

Dynamics of ion-molecule reactions for astrochemistry; study of isomerism and internal or collision energy

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HCO⁺ and HOC⁺ are two isomeric cations detected in Photon Dominated Regions [1], diffuse clouds [2], and Mars atmosphere [3,4]. They correspond to the protonation of carbon monoxide on either the carbon or oxygen atom and are important intermediates in the formation of complex molecules as HCO⁺ is the most abundant ion in molecular clouds. There is a difference in reactivity between the two isomers and isomerization is possible when energy is provided or through collision. The isomers have a difference of energy of 1.7 eV (HCO⁺ being the more stable) and are separated by an isomerization barrier of 3.2 eV [5]. Previous studies of their reactivity have mostly been obtained by electron ionization [6,7] which does not allow the formation of pure HOC⁺ nor precise internal energy determination.

The CERISES [8] instrument, connected on the DESIRS beamline at SOLEIL Synchrotron, was used to produce (i) HCO⁺ from formaldehyde (H₂CO) and (ii) HOC⁺ from deuterated methanol (CD₃OH). We have studied the reactivity of the two isomers with a series of neutral targets to (i) characterize the ionic purity and internal energy content of the two isomers and (ii) study complex reactivity (with a potential increase in chemical complexity). From this extensive data set, we have determined the isomeric purity, the evolution of internal energy as a function of photon energy, and that the reactivity of both isomers with methanol is dominated by Proton Transfer (PT) and dissociative PT. Attempts to evaluate the collision-mediated isomerization are also being performed through an innovative method that aims to combine time-of-flight spectrometry with SIMION simulation.

References

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