FIRST OBSERVATIONS OF THE HONO · H_2O COMPLEX WITH MICROWAVE SPECTROSCOPY

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The impact of gaseous nitrous acid (HONO) in atmospheric chemistry is well described, being a major source of OH radicals acting as a strong oxidant[a]. In standard conditions, HONO is in equilibrium with various nitrous oxides under rapid decomposition at daytime. However, results by Lammel and Cape describe a steady production of OH radicals by HONO in the atmosphere whose source might be the complex of HONO with water[b]. Recent experiments have revealed that HONO remains stable in an aqeous environment as the HONO · H_2O complex, supporting studies of its greater stability in environments with higher humidity[c]. In the present work, gaseous HONO · H_2O was generated in a laboratory scale and investigated with two molecular jet Fourier transform microwave spectrometers operating from 2 to 40 GHz. To guide the experimental observation, geometry optimizations were performed to obtain rotational constants using the standard coupled-cluster theory with single and double excitations. The HONO · H_2O spectrum has been assigned with the ^{14}N quadrupole coupling taken into account. Further splittings by the ortho-hydrogens, resulting from spin-spin coupling interactions, could be fully resolved. Comparing the results to those of the dimethylamine-water complex[d] confirmed an absence of the water tunnelling motion.

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