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Vibrational Spectra, Theoretical Calculations, and Two-Dimensional Potential Energy Surface for 2,4,7-trioxa(3.3.0)octane HYE JIN CHUN, Dept. of Chemistry, Texas A&M University, College Station, TX 77843-3255, NIKLAS MEINANDER, Dept. of Military Technology, Finnish National Defense University, Helsinki, Finland, JAAN LAANE, Dept. of Chemistry, Texas A&M University, College Station, TX 77843-3255 — 2,4,7-Trioxa(3.3.0)octane (247TOO) is an unusual bicyclic molecule which can exist in four different conformational forms which are determined by which directions the two rings pucker. The vibrational assignments of 247TOO have been made based on its infrared and Raman spectra and theoretical density functional theory (DFT) calculations. The two ring-puckering motions (in-phase and out-of-phase) were observed in the Raman spectra of the liquid at 249 and 205 cm^{-1} and these values correspond well to the DFT values of 247 and 198 cm^{-1}. *Ab initio* calculations were utilized to calculate the structures and conformational energies for the four energy minima and the barriers to interconversion, and the data were utilized to generate a two-dimensional potential energy surface (PES) for the two ring-puckering motions. The resulting quantum state energies for this PES were then calculated in order to better understand the patterns that are produced when the PES has four energy minima at different energy values. The wavefunctions corresponding to the different quantum states were also calculated. For lower energy states these clearly correspond to just one of the wells in the PES. For higher energy states the probability is distributed over more than just one conformational form.

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