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Conformer-sensitive nuclear dynamics of the ammonia dimer cation probed by femtosecond time-resolved Coulomb explosion

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Unlike in the liquid phase, the debate of whether and how hydrogen-bonded structures exist in a neutral ammonia dimer (NH3)2 in the gas phase has been ongoing for several decades. Here we distinguish the structures of neutral ammonia dimers with and without hydrogen bonds by photoionization, because the ions inherit initial structures from the
neutral dimers and lead to significantly different Coulomb explosion channels in our pumpprobe experiment, i.e., the direct dissociation (NH3
+ + NH3+) and indirect dissociation with
proton migration (NH2+ + NH4+).
With quantum chemical and molecular dynamics simulation, we showcase that these two different Coulomb explosion channels originate from the ammonia dimer cations with
different structures. The dimer cations without hydrogen bonds correlate with the direct Coulomb explosion channel. In contrast, dimer cations with hydrogen bonds are likely to undergo ultrafast proton migration in ~48 fs which has no potential barrier and correlate
with the indirect dissociation channel in the Coulomb explosion. The 48 fs characteristic time is used to exclude the slower indirect dissociation initiating from non-H-bonded cations.
Our work demonstrates a highly sensitive approach to probe weakly bonded and fluxional structures of gas phase molecular clusters by utilizing both channel- and time-resolutions of Coulomb explosion.

Keywords

This abstract is submitted for....

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