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Vibrational Spectra, Theoretical Calculations, and the Two-Dimensional Potential Energy Surface of 2-Cyclopenten-1-one Ethylene Ketal HONG-LI SHEU, Dept. of Chemistry, Texas A&M University 77843-3255, NIKLAS MEINANDER, Dept. of Military Technology, Finnish National Defense University, Helsinki Finland, JAAN LAANE, Dept. of Chemistry, Texas A&M University 77843-3255 — The bicyclic spiro molecule 2-cyclopenten-1-one ethylene ketal (CEK) was studied by infrared and Raman spectroscopy. Density functional theory (DFT) calculations were utilized to compute the theoretical spectra and excellent agreement with the experimental spectra was observed. The structures and conformational energies for the two pairs of conformational minima, which can be defined in terms of ring-bending (x) and ring-twisting (τ) vibrational coordinates, were also calculated. Utilizing the results from *ab initio* MP2/cc-PVTZ computations, a two-dimensional potential energy surface (PES) was established. The energy levels and wavefunctions of the PES were then calculated and their characteristics were analyzed. At lower energies all of the quantum states are doubly degenerate and correspond to either the lower energy conformation L or to conformation H which is 154 cm^{-1} higher in energy. At energies above the 264 cm^{-1} barrier, the wavefunctions show that the quantum levels have significant probabilities for both conformations.

Jaan Laane
Dept. of Chemistry, Texas A&M University

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