COMPLETION OF THE FIRST SOLVATION SHELL OF CARBON DIOXIDE IN ARGON: ROTATIONALLY RESOLVED INFRARED SPECTRA OF CO_2-AR_{15} AND CO_2-AR_{17}

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There have been a number of theoretical papers on the structures and energetics of CO_2-Ar_n clusters. But in terms of experiment, the only previous spectroscopic results are for n = 1 (extensive work on the CO_2-Ar dimer) and n = 2 (microwave and infrared spectra of CO_2-Ar_2). We have now obtained and analyzed infrared spectra in the CO_2 ν_3 region for a number of clusters in the range n = 3 to 17. Notable among these are CO_2-Ar_{15} and CO_2-Ar_{17}, which mark completion of the first solvation shell for CO_2 in argon. These clusters have highly symmetric structures with D_{3h} and D_{5h} symmetry, respectively, in good agreement with theory. For n = 15, CO_2 is surrounded by five argon rings, each containing three Ar atoms. For n = 17, there are three rings of five atoms each, plus two additional Ar atoms located on the symmetry axis at each end. The observed spectra are symmetric top parallel bands, and both exhibit distinct intensity alternation which helps to confirm their assignment. Observed B-values are 69.93 MHz for CO_2-Ar_{15} and 54.52 MHz for CO_2-Ar_{17}. As usual for symmetric rotors, the spectra are not sensitive to the A constant, but we do obtain precise values for the band origins, and hence the vibrational shifts (relative to free CO_2) as induced by the argon cages.