



Contribution ID: 44

Type: Poster

Dynamics of Furanosides: Inelastic Neutron Scattering and Raman Study of Methyl- β -D-Ribofuranoside

Monday 20 March 2023 16:00 (2 hours)

The biological functionality and structure of DNA and RNA,[1] as well as the activity of various nucleoside-processing enzymes,[2] are all deeply linked to the properties of the underlying five-membered ring sugars, particularly furanosides. The study of five-membered rings is more challenging because of the strain of the ring in all conformations which leads to a small energy difference between twisted and envelope forms, ultimately giving rise to pseudo-rotation.[3] This is opposed to a six-membered ring, in which there is enough freedom to adopt a strain free chair conformation with bond lengths, bond angles, and dihedral angles kept at minimum energy.

While much effort has been put into the conformational study of five-membered rings,[4,5] the dynamics of such sugars, including ring-puckering, intermolecular hydrogen bonding, hydroxyl group dynamics, rotations of methyl groups and other effects, are still unclear and need further research. To this aim, in the current work, inelastic neutron scattering on TOSCA[6,7] and Raman spectroscopy are employed to learn more about the dynamics and various interactions in methyl- β -D-ribofuranoside. The empirical data will be compared to simulated spectra using Density Functional Theory in order to provide a better understanding of this biomolecular building block.

[1] A. G. Evdokimov et al., *J. Phys. Chem. A*, 1999, **103**, 744; [2] V. E. Marquez, Jr. et al., *Nucleosides, Nucleotides, Nucleic Acids*, 2001, **20**, 451; [3] J. Laane, *Vibrational Spectra and Structure*, ed. J. R. Durig, Marcel Dekker, Inc., New York 1972, 26-50; [4] J. B. Houseknecht et al., *J. Phys. Chem. A*, 2003, **107**, 5763; [5] Z. Dzakula et al., *J. Am. Chem. Soc.*, 1996, **118**, 12796; [6] R. S. Pinna et al., *Nuclear Inst. And Methods in Physics Research, A*, 2018, **896**, 68; [7] S. Rudić et al., *Molecular Physics*, 2012, **110**, 1609.

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Session Classification: Poster Session MONDAY

Track Classification: Chemistry of Materials (Structure and Spectroscopy)