STUDYING CO_2 SOLVENT PROPERTIES BY MICROWAVE SPECTROSCOPIC INVESTIGATION OF FLUOROETHYLENE...CO_2...CO_2 TRIMERS

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Supercritical carbon dioxide (*sc*-CO_2) is an increasingly common green solvent, so it is important that its physical properties are well understood. In the present study, chirped-pulse Fourier-transform microwave (CP-FTMW) spectroscopy was used to study weak hydrogen bonding interactions in complexes of fluoroethylene (FE) with CO_2. Previous investigations of 1:1 dimers of CO_2 with FE observed two isomers for FE...CO_2. Our current focus is analysis of weakly bound trimers, and FE...CO_2...CO_2 was recently observed in the 2 – 8 GHz range using the CP-FTMW spectrometer at the University of Virginia. Four structures were optimized at the MP2/6-311++G(2d,2p) level. As with FE...CO_2 dimer, spectra of two trimer isomers were observed experimentally, corresponding to the two lowest energy ab initio structures, which lie within 25 cm^{-1} of each other. Although only planar forms of the isolated FE...CO_2 dimer were observed experimentally, both trimer structures trap a nonplanar dimer fragment, with one CO_2 molecule located above the plane of FE. Current work involves analysis of isotopic data to allow detailed structural comparisons, as well as searching for larger CO_2 clusters to explore structural changes as the number of solvating CO_2 molecules increases. Extended cross correlation and other techniques are being applied to assist assignment of the thousands of lines remaining in the scan and to suggest the carrier of a recently identified spectrum in the FE/CO_2 mixture.