SHORT TERM SCIENTIFIC MISSION (STSM) SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CM 1405
STSM title: Determination of the robivrational spectra of astrophysical relevant anions
STSM start and end date: 18/02/2019 to 26/02/2019
Grantee name: Majdi Hochlaf

PURPOSE OF THE STSM:

Last year, we generated an accurate 3D potential energy surface (3D PES) for the HCO^- anion using state-to-the-art ab initio methodologies. Two stable forms are located in this PES: rigid HCO^- and H^- --CO^- van der Waals complex. The aim of this STSM is to deduce accurate rotational and vibrational spectroscopic parameters for these anions. These data are required in order to help for the identification of these species in laboratory and in astrophysical media.
The identification of this negative ion is of primary importance in astrophysics since the formation and the presence of HCO^- there is closely related to the detection of H^- negative ion, which was never identified in interstellar regions. Whereas several scenarios suggest the implication of H^- in the physical and chemical processes occurring there.
To achieve these goals, we need the treatment of the nuclear motions using a quantum time-independent approach as available in France and the Coupled Cluster (CCSD(T)) based energy-gradient composite scheme as available in the group of Prof. C. Puzzarini at the University of Bologna.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

The newly developed 3D potential energy surface (3D PES) of $[H,C,O]^-$ covers the regions of the equilibrium structures of the H^- -- CO weakly bound cluster and of the covalently bound HCO^- anion. Both of them are stable with respect to autodetachment (i.e. $HCO^- \rightarrow HCO + e^-$).
The rotational spectroscopy of both species was performed. The starting point was the geometries, which were derived from the 3D PES. For that purposes, we used the Coupled Cluster (CCSD(T)) based energy-gradient composite scheme. The pattern of the rovibrational energies of rigid and weakly bound forms of HCO^- are also computed. Special cares were taken to avoid the regions of spontaneous electron detachment.
While the computations were strightforward for the HCO^- rigid isomer, several benchmarks were performed in order to converge the computations and to adapt the composite scheme for the weakly bound H^- --CO isomer. In fine, these benchmarks were successful. This shows the applicability of the composite scheme, firsly developed for rigid molecular systems, to weakly bound complexes.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

In order to help for the identification of HCO^- species, we generated the rovibrational spectrum of HCO^- and of $[H—CO]^-$ van der Waals complex. We also derived a set of very accurate rotational constants including the vibrational ground- and excited-state rotational constants, and the anharmonic spectra. For validation, we also derived the corresponding data for the neutral species (i.e. rigid HCO and weakly bound H—CO van der Waals cluster).
We are currently working on gathering these data and filling the appropriate tables. A common publication is in preparation.
Another main result of this STSM is the validation of the use of the Coupled Cluster (CCSD(T)) based energy-gradient composite scheme for weakly bound clusters. This allows its applicability to a large class of molecules and not only to the rigid ones.

FUTURE COLLABORATIONS (if applicable)

My visit to the lab of Pr. Cristina Puzzarini (University of Bologna) is highly beneficial for both parties. It reinforced the collaboration between our groups. It allowed the achievement of the ongoing projects on the accurate theoretical spectroscopy of astrophysical relevant molecular systems. For instance, we are planning to treat molecular systems containing heavy atoms (e.g. iodine) relevant for atmospheric chemistry. New approaches should be developed mutually to consider relativistic corrections on the spectroscopic terms.