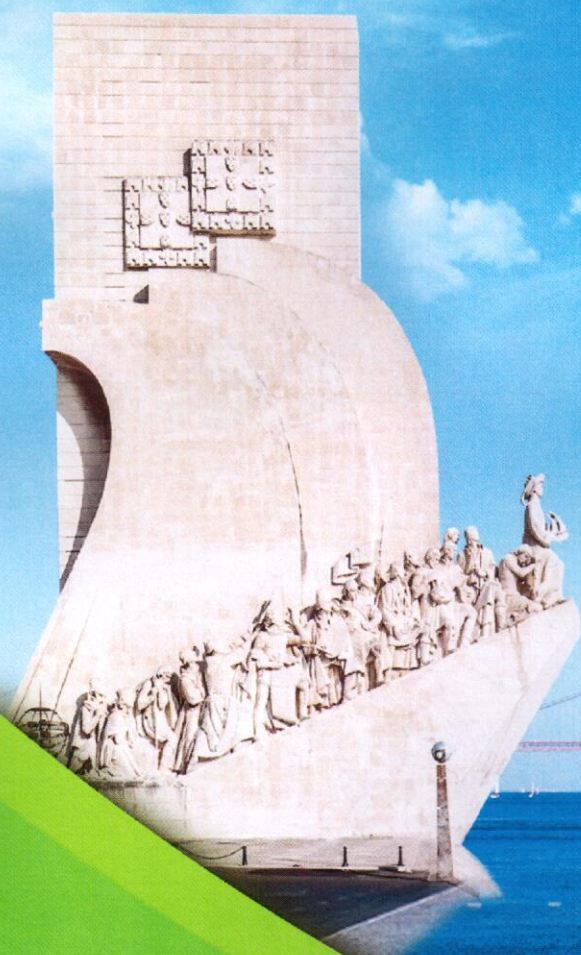


# *1<sup>st</sup> International Conference on Noncovalent Interactions*



## **ICNI 2019**

2 - 6 september, 2019 | Lisbon, Portugal

### **PROGRAM**

<https://icni2019.eventos.chemistry.pt/>



1<sup>st</sup> International Conferences on Noncovalent Interactions (ICNI-2019)

## Noncovalent interaction in cyclic heterocomplexes of phosphinic and phosphoric acids studied by <sup>1</sup>H NMR spectroscopy

Valeriya Mulloyarova,<sup>1</sup> Peter Tolstoy<sup>1</sup>

<sup>1</sup>Institute of Chemistry, St. Petersburg State University, Russia  
e-mail: [mylllerka20071993@gmail.com](mailto:mylllerka20071993@gmail.com)

The monomers of phosphorous-containing acids form cyclic dimers and cyclic trimers [2] by noncovalent interactions namely hydrogen bonds in aprotic solution (CDF<sub>3</sub>/CDCIF<sub>2</sub>). [1] All hydrogen bonds in each type of complexes are equivalent and signals of bridged protons in <sup>1</sup>H NMR spectrum have single chemical shift (Fig. 1b).

In this work the hydrogen bonds in different cyclic heterocomplexes were studied by <sup>1</sup>H NMR spectroscopy. In a mixture of two different acids (for example (MeO)<sub>2</sub>POOH and (PhO)<sub>2</sub>POOH) the monomers form a cyclic heterodimer and two different heterotrimers in almost equal ratios (Fig. 1a). Hydrogen bonds in heterotrimers are non-equivalent and are stronger than bonds in individual self-associates, the chemical shifts of protons are different and there are in lower field (Fig. 1b). In mixture of cacodylic and diphenylphosphoric acids cyclic dimer and trimer are formed. In this case was recorded maximum of <sup>1</sup>H NMR chemical shift of bridged proton in neutral cyclic complexes (17.5 ppm).

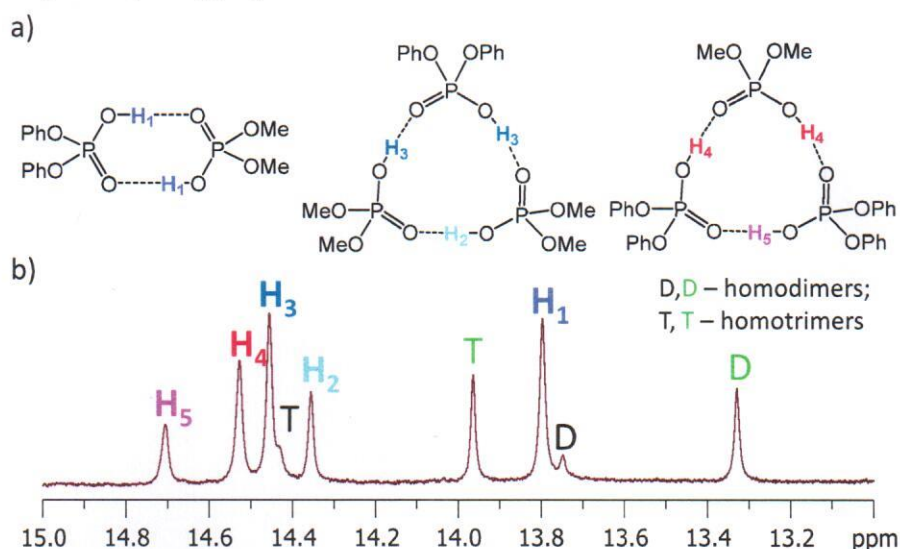


Fig. 1. Structures of the heterodimer and heterotrimers (a) of (MeO)<sub>2</sub>POOH and (PhO)<sub>2</sub>POOH. <sup>1</sup>H NMR spectrum (b) of these acids mixture at 100 K.

### References

- [1] Detering, C.; Tolstoy, P.M.; Golubev, N.S.; Denisov, G.S.; Limbach, H.H., *Dokl. Phys. Chem.*, **2001**, 379, 191–193.  
[2] Mulloyarova, V.V.; Giba, I.S.; Kostin, M.A.; Denisov, G.S.; Shenderovich, I.G.; Tolstoy, P.M., *Phys. Chem. Chem. Phys.*, **2018**, 20, 4901–4910.

**Acknowledgement:** This work has received financial support from the RFBR Grant 18-13-00050.