

Abstract Submitted  
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**First Principles Study of Nuclear Quadrupole Interactions in Single and Double Chain DNA and Solid Nucleobases** T.P. DAS, R.H. PINK, S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, H.P. SAHA, LEE CHOW, UCF Orlando, M.B. HUANG, SUNY Albany — Nuclear Quadrupole Interactions (NQI) of  $^{17}\text{O}$ ,  $^{14}\text{N}$  and  $^2\text{H}$  nuclei have been studied for free nucleobases and nucleobases in single strand and double strand DNA and in solid state. Our first-principles investigations were carried out using the Gaussian 2003 set of programs to implement the Hartree-Fock procedure combined with many-body effects included using many-body perturbation theory. As expected for NQI in general, many-body effects are found to be small. Results will be presented for the quadrupole coupling constants ( $e^2qQ$ ) and asymmetry parameters ( $\eta$ ) for the nucleobases in the various environments. Trends in  $e^2qQ$  and  $\eta$  in the different environments will be discussed. In the case of the solid nucleobases, comparisons will be made with available experimental data [1] for  $^{17}\text{O}$  nuclei.

[1] Gang Wu et al., J. Am. Chem. Soc. 124, 1768 (2002)

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