Spectroscopy and collisional dynamics of medium sized molecules

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I will present several examples of the use of high-level theoretical characterization of low-energy isomers of molecular species (MS) relevant in interstellar media (ISM) and the subsequent collision treatment to deduce their abundances in these media. First, we explore their ground state potential energy surface using coupled cluster (CC) theory. Next, precise equilibrium structures and relative energies are determined using composite schemes based on CC theory and taking into account extrapolation to the complete basis set limit and core correlation effects. For all stable forms, rotational spectroscopy parameters as well as fundamental vibrational frequencies and infrared intensities are also determined. Furthermore, to support astrophysical modeling and improve abundance estimates of these MSs in the ISM, we conduct extensive theoretical investigations on the collisional excitation and de-excitation of these molecules by the most abundant species in the ISM (i.e., X = H_2, H, and He). Our strategy is as follows: first, we generate an accurate multidimensional potential energy surface for the weakly bound MS–X complex at the CCSD(T)-F12/aug-cc-pVTZ level, where we also take into account basis set superposition error corrections. Next, an analytical form of this potential is derived, which is then incorporated into close-coupling quantum scattering calculations for MS colliding with X, yielding state-to-state cross sections and temperature-dependent rate coefficients under conditions relevant to the ISM (5–100 K).

Our work should contribute to the identification of MS in laboratory and astrophysical environments. In particular, it should enable a more accurate interpretation of current and future astronomical observations dealing with MS relevant to astrophysics

Several examples will be presented, including the spectroscopic characterization of protonated HNCO species (in collaboration with Prof. C. Puzzarini group, U. Bologna, Italy),[a] the rotational (de-)excitation of cis-/trans-HONO colliding with He (in collaboration with Prof. D. Ben Abdallah group, U. Tunis, Tunisia) [b] and the rotational (de-)excitation of cis-HNSO colliding with He (in collaboration with Dr. B. Mehnen and Prof. P. Zuchowski group, U. Torun, Poland) [c].

References:

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