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Dynamics in Confinement: a study of CH₄@C₆₀

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Endofullerenes are substances in which small molecules or atoms are encapsulated in highly symmetrical cages of carbon atoms. Each encapsulated atom or molecule behaves as a textbook ex-ample of a quantized particle-in-a-box. The newest and largest member of the endofullerene fami-ly tree, namely CH₄@C₆₀, is the first organic molecule trapped inside the cage and the main interest of this abstract. The use of various spectrometers at ILL, namely PANTHER, IN5 and IN1-LAGRANGE, have allowed us to probe a large energy window up from 1 to 100 meV. The goal from these experiments was to probe the rotational and translational states of the confined CH₄ molecule, and observe the coupling between said states due to the confinement. A novel result that we have observed in this endofullerene, was the effect of the I_h symmetry of the C₆₀ on the rotational states of the CH₄ using inelastic neutron scattering, an effect that was absent in previous endofullerene studies. We have also performed QENS measurements, using PANTHER, that have allowed us to observe slight differences in the rotational dynamics of both the C₆₀ and CH₄, confirming the stronger guest-host coupling that we observed in our INS measurements.

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