universität innsbruck
Institut für Ionenphysik
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# Institutsseminar

# Blackbody Infrared Radiative Dissociation Kinetics and Master Equation Modelling of Hydrated Carbonate Ions

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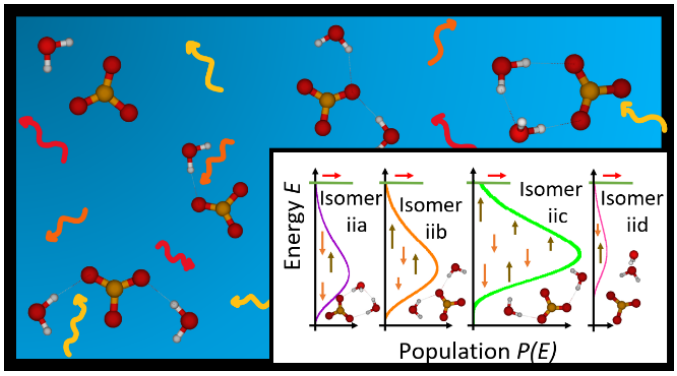


Blackbody infrared radiative dissociation (BIRD) is the dissociation of molecules in a low pressure environment due to surrounding blackbody radiation. As blackbody radiation depends on temperature, also the resulting dissociation channels show a strong temperature dependence.

Here, BIRD of $CO_3^{\bullet-}(H_2O)_{1,2}$ is investigated. The ions are trapped in a FT-ICR mass spectrometer, mass selected and their BIRD induced fragmentation is recorded at temperatures in the range from 250 K to 330 K. Dissociation rates can be modelled with Master Equation Modelling (MEM), considering three processes, namely absorption and emission of photons (leading to changes in the energy content of the molecule), and dissociation of molecules above a certain energy level. To describe the process, we consider not only the isomer with the lowest energy, but also other local minima.
Precise experimental measurements of BIRD kinetics at different temperatures and the multiple-well approach for Master Equation Modelling are combined, providing water binding energies of the investigated clusters. These energies are consistent with ab initio calculations. Comparison with the use of a single-well-MEM approach shows that the multiple well approach is better suited for the description of the BIRD process of hydrated carbonate ions.

**HS D** **16:15 Uhr** **14.12.2022**