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HCOOH-NH3-H2O, a prototypical acid-base-water cluster revealed by rotational spectroscopy

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The ternary complex HCOOH-NH3-H2O, serving as a prototypical acid-base-water cluster relevant to atmospheric nucleation processes, was investigated using rotational spectroscopy in conjunction with theoretical calculations. The complex adopts an effective Cs symmetry with two tunneling motions: NH3 internal rotation and free -OH wagging. Ammonia acts as the proton acceptor to formic acid, resulting in a transitionary chemical bond with both hydrogen bond and ionic bond characteristics. The measured 14N nuclear quadrupole coupling constants indicate that the ionicity of the ternary complex (27%) is higher than that of binary complexes such as HX-NH3, (X = -COOH, F, Cl, Br, I). These results suggest that the inclusion of a single water molecule significantly enhances proton and electron transfer between the acid and base molecules by reinforcing the hydrogen bond network. This model could serve as a prototype of acid-base-water ternary aggregates, offering valuable insights into the gas-to-particle phase transition mechanisms.

Keywords

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