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**Hartree-Fock Cluster Study of Electronic Structures and Nuclear Quadrupole Interactions in Solid Nucleobases.** R.H. SCHEICHER, Uppsala University, Sweden, ARCHANA DUBEY, UCF Orlando, S.R. BADU, SUNY Albany, H.P. SAHA, UCF Orlando, R.H. PINK, SUNY Albany, K. NAGAMINE, UC Riverside, E. TORIKAI, Yamanashi University, Japan, LEE CHOW, UCF Orlando, T.P. DAS, SUNY Albany, UCF Orlando — In recent work [1] we have studied nucleobases attached to a $CH_3$ group to simulate the influence of their binding to the sugar rings and the phosphate groups in DNA and RNA and the effect of this binding on the nuclear quadrupole interactions of $^{14}N$, $^{17}O$ and $^{2}H$ nuclei. Our results from this work have indicated that for $^{17}O$, the binding to the $CH_3$ group moves our results from the free nucleobases closer to the experimentally observed data [2] in the solid nucleobases. We are now investigating the solid nucleobases by the first –principles Hartree-Fock cluster procedure that we have employed earlier for the halogen molecular solids [3]. Our results for the binding energy of an imidazole molecule in the molecular solid system and the $^{14}N$, $^{17}O$ and $^{2}H$ nuclear quadrupole interaction parameters will be presented.
[1] T.P. Das et al (at this APS meeting), [2] Gang Wu et al, J. Am.Chem. Soc. 124, 1768(2002). [3] M.M. Aryal et al Hyperfine Interactions (to be published).

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