

Collisions of low-energy helium cations with furan molecules

Tomasz J. Wasowicz^{1*}, Marta Łabuda², Bogusław Pranszke³

¹Department of Physics of Electronic Phenomena, Gdańsk University of Technology, ul. Narutowicza 11/12, 80-233 Gdańsk, Poland

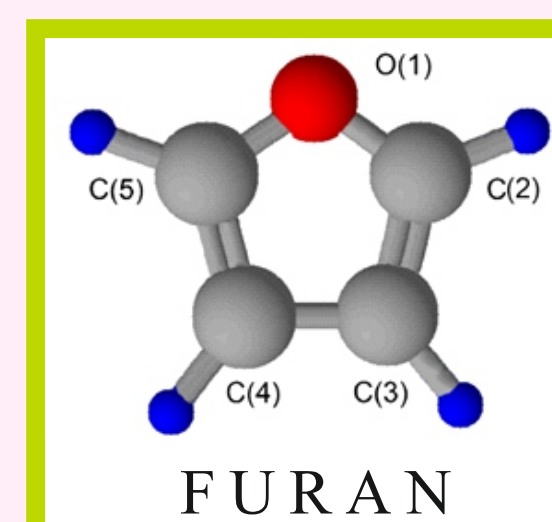
²Department of Theoretical Physics & Quantum Information, Gdańsk University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk, Poland

³Institute of Experimental Physics, University of Gdańsk, ul. Wita Stwosza 57, 80-952 Gdańsk, Poland

*Corresponding author: twasowicz@mif.pg.gda.pl or tomwasowl@pg.edu.pl

Abstract

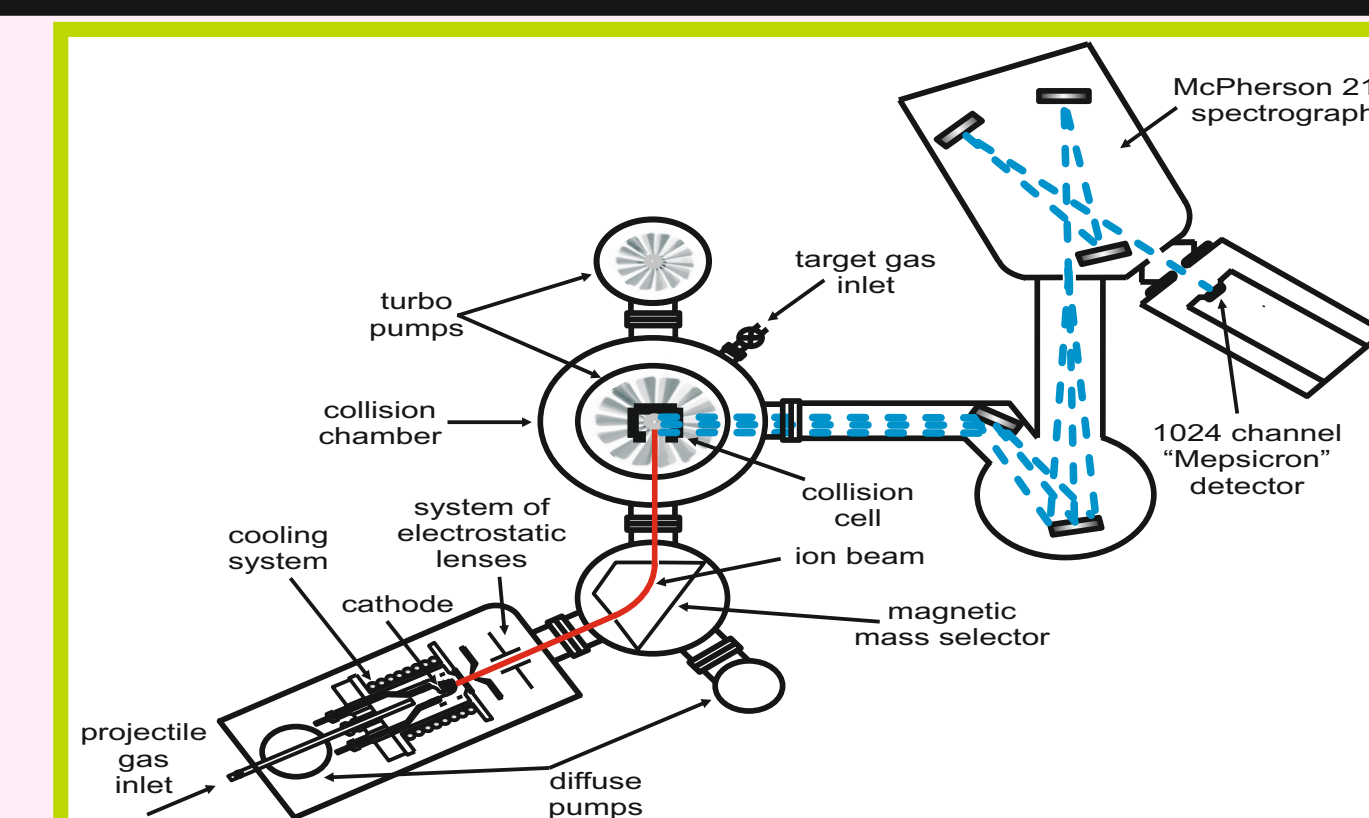
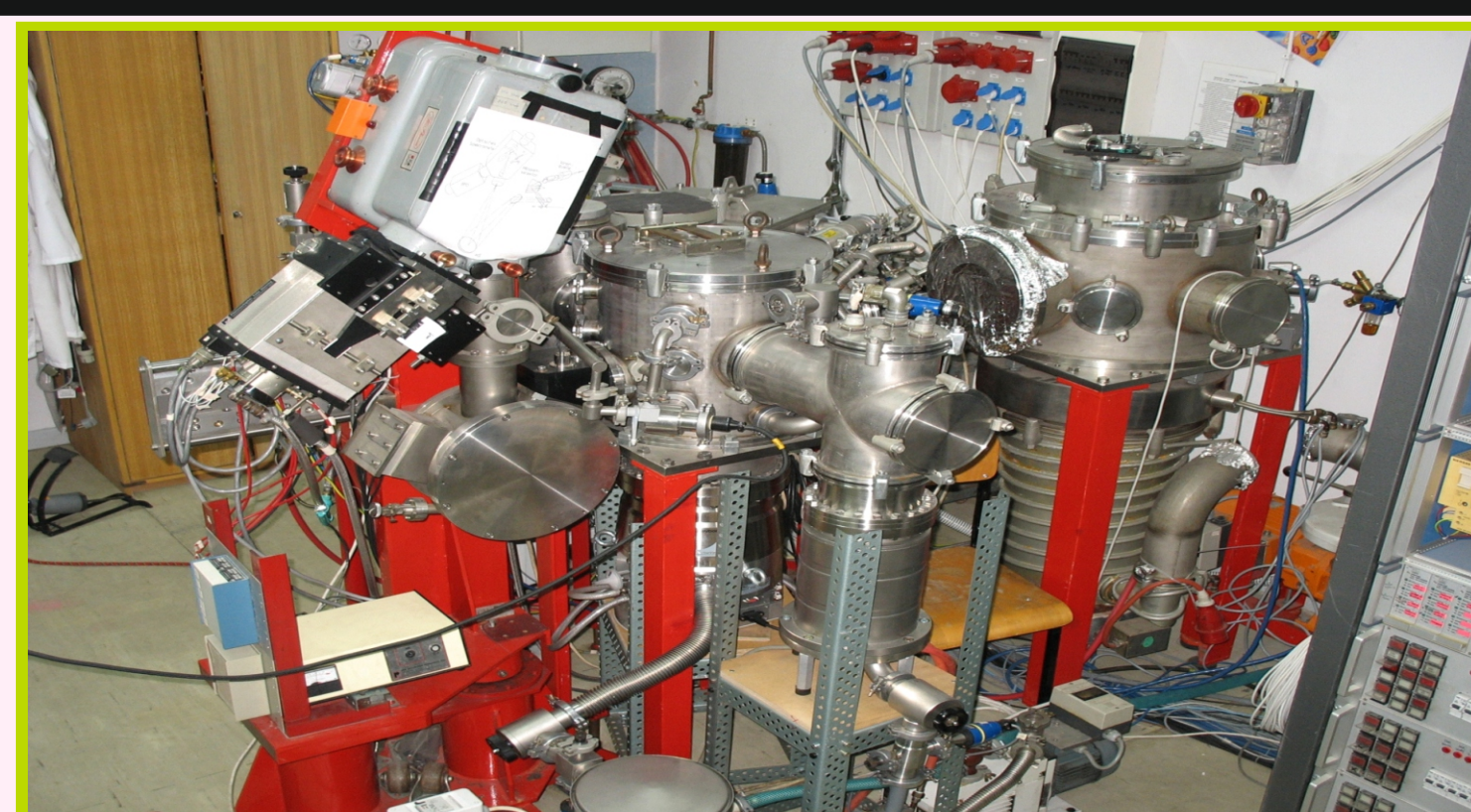
In this communication we present studies of charge transfer and complex formation processes observed in fragmentation of furan molecules in collisions with He⁺ cations applying collision-induced luminescence spectroscopy [1]. For comparison, we also report results of studies of fragmentation processes of furan molecules in collisions with the He²⁺ ions. Furan (C₄H₄O) has a special significance for biology and chemistry, since its ring forms the basis of the simple sugars, ribose and deoxyribose, in backbone of the RNA and the DNA helix. This is important because the interaction of the primary ion beam and the secondary particles, low energy electrons, radicals and ions which are formed along the beam track in the biological cell [2], in medical hadrontherapy, may produce structural and chemical modifications by bond cleavages in the DNA helix [3].



Experimental technique

The measurements were carried out using collision-induced luminescence spectroscopy [1]. This technique allows to investigate the molecular dissociation through detection of the luminescence decay of the excited neutral fragments.

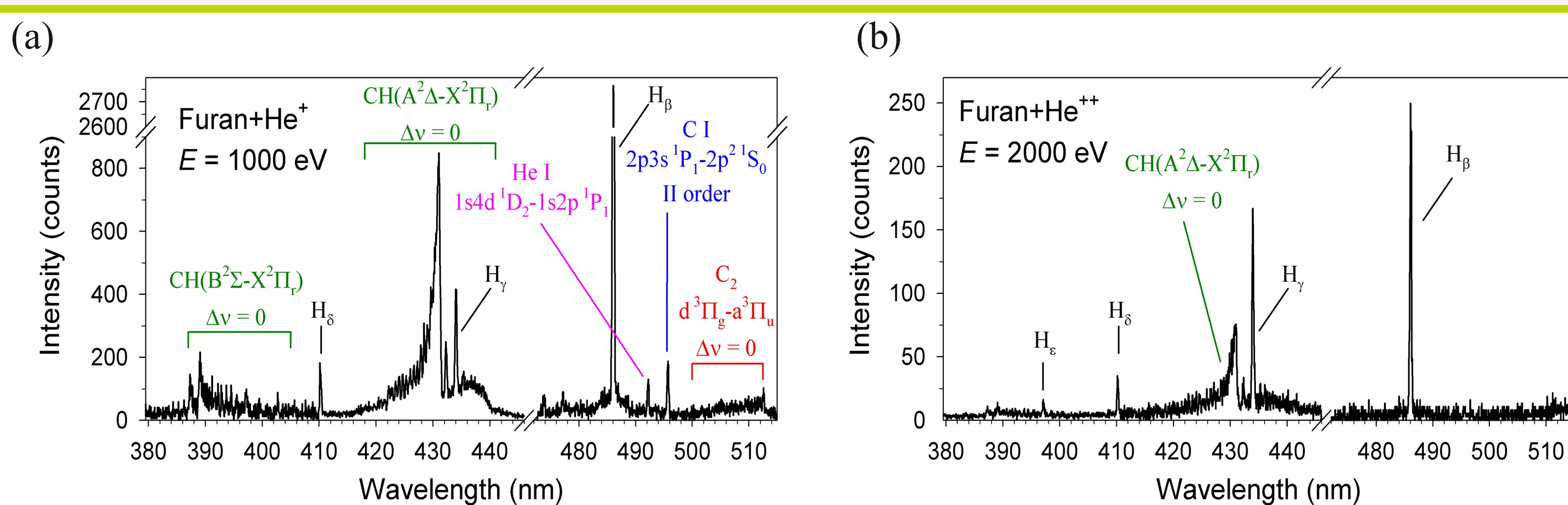
The apparatus consisted of a Colutron-type ion source, magnetic mass selector, reaction cell, and an optical spectrometer equipped with a multichannel photon-counting system to detect luminescence from the excited fragments. The collision energies of the incident cations were varied between 5 and 2000 eV and thus covered a velocity range from 15 to 310 km/s.



Theoretical method

The molecular calculations have been performed by using a high level of ab initio quantum chemistry methods. The molecular calculations were carried out employing the MOLPRO package of ab initio programs. The geometry of the ground state of the furan molecule has been optimized by means of density-functional-theory (DFT) calculations using the Becke-Lee-Yang-Parr density functional (B3LYP). Particular attention was paid to investigate the charge transfer process and possible formation of the quasi-molecular clusters between the colliding ions and target molecule. Molecular description of the charge transfer process is based on the collision model at relatively low velocities in which the nuclear motion is slow compared to the bound electron being captured. Under such conditions, the electron has sufficient time to adjust to the changing interatomic field as the nuclei approach and separate, and quasi-molecular description of the collision becomes necessary for a detailed treatment of the problem. Thus, the capture of electron process is represented as a transition between the stationary states of the quasi-molecule, and the dynamics (cross-sections) of the process depends strongly on the detailed analysis of the potential energy curves representing the particular quasi-complex and on the couplings between them. In this model, detailed calculations for specific collision partners are performed utilizing the one-dimensional reaction coordinate approximation in which a projectile ion is approaching the corresponding target molecule by single straight-line trajectory. Under such assumption, the interaction of the heterocyclic furan molecule with helium ions can be represented as the evolution of the polyatomic He-C₄H₄O^{q+} (q=1, 2) quasi-molecular complex with the reaction coordinate corresponding to the distance R between the centre of mass of the C₄H₄O molecule and the colliding ion. The rearrangement of the C₄H₄O molecule when approaching the He⁺²⁺ ion can be taken into account by relaxation of the geometry of the He-C₄H₄O^{q+} complex along the chosen reaction path.

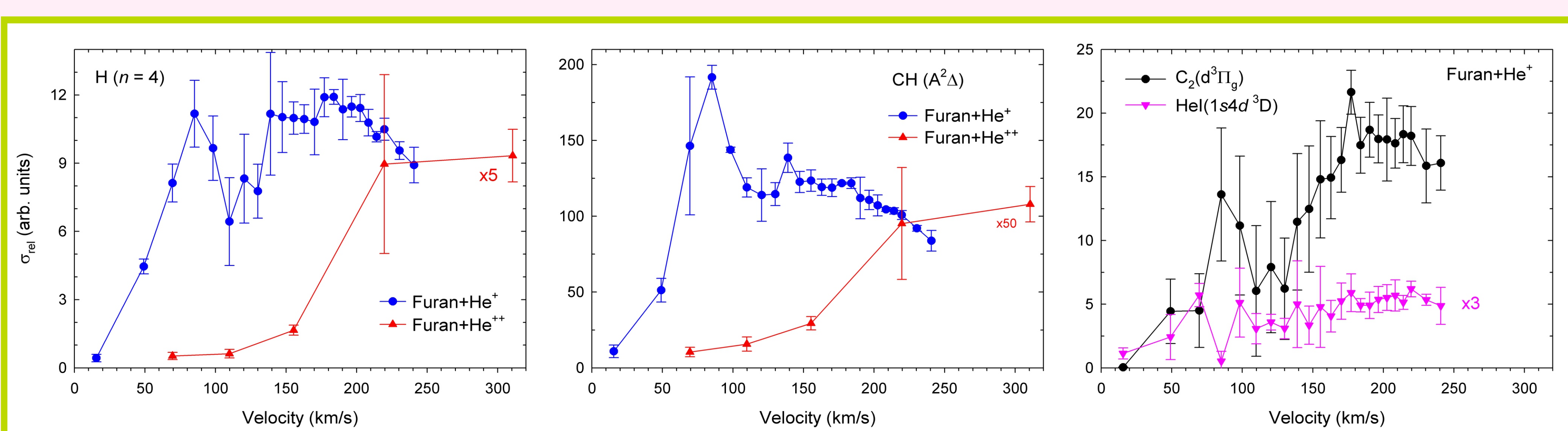
Luminescence spectra



(a) The emission spectrum obtained for collisions with the He⁺ ions reveals formation of hydrogen H(*n*), *n*=4–9, and carbon C(2*p*3*s* ¹P₁) atoms, and rotationally and vibrationally excited diatomic CH(A²Δ, B²Σ) and C₂(d³Π_g) fragments from furan. It also shows production of helium atoms excited to the 1*s*4*d* ¹D₂, ³D states. Since He atom is not incorporated into chemical structure of the furan molecule, the observation of its emission lines clearly indicates transfer of an electron from the furan molecule to the He⁺ cation.

(b) The emission spectrum obtained for collisions with the He²⁺ ions is presented for comparison.

Fragmentation yield spectra

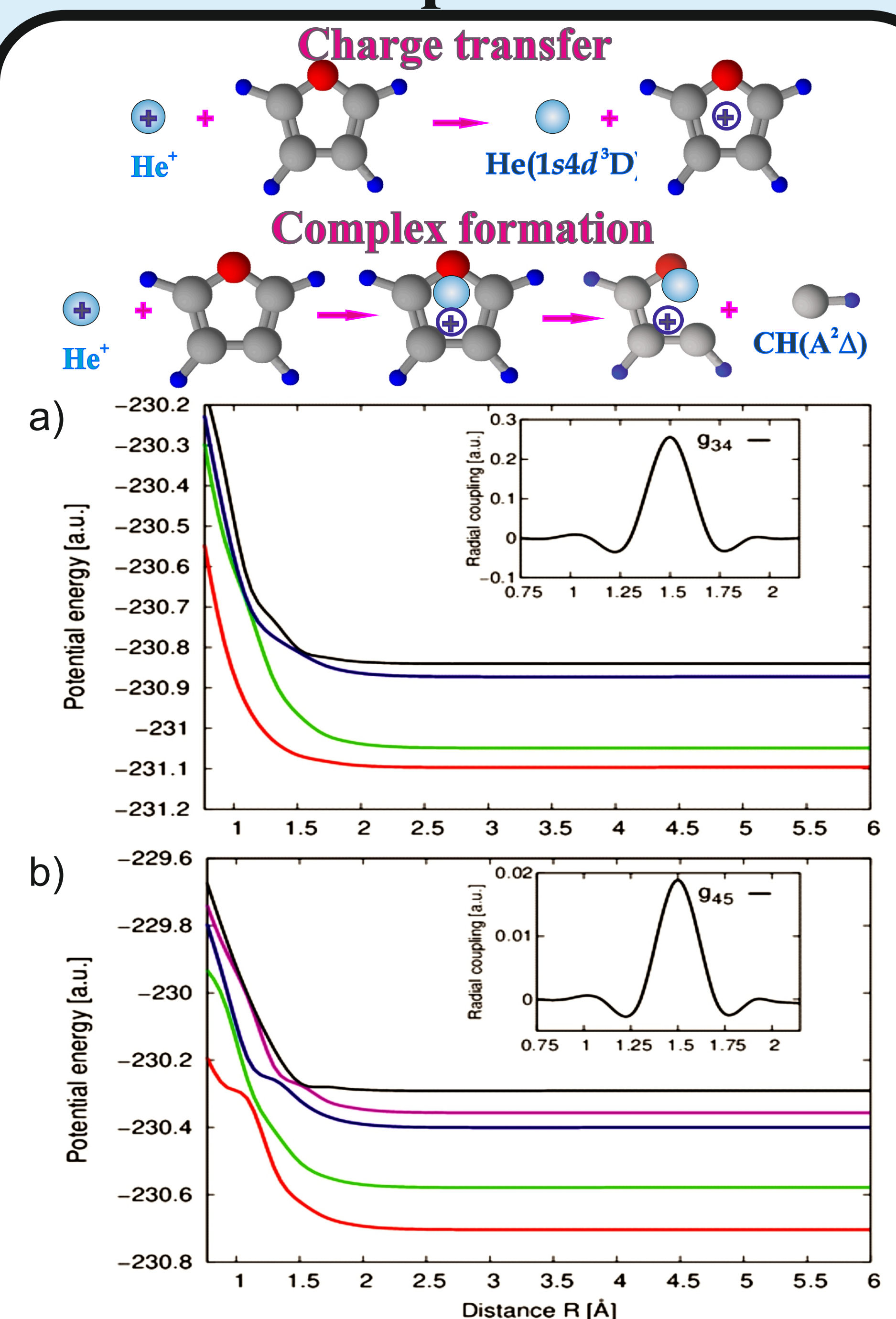


Figures display the velocity dependences of the fragmentation yields (σ_{rel}) for the excited H(*n*=4), CH(A²Δ), C₂(d³Π_g) and He(1*s*4*d* ³D) fragments obtained in collisions of furan with the He⁺ and for comparison with the He²⁺ cations. The observed rapid increase of the CH(A²Δ) fragmentation yield occurring at lower velocities may be regarded as an indication of the [He-C₄H₄O]⁺ complex being formed prior to dissociation of furan molecules [1].

Acknowledgements

This work was conducted within the framework of the COST Action CM1204 (XLIC).

Collisional processes



a) Adiabatic potential energy curves of the ²A₁ states in the collision of He⁺ with furan (C_{2v}) in-the-plane orientation along the *y* axis. The inset shows the most important coupling. b) Adiabatic potential energy curves of the ¹A states in the collision of He²⁺ with furan in-the-plane orientation along the *x* axis.

The calculated PECs in each case show an occurrence of avoided crossings around the nuclear distance of 1.5–2 Å. Such a region corresponds to the strong interaction between electronic states and exhibits the interplay between approaching electronic clouds of both species.

References

- [1] T. J. Wasowicz et al 2015 J. Phys. Chem. A **119** 581.
- [2] M.C. Fuss et al., Chem. Phys. Lett. (2010), **486**, 110.
- [3] U. Amaldi, G. Kraft, Rep. Prog. Phys. (2005), **68**, 1861.