Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Peroxynitrous Acid Dimer: Ab Initio Density Functional Study
RAJEEV PATHAK, Department of Physics, University of Pune, Pune 411007, MH, India — Peroxynitrous acid (PNA) HOONO, isomeric to nitric acid, is a very strong oxidant. A novel *dimeric* hydrogen-bonded cluster of peroxynitrous acid (PNA-D) is proposed herein; *ab inito* quantum chemical investigations performed whereupon lead to several stable structures that have a direct bearing on the reactivity of the participating monomers, quantified in terms of the molecular electrostatic potential. The electron-correlation lending stability to PNA and its dimers is gauged through several density functionals namely B3LYP, B3PW91, M06-2X, M06-L, and ω-B97X, etc.; as well as from popular wave-function based second order Møller-Plesset (MP2) perturbation theory, using the basis sets 6-311++G(d,p) and 6-311++G(2d,2p). The infra-red vibrational spectra reveal spectral shifts and intensity redistribution after dimerization. While the lowest energy PNA-D has a perfect inversion symmetry; the other stable dimers emerge as combinations of monomers in different orientation.

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Date submitted: 31 Oct 2011 Electronic form version 1.4