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Spectroscopy of C60 Endofullerenes

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Endofullerenes are supramolecular complexes where one small (endohedral) atom/molecule is completely confined within a bigger, fullerene, molecule which acts as an enclosing cage.1 Endofullerenes offer an ideal "particle in a box" nano-laboratory to observe quantum mechanical phenomena.

The noble gas endofullerenes He@C_{60} and Ne@C_{60} have been investigated using INS (Inelastic Neutron Scattering) and THz (far-Infra Red) spectroscopy.2 Surprisingly, He@C_{60} is observed to absorb THz light and scatter neutrons, which translationally excite the Helium atom. The atomic translational quantization arising due to confinement is probed using these techniques. Simulating the experimental results delivers the confining interaction potential between the noble gas atom and the confining C_{60} fullerene cage; providing valuable non-covalent interaction parameters, which serve as benchmark for quantum chemistry calculations.
An unexpected NMR (Nuclear Magnetic Resonance) interaction, J-coupling, between ^{3}He and ^{13}C in the C_{60} cage was observed due to confinement, in the ^{3}He@C_{60} endofullerene.3 This is attributed to a scalar $^{0}J_{HeC}$-coupling, where the "zero" represents the number of chemical bonds between Helium and Carbon. Indication of similar ^{0}J-couplings between ^{1}H and ^{13}C are also observed in endofullerenes containing endohedral hydrogen.
When the C_{60} molecule is filled with an endohedral species, the C_{60} ^{13}C NMR resonance is shifted downfield, relative to C_{60}, depending on the species (endohedral shift). The magnitude of the shift scales proportionally with the size of the endohedral species. The endohedral shift appears to reflect the "pressure" a single atom/molecule exerts on its container, in this case the C_{60} molecule. Solution and solid state NMR measurements together with an interpretation of the endohedral shifts will be presented.

1-Y. Murata et al., Science, 2005, 307, 238
2-G. R. Bacanu et al., JCP, 2021, 155, 144302
3-G. R. Bacanu et al., JACS, 2020, 142, 16926

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