Work plan

Last year, we published an accurate global potential energy surface (PES) of HCO^- anion, which is of astrophysical interest. [1] Indeed, the formation and the presence of HCO^- is closely related to the detection of H^- negative ion, which was never identified in interstellar regions. This new PES covers the regions of the covalently bound HCO^- and the weakly bound $[H—CO]^-$ complex. Special cares were taken to treat the regions of spontaneous electron detachment (i.e. $HCO^- \rightarrow HCO + e^-$). In order to help for the identification of HCO^- species, we plan to generate the rovibrational spectrum of HCO^- and of $[H—CO]^-$ van der Waals complex. The nuclear motions will be treated using either a quantum time-independent approach [2,3] or the Coupled Cluster (CCSD(T)) based energy-gradient composite scheme [4]. Note that this composite scheme has been largely validated for rigid molecular systems by Prof. C. Puzzarini at the University of Bologna, in particular for structural and spectroscopic applications [5,6]. Thus, benchmark studies are required in order to test the validity of this approach in deriving accurate structural and spectroscopic parameters of van der Waals molecular systems. The results will be published jointly.

1. T. Stoecklin, P. Halvick, M. Lara-Moreno, T. Trabelsi and M. Hochlaf. On the gas-phase formation of the HCO^- anion: accurate quantum study of the H^- + CO radiative association and HCO radiative electron attachment. Faraday Discuss. 212, 101-116 (2018).
2. T. Stoecklin, F. Lique and M. Hochlaf. A new theoretical method for calculating the radiative association cross section of a triatomic molecule: application to N_2–H^-. Phys. Chem. Chem. Phys., 2013, 15, 13818–13825 (2013).
3. T. Stoecklin, P. Halvick, H.-G. Yu, G. Nyman and Y. Ellinger. On the gas-phase formation of the HCO radical: Accurate quantum study of the H + CO radiative association. Mon. Not. R. Astron. Soc. 475, 2545–2552 (2018).
4. M. Heckert, M. Kállay, D.P. Tew, W. Klopper and J. Gauss. Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory. J. Chem. Phys., 125 (2006) 044108.
5. C. Puzzarini. Astronomical Complex Organic Molecules: Quantum Chemistry meets Rotational Spectroscopy. Int. J. Quantum Chem. 117 (2017) 129
6. C. Puzzarini. Accurate molecular structures of small- and medium-sized molecules. Int. J. Quantum Chem., 116 (2016) 1513.