

# **Book of Abstracts**

## **XXIth International Conference on Horizons in Hydrogen Bond Research “HBond2015”**

**13-18 September, 2015**

## FTIR study of fluoroform and methyl fluoride trapped in low temperature matrices. Evidence of a weak complex formation stabilized by blue shifting H-bond

Ruslan E. Asfin, Sonia M. Melikova, Konstantin S. Rutkowski

*Department of Physics, St. Petersburg State University, R.Asfin@molsphys.spbu.ru*

Fluoroform and fluoroform complexes with methyl fluoride were studied by means of infrared matrix isolation spectroscopy. Ar and N<sub>2</sub> were used as matrix gases. The F<sub>3</sub>CH/M, FCD<sub>3</sub>/M (within (0.5 – 7):1000 ratio) and F<sub>3</sub>CH/FCD<sub>3</sub>/M mixtures were prepared by the standard manometric technique (M = Ar or N<sub>2</sub>). The gas mixtures were sprayed onto gold-plated copper mirror held at 15 or 20 K by a closed cycle He refrigerator. FTIR spectra (resolution 0.1 cm<sup>-1</sup>) were studied at 10 K in a reflection mode with a Bruker IFS 125 FTIR spectrometer. The spectra were recorded directly after matrix deposition and after its annealing to 28 – 32 K for 20 – 40 min. Results obtained for fluoroform in N<sub>2</sub> matrix have shown noticeable blue frequency shift effect for CH stretching vibration as compared to the gas phase<sup>1</sup> and Ar matrix results. Additionally lifting degeneracy effects were found which resulted in noticeable splitting the C-H bending and C-F stretching bands of *E* symmetry. Analyzing the IR spectra of F<sub>3</sub>CH/FCD<sub>3</sub> mixtures in N<sub>2</sub> matrix it was concluded that the interaction between F<sub>3</sub>CH and FCD<sub>3</sub> is of a blue shifting H-bond type, with the frequency shift  $\Delta\nu^{c-m}$  of c.a. +16 cm<sup>-1</sup> for CH stretching vibration of fluoroform. This value was compared with the data obtained earlier in the gas phase<sup>1</sup> and in liquefied noble and atmospheric (Ar, Kr, Xe, N<sub>2</sub>) gas solutions<sup>2,3</sup>. The environment effect on the frequency shift has been shortly discussed.

### Acknowledgements

This work was supported by the Russian Foundation for Basic Research, project no. 14-03-00111. The spectra were recorded in the Center for Geo-Environmental Research and Modeling (GEOMODEL) of Research park of St. Petersburg State University.

### REFERENCES

1. K.S. Rutkowski, S.M. Melikova, R.E. Asfin, B. Czarnik-Matuszewicz, M. Rospenk, *J. Mol. Struct.* **2014**, *1072*, 32
2. K.S. Rutkowski, S.M. Melikova, P. Rodziewicz, W.A. Herrebout, B.J. van der Veken, A. Koll, *J. Mol. Struct.* **2008**, *880*, 64
3. K.S. Rutkowski, P. Rodziewicz, S.M. Melikova, W.A. Herrebout, B.J. van der Veken, A. Koll, *Chem. Phys.* **2005**, *313*, 225