been proposed based on the radical formation by initiation of polystyrene decomposition. Feasible main products that could be generated from propagating all these pathways include free radicals, styrene, and toluene. The influence of free radical formation on initiation of the pyrolysis mechanism is further investigated to understand the thermal decomposition of polystyrene by potential energy surface scan calculation. Continuous investigations will be carried out to study polystyrene's most feasible pyrolysis mechanism to develop pyrolysis technology for waste plastics.

Keywords: polystyrene, density functional theory, thermal degradation, bond dissociation energy, pyrolysis

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Determination of descriptors for methyl 3-nitrobenzoate using solvation parameter model

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Advancements in chemical industries have introduced many harmful organic chemicals into the environment. It is essential to determine the distribution of these chemicals in the ecosystem for risk assessment. However, some toxic organic substances lack effect or exposure assessment data due to limitations of required experimental data. To overcome this problem, quantitative structure-property relationships (QSPR) can be used to estimate the environmental endpoint values. Abraham solvation parameter model is used as the QSPR model in this research study to determine the descriptors for methyl 3-nitrobenzoate. Methyl 3-nitrobenzoate is a common compound used in the textile industry to produce azo dyes and as a crop protection agent. Descriptor values for methyl 3-nitrobenzoate were determined using gas-liquid chromatographic retention factor values and liquid-liquid partition coefficient values. Isothermal retention factors of methyl 3-nitrobenzoate were determined at 20 °C intervals over the temperature range of 100 °C - 260 °C for 14% cyanopropylphenyl dimethyl polysiloxane gas chromatographic column, and over 100 °C - 240 °C for the 5%-Phenyl 95%-methylpolysiloxane gas chromatographic column. Calibration curves for stationary phases were constructed for each temperature by plotting experimental log (retention factor) versus standard log (retention factor) values considering a wide range of polarities. Standard log (retention factors) for methyl 3-nitrobenzoate at each temperature were determined by determining the experimental log (retention factor) for methyl 3-nitrobenzoate and correlating it to the standard value using the calibration curves. Partition coefficients were determined using eleven different biphasic systems. Descriptor values were determined using solver algorithm in excel such that the standard deviation would be minimum. Determined descriptor values are E = 1.15, S = 1.47, A = 0.00, L = 6.08, B = 0.61, V = 1.25 with 0.06 standard deviation.

Keywords: Methyl 3-nitrobenzoate, QSPR, Solvation parameter model, Descriptors, Gas-liquid chromatography