

## Measurements and Modeling of Adsorption Enthalpies of Explosives and Taggants on Polymer Surfaces

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Increased efforts to detect and identify explosive residues are hampered by the limited availability of experimentally determined thermophysical data for explosive compounds and their degradation products. Gas chromatographic (GC) techniques are used to determine the enthalpy of solution,  $\Delta H_{Sol}$ , for a series of nitroaromatic explosives and explosive degradation products. Five stationary phases, namely polydimethylsiloxane (PDMS), 80 % dimethyl – 20 % diphenyl polysiloxane (DM80.DP), 14 % cyanopropylphenyl – 86 % dimethyl polysiloxane (CP14.DM), 50 % phenyl – 50 % methyl polysiloxane (P50.M) and polyethylene glycol (PEG) were evaluated with the 13 nitroaromatic compounds. Isothermal Kováts retention indices are also reported for the nitroaromatics as well as the  $\Delta H_{Sol}$  of several n-alkanes. Using the experimental data, an empirical correlation was found relating the  $\Delta H_{Sol}$  of nitroaromatic compounds to their relative molecular mass (RMM) and a parameter involving McReynolds constants for each of the stationary phases. The model was tested over a range of temperatures. At 160°C, the predicted versus experimental  $\Delta H_{Sol}$  values using this model had an  $R^2$  value of 0.9266. It is proposed that this model serves as a first order approximation for predicting  $\Delta H_{Sol}$  on polymer surfaces similar to GC stationary phases where direct measurements are unavailable.