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Theoretical Study of Chemical Warfare Agent and Reaction Byproduct Molecular Structure: Enabling FTIR Analysis

Alex Balboa US Army DEVCOM Chemical Biological Center **Matthew Browe** US Army DEVCOM Chemical Biological Center
Margaret Hurley US Army DEVCOM Army Research Laboratory **Wesley Gordon** US Army DEVCOM Chemical Biological Center

Vibrational spectroscopy is a valuable tool that enables the study of adsorption and reaction of chemical warfare agents and simulants with surfaces of interest such as existing and emerging filtration and protection materials. Fourier Transform Infrared Spectroscopy (FTIR) studies have been performed of chemical warfare agents (CWAs) interacting with militarily relevant surfaces; however detailed assignments of vibrational modes have often been based on a qualitative understanding of the spectroscopic results without a strong theoretical base to support conclusions about interaction and reaction of CWAs with surfaces. To assist in bridging this knowledge gap, high level calculations were performed of the lowest energy structure of an isolated molecule in the gas phase and at 0 K. Vibration harmonic frequency calculations were performed in Gaussian 16 at the B3LYP/def2TZVPPD level of theory. Infrared spectra of CWAs such as VX and its byproducts were determined theoretically and analyzed to perform mode assignments to assist in the interpretation of experimental test results involving emerging protective materials such as metal oxides, metal organic frameworks, and composite materials.

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