Microwave spectrum of 3-amino-2-propenenitrile (H_2N-CH=CH-CN), a molecule of astrochemical interest.

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Ammonia easily reacts on cyanoacetylene in gas-phase or in a solvent to form the $Z$and E-isomers of aminoacrylonitrile (3-amino-2-propenenitrile). This kinetically stable enamine presents interest for its possible presence in the interstellar medium, the comets, the atmospheres of Planets including the Primitive Earth, and from a theoretical point of view. B3LYP/6-311+G(3df,2p) and G2 calculations indicate that the imine isomer is significantly less stable than the enamine. DFT and G2 calculations indicate that the Z-isomer of the enamine lies ca. 8.0 kJ mol^{-1} lower in energy than the E-isomer.[1]

(Z)-H_2NCH=CHCN has been investigated by microwave Stark spectroscopy in Oslo in the 10-80 GHz spectral range and by Fourier transform microwave spectroscopy in Lille in the 6-20 GHz region. The ground vibrational state and several vibrationally excited states have been assigned for the parent species. The ground vibrationally state of eight isotopomers have so far been assigned. Some of these species were studied in natural abundance, while several isotopomers have been synthesized. The nuclear quadrupole coupling constants of both nitrogen atoms have been determined. Extensive quantum chemical calculations have been performed. The molecule is planar or nearly planar. We expect to present a substitution structure of the molecules as well as its equilibrium structure at the time of the conference. It is also expected that a plausible reaction path for the generation of this compound from ammonia and cyanoacetylene will be available.[2]

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2. Möllendal, H.; Askeland, E.; Avles-Moreno, J.R.; Huet, T.R.; Demaison, J. ; Guillemin, J.-C. ; manuscript in preparation.