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Editorial: Structure and dynamics of atmospheric, plasma, and astrochemical molecular processes

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Editorial on the Research Topic

[Structure and dynamics of atmospheric, plasma and astrochemical molecular processes](#)

This Research Topic provides new data on chemical systems ranging from the smallest triatomic molecule (and the most common molecular ion in the universe) to complex polycyclic aromatic hydrocarbons (PAHs), passing through atmospheric collisions and positron–molecule interactions. The methods employed are also impressive: extraordinarily high convergence accuracy is achieved for the rovibrational levels of the H_3^+ ion, a new approach to study positron–molecule interactions is presented, global optimization methods (Tabu Search) are employed, and highly accurate calculations for the H_2O_2 system are carried out. The data provided here by computational methods are important for a better understanding and modeling of atmospheric, plasma, and astrochemical environments.

In spite of its paramount importance for astrochemistry and its simplicity, the complete spectrum of H_3^+ is still unassigned. The work of [Sarka et al.](#) calculates rovibrational levels for this molecule, pushing the convergence accuracy to an unprecedented level of a few 10^{-5} cm^{-1} . This allowed them to unambiguously label the energy levels using a fully *ab initio* scheme. Given the ever increasing number of detected molecules in the interstellar medium (ISM), the spectral lines from different molecules can overlap, and the data provided here on the transition of the abundant trihydrogen cations will help the astrochemical community in better identifying the observed spectra.

Increasing the complexity of the system, we have the HO_2 molecule, which is a key player in the whole range of interest to our Research Topic: atmospheric, plasma, and astrochemical environments (not to mention combustion). In all such environments, H atoms are important in the reactivity and chemical evolution of the medium. For this reason, a fundamental understanding of the $H + HO_2$ reaction is crucial. In the work

presented by Jasper *et al.*, in addition to calculating highly accurate *ab initio* energies, modeling a potential energy surface, and computing rate coefficients for this reaction, the authors show that it behaves in a very unexpected way. In spite of being a very powerful tool for guiding the way we think of chemical kinetics, the transition state theory is based on the local equilibrium assumption. As found in the above-mentioned work, after the deep H₂O₂ minimum is achieved on H + HO₂ collisions, one would expect efficient intramolecular vibrational energy redistribution, which is shown to not be the case here. Among the unexpected consequences, the rate constant shows a negative dependence on the internal energy of the reactants.

When polycyclic aromatic hydrocarbons (PAHs) are abundant in the ISM and relevant to elucidate the chemical evolution of the universe, their experimental identification is a daunting task due to their metastability. Furthermore, although PAHs can be associated with unassigned infrared emission bands from astronomical observations, it is still debatable if these bands originate from any specific molecule or a structurally similar species. In this context, Roy *et al.* have studied the structurally similar bicyclic C₁₁H₈ isomers *via* a computational study of their thermodynamic and spectroscopic properties. A global optimization method (Tabu Search) is employed to find more than 400 structures, and the key IR spectroscopic signatures of low-energy isomers are computed to compare with the astronomical emission features. The data provided here proposed that the C₁₁H₈ isomers are crucial reactive intermediates for the formation of PAHs, and thus, experimental investigations are needed.

From the antimatter side, the positron–matter interaction is a widespread phenomenon in astrophysics and plasma. When the annihilation of high-energy positrons is studied and observed in various astronomical observations, fewer low-energy positron–molecule interactions are explored in the literature. This is primarily due to the difficulties in producing sufficient low-energy positrons. However, a comprehensive knowledge on the low-energy positron molecule collisions and thermalization processes is central to developing experimental techniques to produce high-density positron plasma and control the positron beams in electromagnetic traps. In the present work, Poveda *et al.* studied the low-energy positron–H₂ and –N₂ interaction by developing a three-dimensional model potential and

using it on time-dependent wave packet propagation. They have shown that the positron responds instantly to a correlation-polarization potential, whose attractiveness oscillates following the vibrational mode of the target. The knowledge provided here can be useful to understand the resonant positron annihilation to polycyclic aromatic hydrocarbons present in the ISM.

We hope the present research topic will be a useful source of new molecular data (such as rovibrational levels, infra-red peaks, reaction rate coefficients, and vibrational-excitation cross sections) and contribute to the development of new methods and ways of dealing with molecular processes.

Author contributions

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