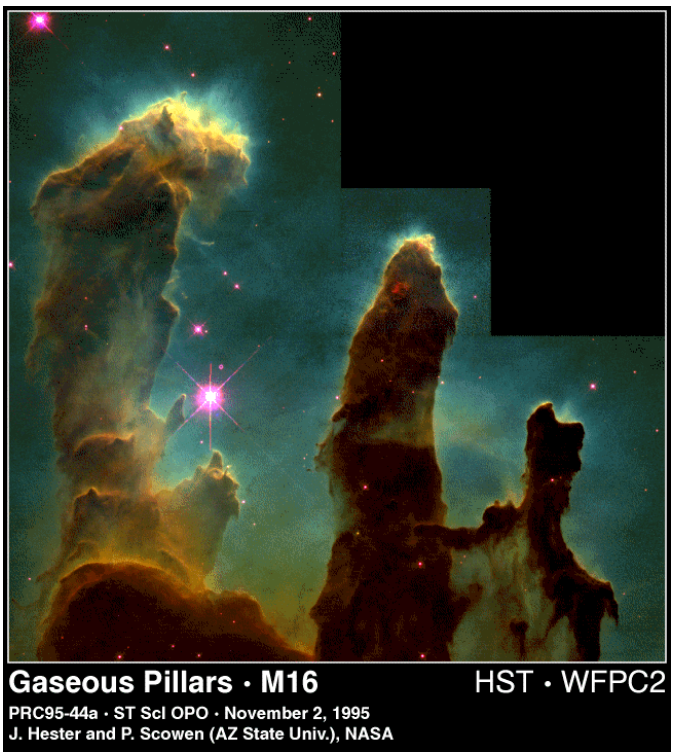

Illustration 1: Molecular Clouds in the Eagle Nebula

I have one project in this general area. This project deals with the formation of (water) ice mantles on dust grains. It is generally assumed that these mantles form *in situ* on the dust grains rather than by accretion from the gas-phase. However, the formation of water is generally considered to be an activated process, which makes it impossible in space, because of the low temperatures of the ambient gas. However, the evidence for this is rather tenuous and you will be performing calculations, using state-of-the-art computer software, to (dis)prove the possibility of forming water on dust grains.

Project 2: Quantum Mechanical Studies of Solution-Phase Reactions

The research in my group is focused on the study of chemical reactions using a variety of computational methods and supercomputers, both here in Sheffield and outside Sheffield. These methods are applied to a variety of molecular systems varying from gas-phase and gas-surface reactions occurring in interstellar space (see above) to solution-phase reactions used in (in)organic synthesis. In this project, you will be applying these methods to investigate the (sometimes surprising) regio-selectivity of Diels-Alder reactions of compounds under current investigation in the Harrity group.

For more details, please see dr. Meijer.