Imaging reaction dynamics of O^- + CH_3I reactive scattering

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We report on ion-molecule reactive scattering studies of the O^- + CH_3I system at collision energies between 0.3-2.0 eV. Here, we combine state-of-the-art crossed-beam velocity map imaging and quantum chemistry calculations to understand the dynamics for the formations of the different ionic products such as I^-, OI^-, CH_2I^-, and CHI^-. The velocity- and angle-differential cross-sections have been obtained for all collision energies. It is observed that reaction outcome depends solely on the collision energy and angle of attack of the O^- ion. Here, the predominant product ion, for all collision energies, is I^- (about 70-80%). We can see that throughout all investigated collision energies, an indirect mechanism dominates in the I^- product distributions. In the experimental velocity- and angular-distribution plots, this process manifests as a uniform I^- distribution without any angular preference of the I^- ions as an isotropic distribution. Our calculated minimum energy pathway for the O^- + CH_3I system shows that the front-side attack does not lead to the direct formation of I^-. Instead, it proceeds via the intermediate OI^- or hypoiodite formation channel. The other two observed channels are proton transfer (CH_2I^- formation) and combined hydrogen/proton transfer (CHI^- formation). The velocity- and angle-differential cross-sections for these channels are dominated by forward scattered events. However, for the CHI^- channel, the data show a lower product velocity than for CH_2I^- channel. This indicates a higher internal excitation for the hydrogen/proton transfer reaction than the single proton transfer reaction. Further, our results suggest the combined hydrogen/proton transfer process proceeds via a two-step process.

References:
1. Khan, A., Ayasli, A., Michaelsen, T., Gstir, T., Ončák, M., & Wester, R. Imaging the Atomistic Dynamics of Single Proton Transfer and Combined Hydrogen/Proton Transfer in the O^-+ CH_3I Reaction. *The Journal of Physical Chemistry A* (2022).
2. Ayasli, A., Khan, A., Michaelsen, T., Gstir, T., Ončák, M., & Wester, R. Imaging frontside and backside attack mechanisms in radical ion-molecule reactive scattering (To be submitted).