

MICROWAVE SPECTRA OF 3-AMINO-2-PROPENENITRILE ($\text{H}_2\text{N-CH=CH-CN}$), A MOLECULE OF ASTRO-CHEMICAL INTEREST

T.R. HUET, J.R. AVILES-MORENO, J. DEMAISON,, *Laboratoire PhLAM, UMR 8523 CNRS-Universite Lille 1, F-59655 Villeneuve d'Ascq Cedex, France*; E. ASKELUND, H. MOLLENDAL, *Department of Chemistry, University of Oslo, 0315 Oslo, Norway*; J.C. GUILLEMIN, *Sciences Chimiques de Rennes, UMR 6226 CNRS-Ecole Nationale Supérieure de Chimie de Rennes, 35700 Rennes, France*.

Ammonia easily reacts on cyanoacetylene in gas-phase or in a solvent to form the Z (cis) 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.

Cis- $\text{H}_2\text{NCH=CHCN}$ 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 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.