VIBRATIONAL FREQUENCIES AND STRUCTURAL DETERMINATIONS OF DI-VINYL SULFONE

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We present a detailed analysis of the structure and infrared spectra of di-vinyl sulfone. The vibrational frequencies of the di-vinyl sulfone molecule were analyzed using standard quantum chemical techniques and compared with recent experimental measurements. Frequencies were calculated at the MP2 and DFT (B3LYP) levels of theory using standard 6-311G* basis set. The molecule exists normally in a C2 configuration. High-energy forms of divinyl sulfone with CS and C1 symmetries also exist. Spectra, structure, and thermodynamics of all three forms of di-vinyl sulfone are presented in detail.