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Investigation of Lignin Solubilization Using Quantum Chemical Calculations in Constrained Media

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UND UNIVERSITY OF NORTH DAKOTA
COLLEGE OF ARTS & SCIENCES

Undergraduate Showcase

Introduction

Lignin is a classification of organic polymers, that makes up of a large portion of vascular plants. They lie typically within the cell wall of plant cells and aid in the structure of the plants, typically taking the form of the xylem tissue. Lignin is more hydrophobic than other components of the cell wall thus aiding in the plants' ability to manage its water content. Lignin is a desirable polymer due to both its uses and its source. It can be functionalized much easier than coal/oil-based products as well as sourced through agricultural waste. This study aims to understand a solution of H2O and supercritical CO2 specifically developed to dissolve lignin that does not follow normal solvation trends.

Methods

- Software Platform used: Gaussian via UND's HPC Talon
- Chemical Visualization software: Gaussview and Avogadro

Basis Sets
6-31g*
6-311++g**

Theories Used
rHF
MP2
wB97XD
HSE06
PBE
B3LYP
CCSD

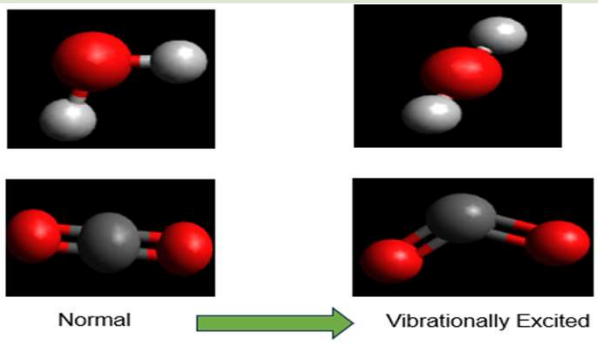

Figure 1 - Example of excited state geometries of both H_2O and CO_2

Results

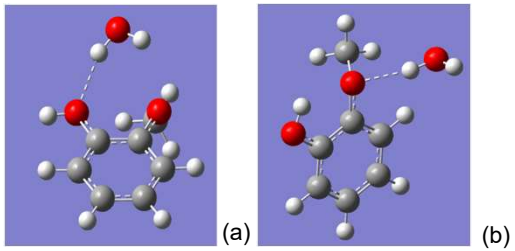

Figure 2 – (Generated by B3LYP (a) and MP2 (b) 6-311++g**) Molecular interactions of Hydroxy group of Guaiacol and Water (a). Interaction of water and methoxy group of Guaiacol (b).

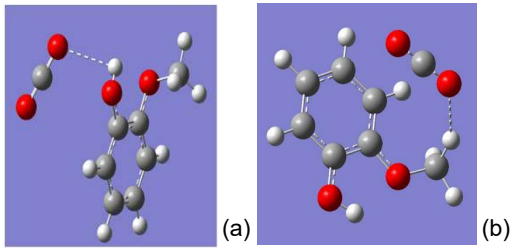

Figure 3 – (Generated by B3LYP (a) and wB97XD (b) 6-31g* and 6-311++g**, respectively) Molecular interactions of Hydroxy group of Guaiacol and CO_2 (a). Interaction of CO_2 and methoxy group of Guaiacol (b).

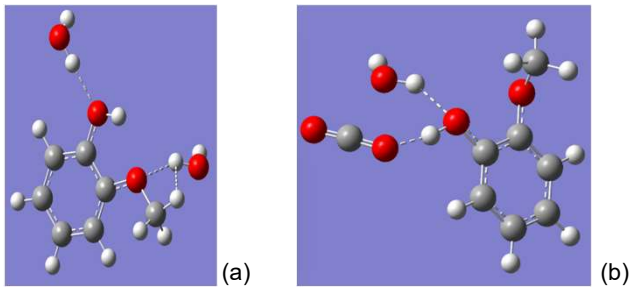

Figure 4 – (Generated by MP2 (a) and rHF (b) 6-311++g** and 6-31g*, respectively) Molecular interactions of two water molecules with methoxy and hydroxy groups of Guaiacol (a). Interaction of CO_2 and H_2O with the methoxy group of Guaiacol (b).

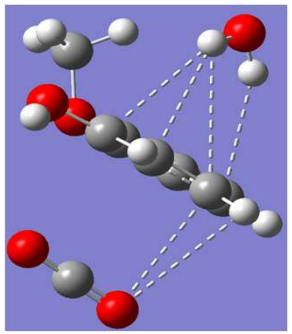

Figure 5 – (Generated by MP2 6-311++g**) Interaction of CO_2 and H_2O with the planer ring of Guaiacol

Future Directions

- Create a simulation of ideally, simulating something as close to the real solution
- Ensemble averaging
- Repeat this process for a more complex Lignin fragment (exp. Vanillin)

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Conclusions

- We have determined the basis of the molecular interactions between Guaiacol and the solvent
- The beginning of the interactions that defy the normal solvation rules (Figure 4b).

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