**European Conference on Neutron Scattering 2023** 



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

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Neutron moderators come in many forms and sizes with water (H2O), methane (CH4) and molecular hydrogen (H2) 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 (C10H14O). 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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