Adsorption Enthalpy of Explosives and Taggants on a Polymeric Surface

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Since many in-the-field explosive sensors rely on vapor-phase detection methods, our ability to effectively verify the presence of explosive materials relies on the assumption that these compounds have a significant enough vapor pressure. Unfortunately, most explosives and their residues have very low vapor pressures. Moreover, it is very rare to find the compounds present in a pure form, where the volatility of the bulk compounds would govern the vapor-phase concentration. Explosive compounds will, in general, be deposited on a surface. Therefore, to develop a predictor of sensor efficiency, one must consider the surface explicitly. The most fundamental parameter that can describe the surface interaction is the respective enthalpy of the interaction, ΔH. On a practical level, this will be either the enthalpy of solution, $\Delta HSOL$, or the enthalpy of adsorption, $\Delta HADS$, for these compounds on the surfaces that they have settled upon. At present, these important physical-chemical data are lacking for explosive compounds. In this talk, we report the $\Delta HSOL$ for four high explosive compounds and three taggants on a polydimethylsiloxane capillary column stationary phase. The $\Delta HSOL$ for the high explosives, TNB, TNT, RDX, and HMX were measured to be 57.85, 59.48, 62.36, and 72.1 kJ/mol, respectively. For the taggants 2-NT, 3-NT, and 4-NT, we measured 49.8, 50.7, and 51.0 kJ/mol, respectively. In addition, the Kováts retention indices, which compare the behavior of these compounds with n-alkanes, were measured over the temperature range used to determine the $\Delta HSOL$. We demonstrate that capillary gas chromatography is an effective metrology, using stationary phase materials as surrogates for representative matrices and surfaces associated with consumer products, personnel, and shipping containers. While preliminary in nature, the report of this extremely valuable data is needed as part of the overall effort to counter immediate terrorist threats.