Fully Coupled Quantum Treatment of a Water Molecule inside a Fullerene C_{60}

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The encapsulation of molecules inside cage compounds has opened new opportunities to investigate the characteristics of these guest-host systems with potential applications in nanoscience and nanotechnology. Recent experiments have been performed showing interesting properties for such systems, motivating us to develop a methodology to treat the full-dimensional quantum problem within the MCTDH framework for any triatomic molecule in a embedded or confined environment [1,2].

In this work, we present a theoretical study of a single water molecule trapped in a highly isotropic C_{60} fullerene cage computing the energy levels and the nuclear spin isomers. For this system the INS spectra results show the splitting of the *J=1* rotational states [3]. The presence of occluded impurities or inhomogeneities due to noncovalent interactions in the interfullerene environment could modify aspects of the potential, causing significant coupling between otherwise uncoupled modes.

The key point of the study lies in the full 9D description of both nuclear and electronic degrees of freedom. Using specific n-mode model potentials, we obtained splitting patterns that confirm the effects of symmetry breaking observed in the ground ortho-H_2O state. These results highlight the importance of accurate and computational demanding approaches for building up predictive models for such nanoconfined molecules.

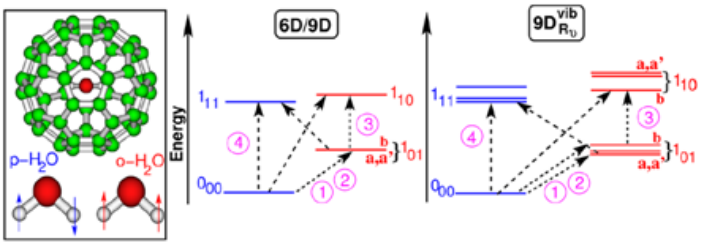

Figure 1: Schematic representation of J = 0 and J = 1 rotational levels for the H2O@C60 system.

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References

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