Guntram Rauhut's Group at the Institut für Theoretische Chemie has built an accurate database of potential energy surfaces (PES) for various polyatomic molecules. These are potentially very useful for the ExoMol group at University College London in the generation of molecular line lists. However, to maximise their utility, they would most conveniently be expressed as functions of internal coordinates such as bond lengths and angles. Currently, the PESs in this database are defined in terms of the molecular normal mode coordinates. This visit will aim at developing an interface between the normal mode and internal coordinates and thus to make the PES database compatible with the ExoMol computational tools (such as e.g. DVR3D and TROVE)

To that end, I have been developing a program designed for this purpose. Here, a user inputs a molecular structure, defines the coordinates, and adds the potential energy surface obtained from the database. The user is then able to provide any set of internal coordinates to obtain an energy. Thus far, the program is able to convert the internal coordinates into the normal coordinates, but there have been difficulties in using the database itself to obtain the correct energy.

To solve this issue, closer collaboration with Guntram Rauhut's group would be desirable. In visiting the group, I would be able better understand the database to program this calculation and I would be able to check and debug the code effectively.

Another aim of this visit is to learn about the so-called Raman wavefunctions method, a very efficient approach to generate cross sections of larger polyatomic molecules. We plan to implement this method into the TROVE package.

Proposed contribution to the scientific objectives of the Action:

The aim of the visit further advances the Action CM1045 (Molecules in motion) by enabling the usage of the potential energy surface database in a custom set of internal coordinates defined in a user defined Z matrix, for the ExoMol group and any other groups from the community using the internal coordinates.

Techniques:

My interface code is written in C++, so I will develop my knowledge of this language further. Of course, I will also properly understand how to use the database.

Time line:

First I will show to Guntram Rauhut what has been done so far. With his guidance and assistance, we aim to complete the final part of the code so the outputted energy is correct. Then the code will be extensively tested. I will also interact with Dr Taras Petrenko regarding the Raman wavefunctions method.