Noble Gases in Fullerenes

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Fullerene compounds with noble gas atoms inside the cage as, e.g., $He_n@C_m^q$ (Ng=He; n=1,2; m=60,70,76,78,84; q=0,-6) exist and their NMR spectra have been measured.[1] Particularly interesting examples are the cages housing the dimers of He atoms.[2]

We use density functional theory to study the energy and chemical shift hypersurfaces of the Ng atoms in such systems with particular aim to find reliable density functional and further data for future molecular simulation studies of these systems and to investigate the existence of some of the claimed endohedral compounds. The interactions between a cage and an Ng atom are mainly dispersion forces and that has to be taken into account in calculations. DFT is inherently not designed to describe dispersion interactions but some functionals have been previously found to work reliably in NMR properties. We calibrate our results against MP2 calculations using Ng…C_6H_6 models to search for the functionals which can properly describe the interactions of an Ng in a fullerene cage, in particular for the NMR properties.

[1] M. Saunders, H. A. Jiménez-Vázques, R. J. Cross: *J. Am. Chem. Soc.* **1994**, *116*, 2193.
[2] T. Sternfeld, M. Saunders, R. J. Cross, M. Rabinovitz: *Angew. Chem.* **2003**, *42*, 3136.