Presentació del MCTDH, exemple d'aplicació en el fluoroform

Juan Manuel Ortiz Sánchez – Unitat de Química Física – Departamet de Química (UAB)

juanma@klingon.uab.es

For my Erasmus stage in the Laboratoire de Structure et Dynamique des Systèmes Moléculaires et Solides (LSDSMS) at the Université des Sciences et Techniques du Languedoc (Montpellier, France), I have collaborated with Fabien Gatti in the study of the dynamics involved in the Intramolecular Vibrational-energy Redistribution (IVR) process on the Fluoroform, applying the Multi-Configuration-Time-Dependant-Hartree (MCTDH) method.

More concretely, we have focused on the physical description of the system with different sets of coordinates and how they can improve the convergence of the calculations, in the continuation of the work already done by Prof. Christophe Iung (LSDSMS).

In addition, as it was my first contact with the MCTDH method, I have not only made the effort of understanding its most basic ideas, but also tried to compile and present them in a very pedagogic way, in order to make a helpful introductory guide for anyone interested in the quantum dynamics simulations with MCTDH.

According with these statements, the main points I will present in this seminary are:

1. - To provide to the new quantum dynamical researchers a comprehensive introduction to the MCTDH method.

2. - To apply this mathematical tool to the study of IVR in the Fluoroform's molecule.

3. - To underscore the importance and the consequences of choosing the adequate set of coordinates for describing our system; i.e. describing the Hamiltonian in Polyspherical Coordinates and comparing the results and the consuming times obtained with Rectilinear Coordinates.