HIGH RESOLUTION SPECTROSCOPY OF HEXAMETHYLENETETRAMINE (HMT) $C_6N_4H_{12}$

V. BOUDON, *Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, 9. Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France*; O. PIRALI[a], *Ligne AILES – Synchrotron SOLEIL, L'Orme des Merisiers, F-91192 Gif-sur-Yvette, France*.

Hexamethylenetetramine, or HMT ($C_6N_4H_{12}$) is a N-substituted derivative of adamantane $C_{10}H_{16}$ which is the smallest sample of the diamondoid molecules family. Thanks to their high stability, diamond-like molecules have long been suspected to be present in space[b] (note that diamond nanocrystals are extracted from Murchinson meteorites[c]), and HMT is known to be an abundant residue of UV irradiated ice analogs[d] and might be present in Titan's atmosphere. Using the Bruker IFS 125 coupled to a multipass cell (absorption path length of 150 m) of the AILES beamline at SOLEIL, we recorded the IR spectrum of gas phase HMT in the 300–3000 cm^{-1} spectral region with an unapodized resolution 0.001 cm^{-1}. HMT is a solid powder with about 0.008 mbar vapour pressure at room temperature, it is a T_d molecule (as adamantane) and has 25 vibrational modes from which only 9 are infrared active. Over the 9 IR active modes, we were able to rotationlly resolved the spectra of 6 of them.

The analysis of all the resolved bands has been performed thanks to the XTDS and SPVIEW softwares developed in Dijon for such molecules[e]. Each band can be considered as isolated and we get very good fits of line positions, with a root mean square deviation better than 5×10^{-4} cm^{-1} for J values up to 80 or more in each case. As for our recent study concerning adamantane[f], the resulting synthetic spectra will permit an active search of this very stable specie in different sources of the interstellar medium.

---

[a] Also at: Institut des Sciences Moléculaires d'Orsay, UMR8214 CNRS-Université Paris-Sud, Bat.210, 91405 Orsay cedex, France.

[b] W. C. Saslaw and J. E. Gaustad, Nature, **221**, 160 (1969)

[c] R. S. Lewis et al., Nature, **326**, 160 (1987)

[d] M. P. Bernstein et al., ApJ, **454**, 327 (1995)

[e] Ch. Wenger, V. Boudon, M. Rotger, M. Sanzharov and J.-P. Champion, *J. Mol. Spectrosc.*, **251** 102–113 (2008).

[f] O. Pirali, V. Boudon, J. Oomens, M. Vervloet, J. Chem. Phys., **136**, 024310 (2012)