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Vibrationally inelastic collisions of slow electrons with cyclopropane and diacetylene

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Synopsis This is a joint experimental and theoretical study bringing new results on vibrationally inelastic electron scattering by cyclopropane and diacetylene.

Some of lighter hydrocarbons are known as sources of carbon atoms during chemical vapour decomposition reactions. The cyclopropane was detected in cooler edges of the fusion plasmas. The diacetylene anion was also detected in interstellar space and in the upper layers of planetary atmospheres of Titan and Uranus. In all the above situations the interaction of such molecules with free electrons is important for initiating variety of processes.

In case of cyclopropane the most marked feature observed by experiments [1] has to do with the excitation of ν_3 vibration, the C-C ring stretching. This finding was confirmed computationally [2] where authors obtained a qualitative agreement of the resonance position but the energy dependence of cross section differed above the resonant energies. Therefore, we employed the Discrete Momentum Representation (DMR) method [3] to calculate cross sections for excitations of all the vibrational modes. Our results seem to indicate that the origin of the broad shape resonance centered around 9-10 eV visible in the experimental data for ν_3 mode is due to a vibrational excitation of HCH twisting mode ν_{13} that has accidentally the same energy loss of 147 meV. These findings are demonstrated in Figure 1 where we plot calculated integral cross sections for electron-impact vibrational excitations of ν_3 and ν_{13} modes together with experimental data [4].

In the recent experimental studies [5] the diacetylene molecule was identified as one of the prototype systems where the π^* resonance forms a doorway state to a dissociative electron attachment (DEA) process. The strong excitation of C-H bending mode indicates that C-H bending is the primary relaxation path that couples the C-H dissociative channel. This mechanism was also recently postulated theoretically for acetylene [6].

Therefore, we decided to carry out vibrational excitation studies of diacetylene to contribute to the ongoing discussion of DEA mechanisms in the literature.

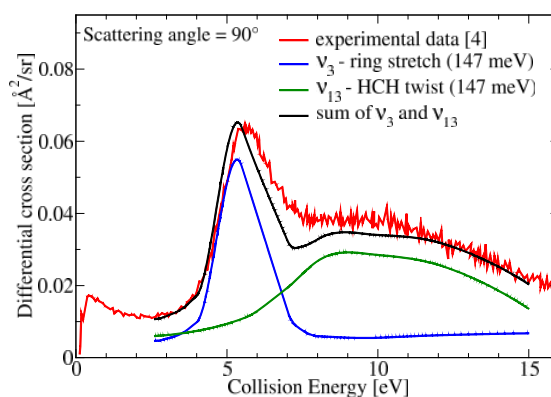


Figure 1. Vibrationally inelastic $0 \rightarrow 1$ differential cross section for cyclopropane. Blue and green lines show calculated cross sections for ν_3 and ν_{13} modes, respectively. Their sum is compared with the experimental data [4].

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