Molecular frame (e, 2e + ion) studies of CH₄ and CF₄

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Synopsis Ionization and fragmentation of the tetrahedral molecules CF₄ and CH₄ is studied at low electron impact energies ranging from E₀ = 35 eV to 67 eV. In kinematically complete experiments, the momentum vectors of the two outgoing electrons and one fragment ion are detected in triple coincidence. Various fragmentation channels are analyzed according to the ionized orbital binding energy (BE) and kinetic energy release (KER). Furthermore, we find electron emission patterns which depend on the spatial molecular orientation in particular for CH₄.

Kinematically complete electron impact ionization studies on atoms and molecules give detailed insight into correlated few-body reactions. Both, CH₄ and CF₄ have tetrahedral symmetry and are relevant in a large range of scientific and practical areas [1, 2].

Experimentally, we use a reaction microscope and a pulsed photoemission electron beam [3]. For the incoming beam energies E₀ between 35 eV and 67 eV were chosen. The momentum vectors of the two outgoing electrons (energies E₁, E₂) and one fragment ion are detected in triple coincidence. E.g., for CF₄ the fragment products CF₃⁺, CF₂⁺, CF⁺, F⁺ and C⁺ are resolved and can be associated to ionized orbitals according to the observed binding energies (BE) (E₀-E₁-E₂) (see [4] for CH₄).

In a two-body molecular dissociation the detected fragment momentum can provide the spatial orientation of the broken bond and, as result, of the whole molecule at the instant of the collision. Thus, molecular orientation resolved (e, 2e) cross sections can be obtained and the influence of the anisotropic molecular potential and multiple scattering of the electrons within the molecule can be studied. In this respect we analyzed fully differential cross sections (FDCS) for the dissociation reactions CX₄⁺ → CX₃⁺ + X where X = H or F. In the illustration in Figure 1 the projectile is coming in from below (p₀) and scattered to the left (p₂). For the CH₄ target and one CH bond being aligned either along the positive or negative x-axis the electron emission patterns in the (grey shaded) xy-plane perpendicular to the incoming beam are shown in Figure 2. Clearly, the cross section is orientation dependent and shows a maximum at 180° for one orientation only. More results and a detailed analysis will be presented at the conference.

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Figure 1. Illustration of the collision kinematics (see main text). Incoming and scattered projectile momenta are p₀ and p₁. The ejected electron (p₂) is observed in the perpendicular xy-plane. (a) and (b) show CH₃⁺ emission along positive and negative x-axis, respectively. Thus, one of the CH bonds of CH₄ is oriented along the x-axis.

Figure 2. FDCS as a function of electron emission angle φₑ₂ in the perpendicular plane. Ejected electron energy E₂ = 4 eV, projectile scattering angle θₑ₁ = - 8°. The black and red solid circles refer to orientation as shown in Figure 1(a) and (b), respectively.

References