NEXT GENERATION CB HAZARD PREDICTION AND CONSEQUENCE ASSESSMENT WITH MULTI-ECHELON DECISION SUPPORT APPLICATIONS

Accurately Predicting Non-covalent Interactions

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There are approximately 5 domains in CBR Defense; Threat Characterization, Detection, Personal Protection, Containment / Decontamination, and Treatment. Understanding non-covalent chemical interactions is a critical part of addressing each of these challenges as they govern how chemicals (agents, biotoxins, TICs, TIMs, and emergent threats) interact with materials present within the local environment; for example, do tires absorb this new agent. Although numerous approaches exist for quantifying molecular interaction energies they are typically computationally expensive, narrow in scope, or provide limited insight into the key parameters governing the interactions. We are utilizing a semi-empirical approach based on 2-body interaction terms to calculate the interaction energy of a given system. Historically, this approach was complicated by the strong dependence of the interaction energy on the separation difference between molecules. Using a homologous (uniformly changing) series, such and linear alkanes, as a reference for the molar volume of a compound with a given molecular weight, the interaction terms can be normalized to a common reference point. This enables the accurate calculation of the interaction energies based on group contributions. A required parameter for the calculation of molecular dispersion forces is ionization energy. Although there is a large amount of data available on adiabatic molecular ionization energies (EI), there are substantial data gaps that hinder the scope of application of the model. To overcome this limitation, we have developed a semi-empirical model for the calculation of EI, based on group additive values based on EIV, where V is the Van der Waals volume of the molecule of interest. The model has very broad applicability (organic compounds containing common functional groups), and has a relative standard error of ≤1.5%, comparable to that of the database from which the terms were derived, outperforming quantum chemical calculations.