Conformational Equilibria and Molecular Structures of Model Sulfur–Sulfur Bridge Systems: Diisopropyl Disulfide

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The conformations and molecular structures of diisopropyl disulfide have been studied by high-resolution microwave spectroscopy and quantum chemical calculations. Three conformers, G′GG′, G′GT, and GGG′,have been observed in the jet expansion. The global minimum, G′GG′, adopts a configuration with the G′ orientation of H−C−S−S and S−S−C−H and the G orientation of C−S−S−C showing the C2 symmetry. The rotational spectra of monosubstituted ^{13}C and ^{34}S isotopologues have also been recorded for G′GG′,leading to an accurate structural determination of this conformer. Two additional

^{34} S isotopologues have also been measured for G′GT. The relative energies of three observed conformers calculated at the MP2/6-311++(d,p) level of theory are within 2 kJ mol−1, while the relative intensity measurements suggested their population ratio to be NG′GG′/N G′GT/N GGG′ ≈ 5:3:2.

Adres publiczny

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https://www.acs.org/content/acs/en.html