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Electron collisions with the $\text{HCOOH}\cdots(\text{H}_2\text{O})_n$ complexes ($n = 1, 2$) in liquid phase: The influence of microsolvation on the π^* resonance of formic acid

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ABSTRACT

We report momentum transfer cross sections for elastic collisions of low-energy electrons with the $\text{HCOOH}\cdots(\text{H}_2\text{O})_n$ complexes, with $n = 1, 2$, in liquid phase. The scattering cross sections were computed using the Schwinger multichannel method with pseudopotentials in the static-exchange and static-exchange plus polarization approximations, for energies ranging from 0.5 eV to 6 eV. We considered ten different structures of $\text{HCOOH}\cdots\text{H}_2\text{O}$ and six structures of $\text{HCOOH}\cdots(\text{H}_2\text{O})_2$ which were generated using classical Monte Carlo simulations of formic acid in aqueous solution at normal conditions of temperature and pressure. The aim of this work is to investigate the influence of microsolvation on the π^* shape resonance of formic acid. Previous theoretical and experimental studies reported a π^* shape resonance for HCOOH at around 1.9 eV. This resonance can be either more stable or less stable in comparison to the isolated molecule depending on the complex structure and the water role played in the hydrogen bond interaction. This behavior is explained in terms of (i) the polarization of the formic acid molecule due to the water molecules and (ii) the net charge of the solute. The proton donor or acceptor character of the water molecules in the hydrogen bond is important for understanding the stabilization versus destabilization of the π^* resonances in the complexes. Our results indicate that the surrounding water molecules may affect the lifetime of the π^* resonance and hence the processes driven by this anion state, such as the dissociative electron attachment.

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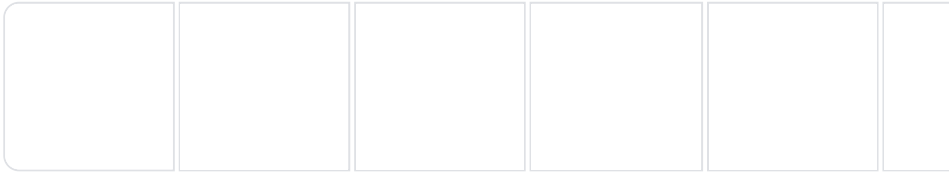
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