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2015

C-13

MEASUREMENT AND CALCULATION OF COMPEXATION CONSTANTS OF VERY WEAK AND VERY STRONG COMPLEXES

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Molecular recognition is an important part of modern organic chemistry[1]. Among UV spectroscopy and potentiometry, ^{1}H-NMR represents an efficient and widespread used tool for determination of complexation constants. [2] As the complexation constants in the region of 100 to 10 000 M^{-1} can be easily measured by NMR, the determination of the constants from 1 to 10 M^{-1} and higher then 10 000 M^{-1} becomes more challenging.

The aspects of measurement and calculations of very low complexation constants can be studied at helicene complexes with various electron- poor aromatics. In these systems, the interaction is based on the charge transfer complex formation[3] with the non- specific π-π bond, with the binding constants lower than 10 M^{-1}.

For the studying of very strong complexes, some calix[4]arene ureido derivatives were synthesized. These compounds are capable of anion binding by hydrogen bonds. The anion binding abilities of these receptors are so pronounced, that their complexation constants are over 10 000 M^{-1} even in such a competitive solvent as DMSO.

In this presentation, the best ways of measurement and calculations of binding constants in such systems will be discussed.

References:

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Acknowledgement:
For the financial support, the Technology Agency of the Czech Republic (TA04010082) and the Czech Science Foundation (13-21704S) is gratefully acknowledged.