

Abstract Submitted
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**Nuclear Quadrupole Interaction Study as a Probe of Interaction
between Nucleobases and Sugar Rings and Phosphate Groups in DNA.**

T.P. DAS, SUNY Albany, UCF Orlando, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Upsala University, Sweden, S.R. BADU, R.H. PINK, SUNY, Albany, K. NAGAMINE, UC, Riverside, E. TORIKAI, Yamanashi University, Japan, H.P. SAHA, LEE CHOW, UCF, Orlando, M.B. HUANG, SUNY, Albany — We have been investigating the influence of the interaction between the nucleobases and sugar rings and phosphate groups in DNA using Nuclear Quadrupole interactions (NQI) of ^{14}N and ^{17}O and ^2H nuclei as probes. We have first simulated the influence of the interaction between a nucleobase and a sugar ring using a CH_3 group attached to the former. For our electronic structure investigations, we have employed the Hartree-Fock-Roothaan procedure using the Gaussian set of programs. Our preliminary investigations have shown that there are comparable indirect and direct effects on the NQI parameters, the former effect referring to the influence of changes in molecular geometries produced by the CH_3 group and the direct effect is due to the electronic interaction between the CH_3 group and the nucleobase. More quantitative results from our current investigations using the actual sugar rings and phosphate groups will be presented as in earlier work by our group[1] for hyperfine interactions of trapped muonium atoms in DNA.[1] R.H. Scheicher et al Physica B 374-375, 448(2006)

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