

This project aims to obtain a better understanding of intramolecular vibrational redistribution. The inspiration is drawn from the work of Rui Fausto's group, specifically the article from 2015 (A. J. Lopes Jesus, I. Reva, C. Araujo-Andrade, and R. Fausto, "Conformational switching by vibrational excitation of a remote NH bond," *Journal of the American Chemical Society*, vol. 137, no. 45, pp. 14240-14243, 2015.). The article successfully demonstrates that it is possible to switch between two conformers of 6-methoxyindole by exciting the first overtone of the NH bond in the molecule in a matrix-isolated experimental setup. This gives a unique opportunity to control the conformer distribution and investigate intramolecular vibrational redistribution (IVR). Previously this sort of conformational switching had only been done by exciting an OH bond close to where the conformational change happens. Since then similar work has continued mostly within the Fausto group.

In this project we wish to repeat the experimental results for 6-methoxyindole, as well as investigate other (similar) molecules. These two molecules are: 4-amino-2,6-dimethoxypyrimidine and 4-amino-2-hydroxy-6-mercaptopyrimidine. The goal is to hopefully gain more knowledge of how the vibrational energy is redistributed in molecules, and how to control this effectively. As for the 6-methoxyindole, we wish to induce the conformational switching by vibrationally exciting the NH bond. For the 4-amino-2,6-dimethoxypyrimidine, it would be interesting to see if the energy barrier for the switch of the OCH₃ group is the same as for the 6-methoxyindole. As well as to examine if there is a difference between which of the OCH₃ groups switch or whether it is random. For the other molecule, 4-amino-2-hydroxy-6-mercaptopyrimidine, the difference between the two functional groups, SH and OH, and their possible switching mechanism and the energy barriers related to each of them (if separable) is of interest.

For the experiments to be optimal, the wavenumber at which the NH bond is excited must be very exact. In our group we calculate these vibrational frequencies but lack experience in executing well set up matrix-isolated experiments. At the MOLIM Work Group 1 Meeting in September, we met Rui Fausto, who was kind enough to give a lot of great advice to improve our experimental setup.

The LaserLabEurope in Coimbra is therefore an ideal location to conduct these experiments, due to the advanced equipment as well as the experienced staff, which could hopefully help us to gain even more knowledge towards advancing our own matrix-isolation research.