MODELLING ENERGY-TRANSFER KINETICS OF SMALL MOLECULAR IONS IN COLD TRAP ENVIRONMENTS WITH DIFFERENT BUFFER GASES:
INTERACTION POTENTIALS, QUANTUM DYNAMICSAND KINETICS FROM AB-INITO METHODS

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In the field of molecular ion spectroscopy, cold He buffer gas cooling in conjunction with ion trapping has been used successfully by several groups for many years , following initial studies with cold argon gas . The rotational and vibrational cooling of molecules leads to a significantly reduced complexity of laser-induced rovibrational and electronic spectra, especially for polyatomic ions, enabling a deeper understanding of their structure and dynamical processes. The method was also applied to anions, OH- being a recent example in our group. A sophisticated variant of buffer gas cooling of molecular ions has been recently demonstrated, where the molecular ions are simultaneously translationally cooled by laser-cooled atomic ions (sympathetic cooling). MgH+ ions, sympathetically cooled by laser-cooled Ca+ ions, were additionally rotationally cooled by He gas at 4 K, in a cryogenic trap. A rotational temperature of 7.5 K was reached in approximately 1 s of buffer gas interaction time.
The study of simple molecular ions, either cations or anions, under the special condition of them being trapped in a cryogenically cooled linear, radio-frequency quadrupole trap, and sometime already translationally cooled through Coulomb interaction with atomic ,heavier ions, can cause the molecular ions to be cooled into their ground rotational state even though a low density of He atoms, ~10^{10} cm−3, is present in the trap. Therefore to be able to then follow ensuing chemical processes in that trap after the initial cooling of the trapped ions requires to have efficiently achieved that initial cooling step with a variety of possible buffer gases.
From the computational standpoint, to complete that initial preparation of the trapped molecular ions requires knowledge of the interaction forces between the trapped ions and the selected buffer gas atoms, the quantum dynamical treatment of the energy-transfer processes to yield the relevant inelastic cross sections at the expected energy range in the traps, and finally the generation of the state-to-state inelastic rate coefficients over the temperatures of interest. The above set of computational data can then be employed to model the relaxation kinetics in the traps and the relative efficiencies of the selected buffer gases as collision partners.
We have undergone an extensive study involving a variety of simple molecular ions of astrophysical interest which have been considered to operate in cold ion traps with different types of buffer gases like He, Ne, Ar and H_2.
Detailed results on a variety of System/NG combinations which we have been considering in recent years will be presented at the Meeting.

1) M. Hernández Vera, F. A. Gianturco, R. Wester, H. da Silva, Jr., O. Dulieu, and S. Schiller, Rotationally inelastic collisions of H2+ ions with He buffer gas.J. Chem. Phys. 146, 124310 (2017).
2) S. Schiller, I. Kortunov, M. Hernández Vera, F. Gianturco, and H. da Silva, Quantum state preparation of homonuclear molecular ions enabled via a cold buffer gas: An *ab initio* study for the H_2^+ and the D_2^+ case, Phys. Rev. A **95**, 043411 (2017).
3) I. Iskandarov, F. A. Gianturco, M. Hernández Vera, R. Wester, H. da Silva, Jr., and O. Dulieu, "Shape and strength of dynamical couplings between vibrational levels of the H^+_2 , HD^+ and D^+_2 molecular ions in collision with He as a buffer gas," Eur. Phys. J. D **71**, 141 (2017)
4) B. P. Mant, F. A. Gianturco, R. Wester, E. Yurtsever, and L. González-Sánchez, "Ro-vibrational quenching of C^-_2 anions in collisions with He, Ne and Ar atoms," Phys. Rev. A **102**, 062810 (2020).
5) L. González-Sánchez, B. P. Mant, R. Wester, and F. A. Gianturco, "Rotationally inelastic collisions of CN^- with He: Computing cross sections and rates in the interstellar medium," Astrophys. J. **897**, 75 (2020).
6) [5]L. González-Sánchez, E. Yurtsever, B. P. Mant, R. Wester, and F. A. Gianturco, "Collision-driven state-changing efficiency of different buffer gases in cold traps: He(^1S), Ar (^1S) and p-H_2 ($^1\Sigma$) on trapped CN^- ($^1\Sigma$)," Phys. Chem. Chem. Phys. (published online) (2020).
7) B. P. Mant, F. A. Gianturco, L. González-Sánchez, E. Yurtsever, and R. Wester, "Rotationally inelastic processes of C^-_2 ($^2\Sigma^+_g$) colliding with He (^{1}S) at low-temperatures: *Ab initio* interaction potential, state-changing rates and kinetic modelling," J. Phys. B: At., Mol. Opt. Phys. **53**, 025201 (2020).
8) B. P. Mant, F. A. Gianturco, R. Wester, L. González-Sánchez, and E. Yurtsever, "Thermalization of C^-_2 with noble gases in cold ion traps," J. Int. Mass Spectrom. **457**, 116426 (2020).