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L-V | Ab initio Analysis of Ti-catalyzed Phosgenation

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Phosgenation represents a pivotal reaction crucial to the synthesis of polycarbonates (PC). PCs are engineering plastics possessing excellent properties e.g., transparency and impact resistance. The C2P project investigates a novel approach for PC production by utilizing carbon-rich blast furnace gases generated in the steel production industry. This approach replaces conventional carbon sources, thereby benefitting two industries simultaneously. The impurities present in the furnace gas tend to cause undesired colouration in the PCs. Hence, the project focuses on optimising the process minimizing the yield of the colour forming species.

1. Phosgenation reaction network

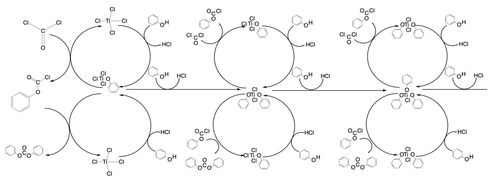


Figure 1: Simplified Phosgenation Reaction Mechanism (Only 3 out of 4 cycles shown, side reactions and impurities are not included in this figure)

Phosgenation is a two-step reaction mechanism:
1. Phosgene reacts with Phenol to form PhenylChloroformate (CASPE).
2. Another Phenol reacts with CASPE to form Diphenyl Carbonate (DPC).

DPC acts as an intermediate for PC production.

To study the reactive system, a comprehensive reaction network is generated and analyzed using Ab-initio calculations.

2. AB initio analyses – A quantum chemistry approach to study reaction kinetics

Following four steps are carried out to calculate reaction rate constants of each reaction in the network:

3. Density Functional Theory (DFT) is used to optimize molecular geometries and find transition states
4. Different conformers are searched
5. Higher level of theory is used to increase accuracy
6. Solvent effects are accounted for in energy calculations

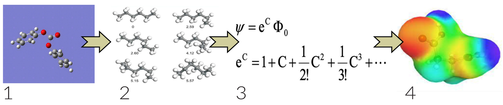


Figure 2: Four-step approach for reaction rate constant calculations

3. Reactor modelling

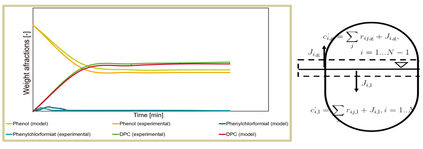


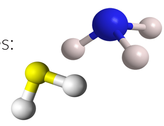
Figure 3: Experimental vs Calculated values

2-phase batch reactor is modelled to help understand relative evolution of the species.
It shows good agreement with the experimental data:
1. Indicates that the key pathways are accurately captured by the computational methodology used.
2. Validates the methodology for the further analysis of the impurities as they have not been studied experimentally.

4. Ongoing work

4.1. Expanding the network

Model compounds for studying impurities:
- Nitrogen based – NH_3
- Sulphur based – H_2S



4.2. UV/Vis spectra

Computational UV/Vis spectra is calculated for all the species postulated in the reaction network. They will be used to determine which species in the system may cause colouration in the system.

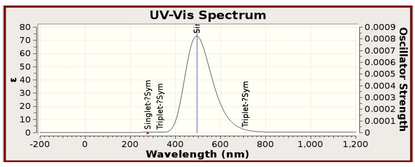


Figure 4: A UV/Vis spectra generated using GAUSSIAN

5. Future Work – Reactor Optimization

- Minimize the yield of the colour forming products
- Control variables = Temperature and Pressure

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