



Inelastic neutron scattering study of thymol as potential neutron-moderating material

Tuesday, 21 March 2023 16:00 (2 hours)

Neutron moderators come in many forms and sizes with water (H_2O), methane (CH_4) and molecular hydrogen (H_2) being the most commonly used moderating materials. These materials have very good neutron moderating characteristics but serious disadvantages as well. As a result, the active search for a new types of moderator materials, and especially cryogenic moderator materials, is underway around the world [1]. This has led to the investigation of thymol ($\text{C}_{10}\text{H}_{14}\text{O}$). Inelastic neutron scattering (INS) spectra of thymol have been recorded with the help of TOSCA neutron spectrometer [2], and the derived experimental data were compared with the theoretical calculations of the molecule optimised geometry and associated vibrational frequencies calculated with the help of Gaussian 16 software package [3]. AbINS software [4] as implemented in Mantid [5] has been used to derive theoretical INS spectra from the Gaussian output. The goal is to use this theoretical and experimental data as a framework to further clarify the moderating capabilities of thymol as well as its possible application within neutron moderators.

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- [3] Gaussian 16, Revision B.01, M.J. Frisch et al., Gaussian, Inc. Wallingford CT, 2016.
- [4] K. Dymkowski et al., Physica B: Condensed Matter 551, 443 (2018).
- [5] O. Arnold et al., Nuclear Instruments and Methods in Physics Research A 764, 156 (2014).

Primary author: ZEPPELIN, Lukas (University of Copenhagen (UCPH))

Co-authors: Dr SKORO, Goran (ISIS facility); Prof. BORDALLO, Heloisa (University of Copenhagen (UCPH)); Dr RUDIC, Svemir (ISIS facility)

Presenter: ZEPPELIN, Lukas (University of Copenhagen (UCPH))

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