

Adsorption Enthalpies of Nitrogen Heterocycles on Polymer Surfaces by Gas Chromatography

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Gas chromatographic (GC) techniques are used to determine solution enthalpies, ΔH_{Sol} , for a series of nitroaromatic explosives and explosive degradation products. Five commercially available GC stationary phases were evaluated with 13 nitroaromatic compounds, including including nitrobenzene, 2-nitrotoluene, 3-nitrotoluene, 4-nitrotoluene, 1,2-dinitrobenzene, 1,3-dinitrobenzene, 1,4-dinitrobenzene, 2,4-dinitrotoluene, 2,6-dinitrotoluene, 3,4-dinitrotoluene, 3,5-dinitrotoluene, 1,3,5-trinitrobenzene and 2,4,6-trinitrotoluene. To facilitate development of a predictive model, the ΔH_{Sol} of several *n*-alkanes were also determined as well as the Kováts retention indices for both the nitroaromatics and *n*-alkanes. Using the experimental data, various empirical correlations were attempted to describe the measured ΔH_{Sol} of nitroaromatic compounds including linear solvation energy relationships. Both solute and solvent descriptors were evaluated; however, the explosive-polymer systems were best described modeling relative molecular mass (RMM) of the explosives with the McReynolds constants for each of the respectively stationary phases. The described model serves as a first order approximation for predicting ΔH_{Sol} on polymer surfaces.