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# Electron Induced Processing at the Molecular Level (EIPAM) Report on work within ESF Exchange Grant Nr. 1288

**Host:** Prof. M. Allan, Department of Chemistry, University of Fribourg, Switzerland **Date:** 15<sup>th</sup> of January to 15<sup>th</sup> of February 2007

# Characterization of the $N_2^{-}(^{2}\Sigma_{g}^{+})$ and the Kr<sup>-</sup>(4p<sup>5</sup> 5s<sup>2</sup>) Feshbach resonances

# Introduction

The narrow  $N_2^{-}(^2\Sigma_g^{+})$  Feshbach resonance [1] (estimated width 0.6 meV [2]) is formed in electron scattering from the ground state  $N_2(X, v = 0)$  at an electron energy close to 11.5 eV, about 0.37 eV below the excited  $N_2^{*}(E^{-3}\Sigma_g^{+}, v = 0)$  state which can be regarded as the neutral parent state. As part of my PhD work at Kaiserslautern, this resonance has been measured in angle-differential elastic scattering and in the angle-integrated yield for formation of metastable  $N_2^{*}$  molecules with a resolution  $\Delta E$  of about 5 meV (FWHM). The instrument involves a high resolution laser photoelectron source at typical currents of 70 pA and a highly-collimated differentially-pumped supersonic molecular beam target [3]. While the Campargue-type supersonic beam virtually eliminates Doppler broadening, care has to be taken with regard to contributions from clusters, as observed for Ar [4]. For studies of the Kr<sup>-</sup>(4p<sup>5</sup> 5s<sup>2</sup> <sup>2</sup>P\_{3/2}) resonance [5] a heated nozzle was used, and an effective resolution of 8 meV was achieved.

Prof. M. Allan at the University of Fribourg has carefully optimized an electron scattering apparatus involving a double hemispherical monochromator and analyzer [6]. With this instrument, resolutions down to 7 meV were demonstrated [7]. A special magnetic angle changer is used to extend the range of measurable scattering angles up to 180° [8]. Absolute differential cross sections are determined using the relative flow method [9]. Elaborate procedures for the determination of the response function and for optimizing the signal to background ratio of the instrument were developed [10].

The primary goal of this work was to obtain an independent set of elastic scattering cross sections in the range of the prominent Feshbach resonances for  $N_2$  and Kr which are guaranteed to be free of cluster contributions by using an effusive target gas beam. Measurements of the differential cross section for angles up to  $180^{\circ}$  promise to provide a sensitive test of the phase shifts for elastic scattering, whose accurate knowledge is important for the determination of the resonance width.

## **Measurements on Nitrogen**

The  $N_2^{-}(^{2}\Sigma_g^{+})$  Feshbach resonance was observed in elastic scattering at the angles 10°, 22.5°, 45°, 90°, 112.5°, 135° and 180° with an energy width of about 13 meV, representing a substantial improvement over previous measurements ( $\Delta E = 35 \text{ meV}$ ) [11]. A combined analysis of the Fribourg and Kaiserslautern elastic scattering data yields a width of 1.0(2) meV for this resonance.



In vibrational excitation spectra of the electronic ground state which have been recorded up to v = 2 at the same angles as in the elastic channel, the resonance is even more prominent. An angular variation in the intensity and shape of the resonance peaks in excitation to the v = 1 state similar to that seen in [12] is clearly observed. The inelastic data will be analyzed using new *ab initio* potential energy curves for the neutral N<sub>2</sub>(X) and N<sub>2</sub><sup>\*</sup>(E) states as well as for the N<sub>2</sub><sup>-</sup>(<sup>2</sup>Σ<sub>g</sub><sup>+</sup>) resonance, calculated with a coupled-cluster method [13].

#### Measurements on Krypton

Compared to previous measurements [14,15], the significantly improved resolution allows for a more accurate characterization of the narrow  ${}^{2}P_{3/2}$  resonance. The broader  ${}^{2}P_{1/2}$  resonance, which lies energetically above the first excited state disappears at a scattering angle of 90°.



### **Measurements on Argon**

In addition to the planned program the  $Ar^{-}(3p^{5}4s^{2})$  Feshbach resonances [5] have been measured at the angles 10°, 22.5°, 45°, 90°, 112.5° and 180°. These data represent a valuable complement of the Kaiserslautern measurements which are influenced by cluster contributions. Absolute

differential cross sections at an energy of 11.2 eV were determined. The data are analyzed using new phase shifts obtained by *ab initio* calculations [13].



## Conclusion

A new set of high-resolution differential scattering cross sections including angles up to  $180^{\circ}$  has been obtained for Ar, Kr and N<sub>2</sub> in the energy range of the lowest sharp Feshbach resonances. A combined analysis of the Fribourg and the Kaiserslautern data will allow for a conclusive determination of the resonance width. Results of this work will be presented at the ECAMP IX conference in Crete and the XXV ICPEAC conference in Freiburg (Germany). Joint publications are in preparation.

I would like to thank Prof. Allan for making difficult measurements look so easy.

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