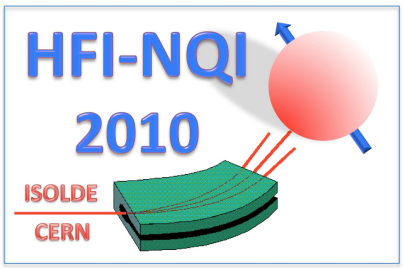

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First Principles Study of Nuclear Quadrupole Interactions in Single and Double Chain DNA and Solid Nucleobases

Summary

free nucleobases and nucleobases in single strand (sDNA), double strand DNA (dsDNA) and in solid state. Our first principles investigation was carried out using the Gaussian 2009 set of programs to implement the Hartree-Fock procedure combined with many-body effects included using many-body perturbation theory. The positions of the atoms were taken from structural data for DNA systems [1], for solid nucleobases from x-ray data [2-5] and by geometry optimization based on the total energy for the free nucleobases. As expected for NQI in general, many-body effects are found to be small. Results will be presented for the nuclear quadrupole coupling constants (e2qQ) and asymmetry parameters (η) for the nucleobases in the various systems, and trends in e2qQ and η in the different systems will be discussed. Our results show that there are substantial changes in the NQI parameters e2qQ and η, at the positions of the nuclei, on going from free nucleobases to the nucleobases attached to single strand DNA (sDNA), between the latter and the nucleobases in double strand DNA (dsDNA) and between free nucleobases and solid nucleobases. Our results for the 17O NQI parameters in the solid nucleobases agree well with experimental results [6] obtained by the magic angle spinning nuclear magnetic resonance technique. Comparison with the results of an earlier theoretical investigation [6] on the solid nucleobases with our theoretical results will be presented and discussed.

It is hoped that the results of experimental measurements of NQI parameters for 17O nuclei in these nucleobases for single strand and double strand DNA and for other nuclei (14N and 2H) will be available in the future to compare with our theoretical predictions.

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