THE BIG CHILL: INELASTIC AND REACTIVE COLLISIONS AT ULTRALOW TEMPERATURES

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Molecules are a much more difficult working environment for BEC experiments but it has been clear from the very beginning that they have more to offer that simply providing an extension of the sort of experiments already performed with atoms. Thus, they have been attracting the interest of both the chemical and physical communities in trying to better understand the large variety of additional effects seen on the way to bringing molecules and atom/molecule mixtures down to very low temperatures and very low velocities. Several fundamental studies [1,2] in which molecules are employed take advantage of the relative ultra-low velocities between molecules achieved in recent experiments. One of the most used approaches [3,4] starts with cold atoms stored in a magneto-optical trap (MOT) and, through the process of photo-association (PA) binds two atoms together. The ensuing molecules are translationally as cold as the atoms from which they are produced but, since the latter get together at rather large internuclear distances, the most favored states of the molecules formed are often high vibrational states just below their dissociation limit. Using a variety of laser schemes, the internal energy distributions of the newly formed molecules can be manipulated in order to transfer them into their rovibrational and electronic ground states. In the second method, a beam of dipolar molecules is decelerated during the passage through an array of time-varying inhomogeneous electric fields [5,6] and then trapped in an electrostatic storage ring or in an electrostatic quadrupole trap [7].

Another possibility for cooling molecules is offered by injecting them in a cold He buffer [8–10] where they can then thermalize after a series of multiple collisions. When ^{3}He is used as a buffer gas, the temperature can be as low as 250 mK and one can still maintain a sufficient buffer gas density to ensure efficient cooling by frequent collisions. One normally expects that the target molecules would be in their electronic and vibrational ground states after the end of the equilibration process, with only a limited number of rotational states populated. It is therefore of importance to have some knowledge of the relative sizes and of the temperature behavior for the corresponding collisionally inelastic cross sections related to a particular molecule injected in the buffer gas to initiate the cooling step of the process. This essentially means that to gather theoretical, and possibly some further information, on the inelastic collisions occurring at ultra-low temperatures demands to have previously acquired reliable information on the anisotropic interactions [11] which drive the collisional cooling and to have set up a computational tool to treat the quantum dynamics that is both numerically and CPU efficient for treating the often numerous molecular states that can be involved in the process at hand [12].

In the present study we have selected three polar diatomics for which we have been able to obtain from previous works a fairly reliable information on their full anisotropic interactions with the He atom. We shall therefore show that numerically converged results for their collisional de-excitation cross sections at very low translational energies allow one to obtain a fairly detailed picture of the cooling efficiency for these three species in the chosen buffer gas and also makes it possible to suggest the environmental parameters that would help to optimize the working conditions in experiments [12,13].

REFERENCES

[1] Arndt, M.; Nair, O.; Vos-Andreae, J.; Keller, C.; van der Zouw, G.; Zeilinger, A. *Nature* **1999**, *401*, 680.

[2] DeMille, D.; Bay, F.; Bickman, S.; Kawall, D.; Jr., D. K.; Maxwell, S. E.; Hunter, L. R. *Phys. Rev. A* **2000**, *61*, 052507.

[3] Gabbanini, C.; Fioretti, A.; Lucchesini, A.; Gozzini, S.; Mazzoni, M. *Phys. Rev. Lett.* **2000**, *84*, 2814.

[4] Nikolov, A. N.; Enscher, J. R.; Eyler, E. E.; Wang, H.; Stwalley, W. C.; Gould, P. L. *Phys. Rev. Lett.* **2000**, *84*, 246.

[5] Bethlem, L. H.; Berden, G.; Meijer, G. *Phys. Rev. Lett.* **1999**, *83*(8), 1558.

[6] Maddi, J. A.; Dinneen, T. P.; Gould, H. *Phys. Rev. A* **1999**, *60*(5), 3882.

[7] Bethlem, L. H.; Berden, G.; Crompvoets, F. M. H.; Jongma, R. T.; van Roij, A. J. A.; Meijer, G. *Nature* **2000**, *406*, 491.

[8] Doyle, J. M.; Friedrich, B.; Kim, J.; Patterson, D. *Phys. Rev. A* **1995**, *52*(4), 2515.

[9] Weinstein, J.; deCarvalho, R.; Guillet, T.; Friedrich, B.; Doyle, J. M. *Nature* **1998**, *395*, 148.

[10] Friedrich, B.; Weinstein, J. D.; deCarvalho, R.; Doyle, J. *J. Chem. Phys.* **1999**, *110*, 2376.

[11] Bodo, E.; Gianturco, F. A.; Martinazzo, R.; Paesani, F.; Raimondi, M. *J. Chem. Phys.* **2000**, *113*(24), 11071.

[12] Bodo E. and Gianturco, F. A.*J. Phys. Chem.* **2003**, *A107*, 7328.

[13] Bodo, E.; Gianturco, F. A. and Dalgarno, A. *J. Phys. B* **2002**, *35*, 4075.