Molecular frame (e, 2e + ion) studies of CH_4 and CF_4

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Synopsis Ionization and fragmentation of the tetrahedral molecules CF_4 and CH_4 is studied at low electron impact energies ranging from E_0 = 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 CH_4.

Kinematically complete electron impact ionization studies on atoms and molecules give detailed insight into correlated few-body reactions. Both, CH_4 and CF_4 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 E_0 between 35 eV and 67 eV were chosen. The momentum vectors of the two outgoing electrons (energies E_1, E_2) and one fragment ion are detected in triple coincidence. E.g., for CF_4 the fragment products CF_3^+, CF_2^+, CF^+, F^+ and C^+ are resolved and can be associated to ionized orbitals according to the observed binding energies (BE) (E_0-E_1-E_2) (see [4] for CH_4).

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 $CX_4^+ \rightarrow CX_3^+ + X$ where X = H or F. In the illustration in Figure 1 the projectile is coming in from below ($\vec{p}_0$) and scattered to the left ($\vec{p}_1$). For the CH_4 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.

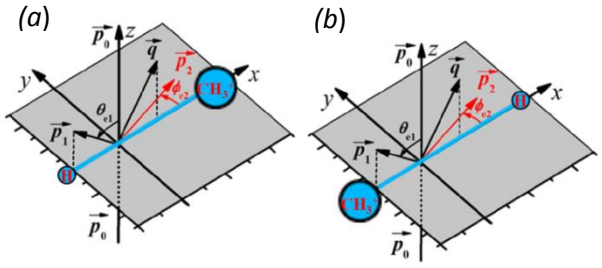

Figure 1. Illustration of the collision kinematics (see main text). Incoming and scattered projectile momenta are p_0 and p_1. The ejected electron (p_2) is observed in the perpendicular xy-plane. (*a*) and (b) show CH_3^+ emission along positive and negative x-axis, respectively. Thus, one of the CH bonds of CH_4 is oriented along the x-axis.

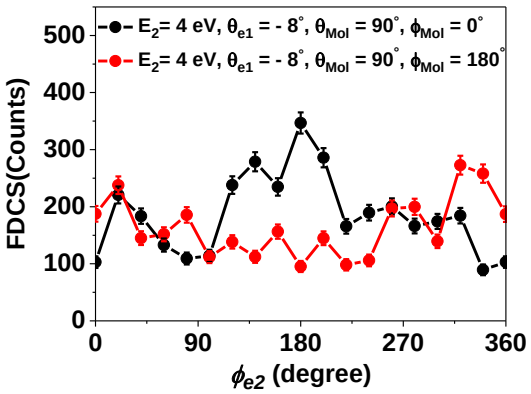

Figure 2. FDCS as a function of electron emission angle ϕ_{e2} in the perpendicular plane. Ejected electron energy E_2 = 4 eV, projectile scattering angle θ_{e1} = - 8°. The black and red solid circles refer to orientation as shown in Figure 1(a) and (b), respectively.

References

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