ROTATIONAL SPECTRA OF N_2OH^+ AND CH_2CHCNH^+ MOLECULAR IONS

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Protonated molecular ions of nitrous oxide (N_2OH^+) and acrylonitrile (CH_2CHCNH^+) have been detected at high spectral resolution in the molecular beam of a Fourier transform microwave spectrometer on the basis of high-level *ab initio* calculations. The ions were synthesized in the throat of a pulsed supersonic nozzle by discharging in a flow of the corresponding precursor gas (either N_2O or CH_2CHCN) heavily diluted in H_2. Two isomers of N_2OH^+ were identified, corresponding to protonation at either the N or O end of NNO. This work contributes precise nitrogen hyperfine coupling constants to existing measurements of ground state $NNOH^+$, and represents the first detection of the higher energy $HNNO^+$ isomer, which is calculated to lie 4.4 kcal/mol above ground[a]. In addition, protonated acrylonitrile has been detected for the first time at high spectral resolution, yielding spectroscopic constants that are in excellent agreement with high-level quantum-chemical calculations[b]. Owing to sizable calculated dipole moments of protonated nitrous oxide and acrylonitrile and the relatively high proton affinities of their neutral counterparts, both cations are plausible candidates for astronomical detection with radio telescopes.

[a] J. M. L. Martin & T. J. Lee, J. Chem. Phys. 98, 7951 (1993)

[b] At CCSD(T)/cc-pwCVQZ level of theory with zero-point vibrational effects at CCSD(T)/cc-pVQZ.