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Absolute cross sections for electron collisions with diacetylene: Elastic scattering, vibrational excitation and dissociative attachment

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Synopsis We present absolute experimental cross sections for elastic scattering, vibrational excitation by electron impact and for dissociative electron attachment to 1,3-butadiyne, as well as calculations of the elastic cross sections.

Electron collisions with diacetylene (1,3-butadiyne, H−C≡C−C≡C−H) are of special interest to astronomers due to the recent discovery of the H−C≡C−C≡C$^-$ anion in interstellar space [1]. We measured absolute cross sections for elastic scattering, vibrational excitation, and for dissociative electron attachment. We also calculated differential and integral elastic cross sections in the fixed-nuclei approximation using a parallel implementation of the Schwinger multichannel method [2]. The calculations employed an extended basis set and included polarization effects.

The measured elastic cross sections show boomerang structure due to the $^2\Pi_u$ resonance at 1 eV, and angle-dependent structure due to the $^2\Pi_g$ resonance around 5.5 eV. The essential features are reproduced by the calculation.

The selectivity of vibrational excitation reveals detailed information about shape resonances as shown in Fig. 1. Excitation of the C≡C stretch and of double quanta of the C−H bend vibrations reveal a $^2\Pi_u$ resonance at 1 eV (autodetachment width about 30 meV) and a $^2\Pi_g$ resonance at 6.2 eV (autodetachment width 1-2 eV). There is a strong preference for excitation of even quanta of the bending vibration. The excitation of the odd and even quanta of the bending vibration within the $^2\Pi_u$ resonance have very different angular distributions: the former has a maximum at 90°, the latter a minimum. Excitation of the C−H stretch vibration reveals σ^* resonances at 4.3, 6.8, and 9.8 eV, with autodetachment widths of about 2 eV. The detailed information about resonances permits conclusions about mechanism of dissociative electron attachment [3].

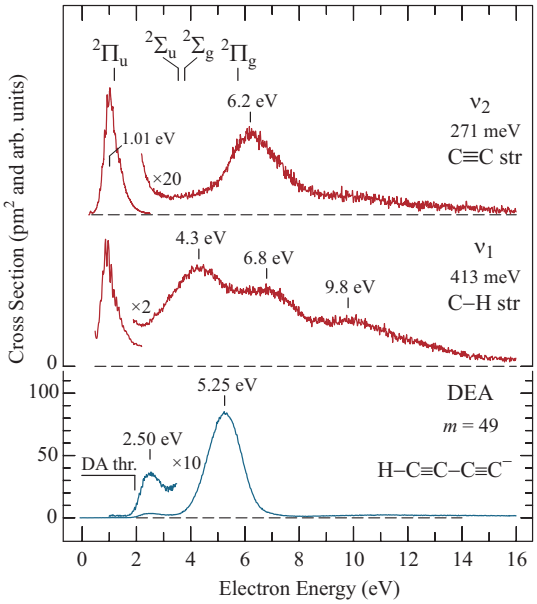

Figure 1. The top two curves show cross sections for exciting the C≡C and C−H stretch vibrations. Predictions from empirically scaled SCF virtual orbital energies are indicated by vertical lines and labels on the top. The DEA spectrum (loss of H) is shown at the bottom.

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