Laboratory Astrophysics: from Observations to Interpretation
Proceedings IAU Symposium No. 350, 2019
F. Salama & H. Linnartz, eds.
doi:10.1017/S1743921319007580

Investigation of rotational state-changing collisions of C_2N^- ions with helium

Jan Franz[1] **and Francesco Antonio Gianturco**[2]

[1]Department of Theoretical Physics and Quantum Informatics, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, ul. Narutowicza 11/12 80-233 Gdańsk, Poland
email: janfranz@pg.edu.pl

[2]Institute for Ion Physics and Applied Physics, University of Innsbruck, Technikerstr. 25/3, 6020 Innsbruck, Austria
email: Francesco.Gianturco@uibk.ac.at

Abstract. The cross sections for rotational inelastic collisions between atoms and a molecular anion can be very large, if the anion has a dipole moment. This makes molecular anions very efficient in cooling atomic gases. We address rotational inelastic collisions of Helium atoms with the molecular anion C_2N^-. Here we present preliminary calculations of the potential energy surface.

Keywords. astrochemistry, molecular processes, scattering

1. Introduction

Molecular anions can be very efficient in cooling an atomic gas. In this project we address the rotational inelastic collisions of C_2N^- with Helium atoms at very low temperature

$$C_2N^-(J) + He \rightarrow C_2N^-(J') + He\,.$$

Here J and J′ are the initial and final angular momenta, respectively. The kinetic energy of the Helium atom is converted into rotational energy of the C_2N^- molecule. In an environment with very low density, the rotational energy of the molecule can be emitted by radiation. As a consequence the atomic gas is cooled. Such a process can be important in star forming regions.

It is well known from experiments and theory that C_2N^- is a stable molecule (Garand *et al.* 2009). It has not yet been found in the interstellar medium. However Millar *et al.* (2017) are listing in their recent review all those molecular anions, which have been identified in the interstellar medium. Among them are nitrogen-containing carbon chains with an odd number of carbon atoms, like CN^-, C_3N^-, and C_5N^-.

In this paper we are presenting preliminary computations of the potential energy surface (PES).

2. Computational details and preliminary results

The electronic ground state of C_2N^- is $X^3\Sigma^-$. The molecular geometry of C_2N^- (linear with $r_{CC} = 1.344$ Å and $r_{CN} = 1.207$Å) has been taken from Garand *et al.* (2009).

The calculations of the PES are done with the program package MOLPRO 2012 (Werner *et al.* 2012). For all calculations the internally-contracted multi-reference configuration interaction method (IC-MRCI) (Werner & Knowles 1988, Knowles & Werner 1988, Shamasundar *et al.* 2011) with the aug-cc-pVQZ basis set (Woon & Dunning 1994)

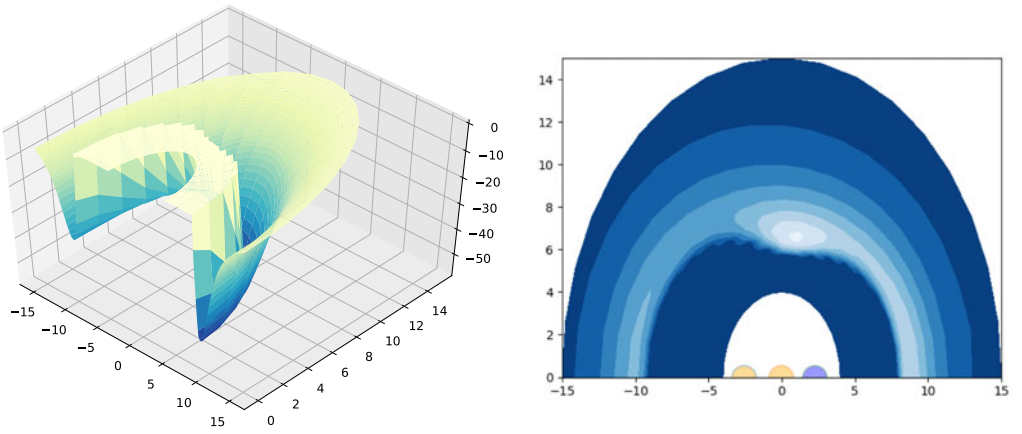

Figure 1. Three dimensional plot (left figure) and contour plot (right figure) of the PES of the system C_2N^- and Helium. The coordinates of Helium are given in Bohr. The energies are given in cm^{-1}.

on all atoms is used. The reference space for the MRCI calculations consists of a complete-active space by distributing 14 electrons in 15 orbitals. All single and double excitations from the reference configurations are included in the variational calculation. The effect of quadruple excitations is estimated by using the Davidson correction.

A scan of the PES of the system is shown in Figure 1. The geometry of C_2N^- is kept fixed. The C_2N^- molecule is placed on the symmetry axis. The center of gravity of the C_2N^- molecule is used as the center of coordinate system.

The global minimum is at a distance of around 6.7 Bohr from the center at an angle of around 80 degrees and has a depth of around 58 cm^{-1}. The PES shows two other local minima at zero and 180 degrees. These minima are seperated by a barrier of a few wavenumbers from the global minimum. The tow local minima could be an artefact, caused by the basis set superposition error, and may vanish after taking into account counterpoise corrections. Such calculations currently in work and the PES will be prepared for the computation of rotational inelastic cross sections.

Acknowledgment

JF thanks the organizers of the symposium, the International Astronomical Union and Europlanet for a travel grant, which made the visit of this symposium possible. JF thanks the European COST action *Our Astro-Chemical History* for financing a short-term scientific mission (STSM) at the University of Innsbruck. The authors acknowledge computational resources made available by the computer center WCSS in Wroclaw through grant number KDM-408.

References

Garand, E., Yacovitch, T. I., & Neumark, D. M. 2009, *J. Chem. Phys.*, 130, 064304
Hauser, D., Lee, S., Carelli, F. *et al.* 2015, *Nature Phys.*, 11, 467
Knowles, P. J., & Werner, H.-J. 1988, *Chem. Phys. Lett.*, 145, 514
Millar, T. J. , Walsh, C., & Field, T. A. 2017, *Chem. Rev.*, 117, 1765
Shamasundar, K. R., Knizia, G., & Werner, H.-J. 2011, *J. Chem. Phys.*, 135, 054101
Werner, H.-J. & Knowles, P. J. 1988, *J. Chem. Phys.*, 89, 5803
Werner, H.-J., Knowles, P. J., Knizia, G., Manby, F. R., Schütz, M., & others, MOLPRO, version 2012.1, a package of ab initio programs, For the current version, see http://www.molpro.net
Woon, D. E., & Dunning, T. H. Jr. 1994, *J. Chem. Phys.*, 100, 2975

https://doi.org/10.1017/S1743921319007580 Published online by Cambridge University Press