Identification of Vapor Pressure Traces of Energetic Materials (EMs) and Cosmetics Nitro Musk Molecules via Signature Spectroscopic Properties for Homeland Security Applications

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The aim of this research project is to explore physical-chemical properties of various explosive materials (EMs) at the microscopic (i.e., quantum mechanical) level. This investigation will address differences and similarities in the vibrational spectra of explosives and common nitro musk cosmetics molecules with particular attention to their spectroscopic behavior in the THz region of the infrared (IR) spectrum (0.1-10 THz, 3.33-333 cm^{-1}). EMs under investigation are TNT, RDX, HMX, TATB, PETN, FOX-7, and EGDN; nitromusks include musk moskene, musk tibetene, musk xylene, ambrette, and musk ketone. Accurate identification of energetic materials has potential for application in homeland security scenarios, especially if distinctions can be made from similar cosmetic and fragrance molecules. The overarching final objective is to contribute to the compilation of a database of physical-chemical descriptors, which can then be analyzed to distinguish trends and isolate features that allow the identification of each specific molecule.