Warsaw Doctoral School in Natural and Biomedical Sciences and the Institute of Physical Chemistry PAS cordially invites you to a **SPOTLIGHT TALK**

Hydrogen bonding

given by

Prof. Poul Erik Hansen
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on 8th November 2022, 11:00 at IChF Aula
Duration: 45 min + question time

Highly recommended to all Warsaw-4-Phd students!

Talk abstract:

Hydrogen bonding is a very important structural parameter for both chemical and biological compounds. Hydrogen bonding influences a number of chemical properties such as boiling points, solubility, pKa values etc. and the interaction between small molecules (drugs) and biomolecules. Hydrogen bonding is a determining factor in the structure of carbohydrates, proteins, DNA and RNA.

The talk will discuss spectroscopic techniques such as Infra Red and NMR to establish the presence of hydrogen bonds and characterize those. A special technique, deuterium isotope effects on chemical shifts to establish the presence of hydrogen bonds will be presented and used to find hydrogen bonds and salt bridges in proteins in solution vs. X-ray structures. Related to intramolecular hydrogen bonding is tautomerism. Tautomerism if often elusive and methods will be given to establish this phenomenon. Examples will be taken from chemistry and biology. In the latter case the importance of having the right structure in relation to biological action is discussed. Finally, theoretical calculations will be touched upon.

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