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Trimerization of sulfur trioxide: a density functional theory study

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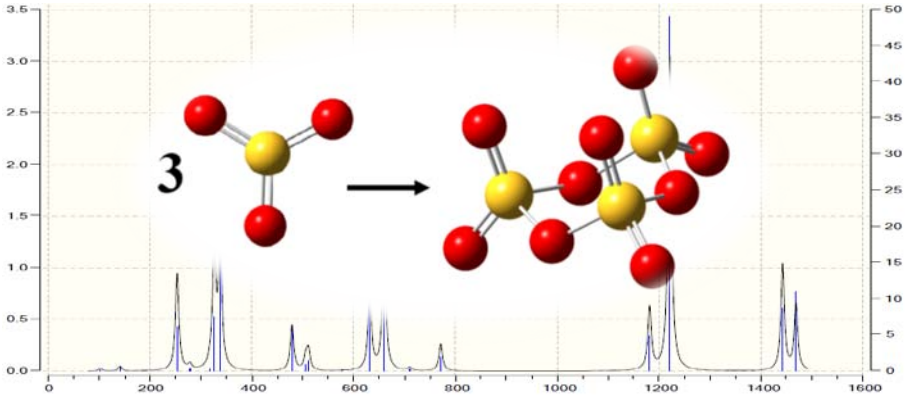
Upon condensation of the pure planar gas SO_3 (D_{3h}) trimerizes spontaneously, which is often called γ-SO_3. It adopts a cyclic structure (C_{3V}) described as $[S(=O)_2(\mu–O)]_3$. The highly electrophilic nature of γ-SO_3 results in insertion reactions into M-C as well as M-O (M = Si**,** Ge, Sn, Pb) bonds under very mild conditions to leave the organic portion of the molecule intact [1-3]. Other experimental and theoretical investigations of γ-SO_3 and its derivatives have been relatively sparse.

Thus, the main objective of the present work is to study the trimerization of SO_3 in the gas phase, with density functional theory (DFT) at the B3LYP/ 6-31G(d) basis set level. The basis set superposition error (BSSE) associated with the polymerization energy was computed via the counterpoise method using the individual bases as fragments [4].



DFT calculations were carried out to predict the structures and vibrational (Raman and infrared) spectra and were compared to the experimental results [5-7]. Theoretical calculations were also carried out for SO_3 and γ-SO_3 for better understanding the intermolecular interactions.

References:

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