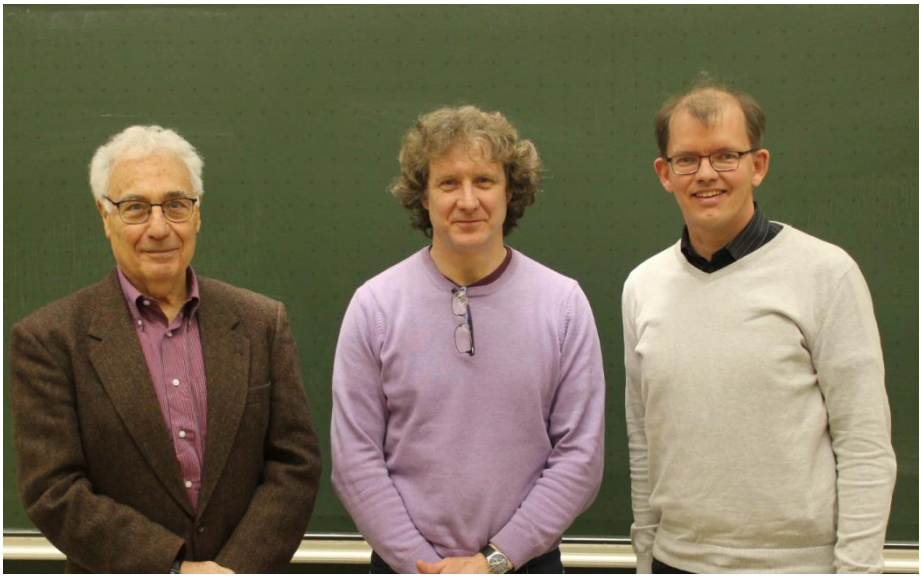
BritInn Fellowship Visit 2020

At the heart of chemistry lies the interaction between atoms to form molecules. Describing this process accurately using computer simulations is surprisingly hard. The present project aimed to bring together two different approaches to study the formation of small molecules found in space. Prof. Gianturco (Innsbruck) uses calculations that examine all the available quantum states of a molecular reaction to see how it then populates some of them under the chosen conditions, whereas Prof. Worth (UCL) directly simulates the time evolution of the atoms as they come together. The challenge for the time-dependent methods is the high accuracy required for studies of atoms colliding in the very cold temperatures of space. The challenge for the time-independent methods is that they cannot treat chemical reactions with more than 4 or 5 atoms involved.

The visit took place over 2 weeks and was planned to be an opportunity for both researchers to learn more about the methods of the other. Calculations were performed on a simple system He + CN^- using both approaches to compare. Preliminary results have already been obtained and the collaboration will now continue by further moving to more challenging calculations.

The visit was hosted at the Department of Ion Physics and Applied Physics at the University of Innsbruck by Prof. Roland Wester. Prof. Worth was able to learn about the highly specialized experiments being carried out there, with many informative discussions with the researchers involved in the various projects. In addition to the research, Prof. Worth presented a well-attended general lecture on "Watching Fundamental Chemistry as it Happens Using Lasers and Computers".

The visit of Prof. Worth was supported by the Academic Network Britain-Innsbruck of the University of Innsbruck.



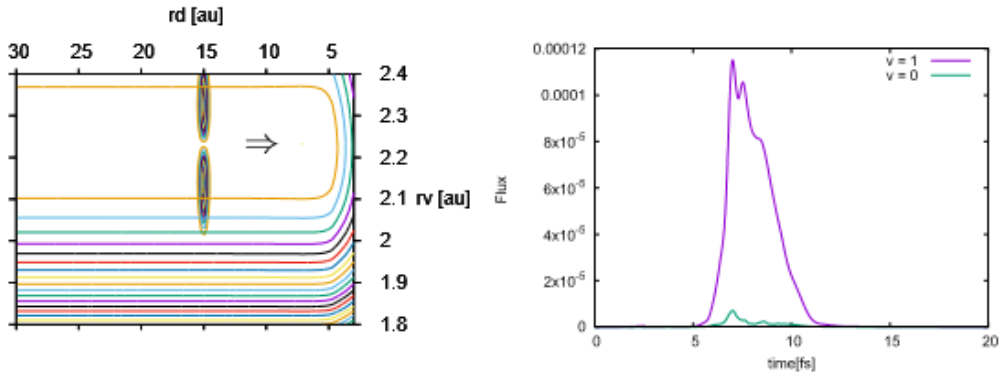


Figure 1: Depiction of He reacting with CN^-. Left panel: He wavepacket approaching CN^-1 in state $v = 1$. Right panel: Outgoing flux after the collision showing some CN^-1 has been cooled into the $v = 0$ state.

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