Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

A Density Functional Study of the Redox Properties of H2TPP Porphyrin[1] DAYLA MORRISON, Physics Department, University of Texas at Arlington, Arlington, Texas, ROBERT THOMAS, Optical Radiation Bioeffects Branch, Bioeffects Division, Air Force Research Laboratory, Fort Sam Houston, Texas, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas — Properties of the ground state of free base meso-tetraphenylporphyrin (H2TPP) have been calculated with various charges using the B3LYP functional and the 6-31+G basis set. The porphyrin skeleton was rippled and saddled and the meso-phenyl rings were twisted to yield the C_{2h}, C_{2v}, D_2, D_{2h} planar and D_{2h} non-planar symmetries and the structures optimized. The ground state structure was found to be of C_{2v} symmetry although the C_{2h}, D_2 and D_{2h} non-planar structures were basically degenerate, a conclusion not supported by experimental data. The C_{2v} structure indicated a nonzero net dipole moment for all levels of charge studied. Increase in negative charge increased the distortion of the H2TPP structure. The Raman spectra was calculated and compared with experimental data.[2] In addition, the results were used to select the most likely binding configuration among a set of solutions yielded by computational docking algorithms. Calculations using higher basis sets will also be presented.

[1] This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525, the Repperger Fellowship Program and the Air Force Office of Scientific Research.

[2] J.E. Parker, R. J. Thomas, D. R. Morrison, L. Brancaleon, *J. Phys. Chem. B*, 2012, 116 (36), pp 11032–11040.

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None

Date submitted: 20 Nov 2012 Electronic form version 1.4