

MODELING CO₂ MICROSOLVATION: MICROWAVE SPECTROSCOPIC STUDIES OF DIFLUOROETHYLENE (DFE)/CO₂ CLUSTERS, (DFE)₁(CO₂)_x, FOR A TRIMER, TETRAMER, AND PENTAMER

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Microwave spectroscopy allows for analysis of weakly-bound clusters in a mixture of difluoroethylene (DFE) and CO₂. The present study probes variations in interactions and orientations of DFE and CO₂ within weakly-bound clusters as cluster size increases. Four chirped-pulse FTMW spectra of DFE/CO₂ mixtures were obtained from 2-8 GHz, where the concentration of CO₂ was varied from 1% to 4%, with a constant DFE concentration of 1%. This experimental design allowed variation in intensity to be observed based on the variation of CO₂ concentration, where the pattern of intensity variation was used to identify transitions belonging to a particular cluster. In addition, patterns of intensity variation provided information about the size and DFE:CO₂ ratio of the cluster. Using these methods based on intensity variation analysis,^a three separate sets of transitions, each with unique intensity variation patterns, were extracted from the original raw spectra. Cluster composition was hypothesized based on further evidence from the intensity variation analyses, leading to compositions of (DFE)₁(CO₂)₂, (DFE)₁(CO₂)₃, and (DFE)₁(CO₂)₄. Fitted rotational constants for the spectra were compared to the results of ab initio calculations, which further supported hypothesized cluster compositions for the trimer, tetramer and pentamer. These results indicate that instead of forming a solvation shell around DFE, CO₂ molecules appear preferably to interact with other CO₂ molecules to form arrangements more closely resembling pure CO₂ clusters, with DFE on the outside of the cluster.

^aH. Fino, R.A. Peebles, S.A. Peebles, C. West, B. Pate, International Symposium on Molecular Spectroscopy (Virtual), Talk FH12, June 25, 2021; R.A. Peebles, S.A. Peebles, P. Kannangara, H. Fino, International Symposium on Molecular Spectroscopy (Virtual), Talk FH13, June 25, 2021