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Ring-Puckering Potential Energy Functions and Structures for Trimethylene Sulfide and Its Monovalent Cation[1] HYE JIN CHUN, ESTHER J. OCOLA, JAAN LAANE, Department of Chemistry, Texas AM University, College Station, TX 77843-3255, USA — The vibrational spectra of trimethylene sulfide (TMS) and the vacuum ultraviolet mass-analyzed threshold ionization spectra of the trimethylene sulfide cation (TMS^+) have been reported. Theoretical computations have been carried out to calculate the structures of both TMS and TMS^+ using ab initio (MP2/cc-pVTZ) and DFT (B3LYP/cc-pVTZ) methods. These calculations were used to predict the coordinate dependent kinetic energy functions for the ring-puckering of both molecules. The kinetic energy functions were then used to calculate the refined ring-puckering potential energy functions for both species based on the previously published spectra. The refined ring-puckering potential energy functions fit the experimental data very well. TMS has an energy barrier of 271 cm^{-1} and energy minima at ring-puckering angles of 29 degree. TMS^+ has a barrier of 60 cm^{-1} and the energy minima at ring-puckering angles of 21 degree. The lower barrier for TMS^+ shows that the cation has lower ring angle strain than TMS itself.

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