

## Theoretical Study of Substituted Pyrrolidines and Phospholanes in Gas Phase and Aqueous Phases

S. Abdalla<sup>1\*</sup> and M. Springborg<sup>2</sup>

<sup>1</sup>*Department of Chemistry, University of Khartoum, Sudan*

<sup>2</sup>*Physical & Theoretical Chemistry, University of Saarland, Germany*

\* Author for correspondence e-mail: sahar.abdalla@uofk.edu

Different isomers and tautomers of substituted cyclic pyrrolidines and phospholanes have been investigated theoretically in gas and aqueous phases. Special emphasis is put on the relative total energies and on the changes in the structure due to substitution or solvation. The calculations were carried through using the B3LYP/6-31+G(d,p) method. To include the effects of the solvent, we used the pure Polarized Continuum and Discrete/Continuum models. In both solvation models, the Integral Equation Formalism (IEF) version of the Polarized Continuum Model (PCM) of Self-Consistent Reaction Field (SCRF) was used. The molecular cavities were constructed using interlocking spheres centered on heavy (that is, non-hydrogen) atoms. The radius of each sphere was obtained by scaling the corresponding van der Waals radius by a factor of 1.2. In the case of Discrete/Continuum calculations, the values of OFac and RMin parameters of the GEPOL algorithm were changed to 0.8 and 0.5 from 0.89 and 0.2, respectively. In gas phase, the cyclic moiety of these molecules shows clear deviations from planarity. Only moderate changes in the structure due to solvation were found. On the other hand, the solvent affects the relative stability of different tautomers and isomers. The inclusion of explicit water molecules changes the order of stability due to the presence of intermolecular hydrogen bonds.