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IR Spectroscopy of Phosphoric Acid Clusters in Helium Nanodroplets

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Phosphates are ubiquitous in nature and play a crucial role in biochemical processes such as protein synthesis, metabolism, and energy production. One unique property of phosphoric acid is that it has the highest intrinsic proton conductivity of any known substance and is used in low-temperature batteries as well as in phosphoric acid fuel cells (PAFCs). The detailed mechanism of the proton transport is, however, not yet fully understood.

In this study, we examine mass-selected ionic clusters containing phosphoric acid in the gas phase using infrared action spectroscopy in helium nanodroplets. Using this technique, spectra can be obtained at a cryogenic temperature of 0.37 K, reducing spectral congestion and yielding well-resolved vibrational bands. Studying hydrogen-bonded systems at these temperatures allows for unique insights into their fundamental properties, enhancing our understanding of phosphoric acid chemistry and its interactions across various environments.

Our investigation reveals molecular structures that can serve as calibration points for quantum chemistry calculations. The elucidation of experimental vibrational bands, the hydrogen-bond interactions between the two moieties, as well as the spectroscopic details, will be discussed.

Keywords

Hydrogen bond: medium, State of system: gas

This abstract is submitted for....

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Primary author: TORRES BOY, América (Fritz-Haber Institut)

Co-authors: Dr TACCONE, Martin (Fritz-Haber Institut); Dr PRABHU, Rakesh (Fritz-Haber Institut); Ms OBER, Katja (Fritz-Haber Institut); Prof. MCCOY, Anne B (University of Washington); Prof. MEIJER, Gerard (Fritz-Haber Institut); Prof. VON HELDEN, Gert (Fritz-Haber Institut)

Presenter: TORRES BOY, América (Fritz-Haber Institut)