THE UREA-WATER COMPLEX OBSERVED BY JET COOLED FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY AND STUDIED BY AB INITIO CALCULATIONS.

J.R. AVILES-MORENO, A. CUISSET, T. DELEPORTE, T.R. HUET, and D. PETITPREZ, *Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 8523 CNRS-Université de Lille 1, F-59655 Villeneuve d'Ascq cedex, France*.

We have recorded the rotational spectra of the urea-water complex using a pulsed-nozzle Fourier-transform microwave spectrometer in the 6-20 GHz range. The spectra were obtained using a mixture of Ne/H_2O carrying away the vapours of urea placed inside a heated nozzle. In order to derive a reliable geometrical structure, we have observed and identified spectral lines for four different species, mixing O=C($^{14}NH_2$)$_2$ or O=C($^{15}NH_2$)$_2$ isotopologues with H_2O or D_2O. The structure and the relative energy of the most stable conformers have been computed by *ab initio* calculations at the B3LYP/aug-cc-pVTZ level of theory. Results of the calculations show that the more stable conformer is stabilized by two hydrogen bonds, the water molecule sitting out of the plane form by the heavy atoms of the urea molecule. These *ab initio* results are in good agreement with the first experimental data which will be presented.