# Gas phase coupling of (thio)urea/urethane: A computational study

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Urea and urethane polymers can be obtained from coupling reaction between [isocyanate, isothiocyanate] and [amine, alcohol, thiol]. Such reaction proceeds spontaneously even without solvent or catalyst, allowing its utilization in vapor-phase methods. It is known that the linker between two terminal functionalities of the monomers can be varied to yield different characteristics of the final polymer products [1]. However, only a few studies so far have systematically investigated the chemistry between different monomers. In this work, reactions between bifunctional reactants were considered using computational chemistry. All calculations were performed using Gaussian 16 with B3LYP functional, D3BJ dispersion correction, and def2-TZVP basis set. It is observed that the activation energy of the reaction is significantly correlated with the proton affinity (gas phase basicity) of the proton-donating monomers (-OH, -NH2, -SH), while the exothermicity of the reaction shows correlation with the gas phase acidity of the proton-donating monomers. Overall, our study provides insights into gas-phase coupling chemistry of (thio)urea/urethane.

[1] Bergsman et al., Chem. Mater. 2017