

WEAK INTERACTIONS AND CO₂ MICROSOLVATION IN THE CIS-1,2-DIFLUOROETHYLENE...CO₂ COMPLEX

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The need for a deep understanding of CO₂ interactions is significant given the importance of supercritical CO₂ (sc-CO₂) as a green solvent. Fluorinated compounds often have higher solubility in sc-CO₂ than their hydrocarbon analogs, and the reasons for this are not well understood. Investigations of dimers of one CO₂ molecule with a simple fluorinated hydrocarbon provide an initial step towards understanding the complex balance of forces that is likely to be present as a larger solvation shell of sc-CO₂ is built.

The weakly bound dimer *cis*-1,2-difluoroethylene...CO₂ is the latest in a series of complexes of CO₂ with fluorinated ethylenes that has recently been studied using chirped-pulse (CP) Fourier-transform microwave spectroscopy. Unlike all previous members of the series, the observed structure of *cis*-1,2-difluoroethylene...CO₂ is nonplanar, with CO₂ sitting above the ethylene plane and crossed relative to the C=C bond. This nonplanar arrangement is consistent with predictions made using symmetry adapted perturbation theory (SAPT), where the dispersion energy of the nonplanar structure is significantly more favorable than for a structure where CO₂ lies in the same plane as the ethylene moiety. Observed transitions are doubled as a result of CO₂ tunneling between equivalent positions above and below the ethylene plane, leading to inversion of the μ_c dipole moment component. Observed transitions for the most abundant isotopologue have been fitted to a two state Hamiltonian to give an energy difference between tunneling states of $\Delta E \approx 333$ MHz, and analysis using Meyer's one dimensional model to determine the barrier to inversion is presently in progress.