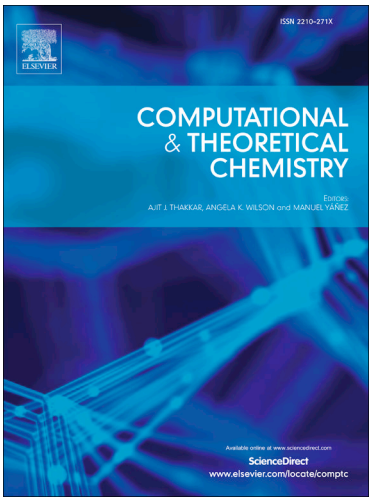

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Abstract

The structural and vibrational analysis of sulfur mustard was performed using second order Møller-Plesset and density functional theory with harmonic and anharmonic force field calculations. The extension to anharmonic calculations provides better agreement between the theoretical vibrational wavenumbers and reported experimental results. At least two conformers co-exist in the experiment is approved by two levels of theory. Based on these possible conformations, most of the relative difference between theoretical and experiment data is less than 1%. The vibrational frequencies were assigned on the basis of potential energy distribution calculation. Furthermore, the terahertz spectrum of sulfur mustard in gas phase was simulated, as well as that of its analogue 2-chloroethylethyl sulfide for comparison.

Key words: Gas phase terahertz spectroscopy; Potential energy distribution; Second-order Møller-Plesset perturbation theory; Density functional theory; Anharmonic calculations