160c Molecular Modeling of Chemical Warfare Agents

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In this work, we present recently developed force fields for the chemical warfare agent sarin and its non-toxic analog dimethylmethylphosphonate (DMMP). Grand canonical histogram-reweighting Monte Carlo calculations are used to determine the phase behavior, critical properties and vapor pressures of DMMP and sarin. Partial charges are determined from a ChelpG analysis performed at the MP2/6-311g++(3d,3p) level of ab initio theory. Lennard-Jones parameters for the phosphorous atom are tuned to reproduce the normal boiling point and liquid density of DMMP at 373 and 303 K at 1 bar. The remaining Lennard-Jones parameters for –O, =O and CH3 functional groups are taken from the TraPPE-UA force field. With no additional parameterization, the liquid density at 298 K and normal boiling point for sarin are predicted within 3% of experiment. These force fields are used in grand canonical Monte Carlo simulations to determine adsorption isotherms for DMMP and sarin in graphite slit pores. While both DMMP and sarin exhibit type I adsorption isotherms, significant quantitative differences are found.