SPECTRA OF C_6H_6-Rg_n (n=1,2) IN THE 3 MIRCON INFRARED BAND SYSTEM OF BENZENE

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Benzene-noble gas complexes were one of the earliest topics of interest in spectroscopic investigation of van der Waals (vdW) complexes. Smalley et al.[a] observed C_6H_6-$(He)_{1,2}$ vdW complexes in the late 1970s by means of electronic spectroscopy. A recent study on the same species was done by Hayashi and Oshima[b] at higher resolution (250 MHz). Here, we present an extensive infrared observation of C_6H_6-Rg_n (n=1,2) with the rare gas being He, Ne, or Ar, in the 3 micron region. The spectra were observed using a tunable optical parametric oscillator to probe a pulsed supersonic-jet expansion from a slit nozzle.

Benzene monomer is known to have a complex band system in this region.[c] The strongest band, centered around 3047.91 cm^{-1}, belongs mainly to the C-H stretching fundamental ν_{12} of symmetry E_{1u}. Other strong perpendicular bands occurring just above the main band as a result of intensity borrowing via anharmonic resonances between the fundamental ν_{12} and the combinations are $\nu_2 + \nu_{13} + \nu_{18}$, occurring near 3079 cm^{-1}, and $\nu_{13} + \nu_{16}$ and $\nu_3 + \nu_{10} + \nu_{18}$, both occurring near 3100 cm^{-1}. The latter two bands are separated by merely 1.45 cm^{-1}. Although data analysis and observation are presently ongoing, we observe analogous bands for C_6H_6-Rg_n (n=1,2). Spectra were assigned to a symmetric top with C_{6v} symmetry with the rare gas atom being located on the C_6 symmetry axis. Spectra of the C_6H_6-Rg_2 trimers are in agreement with a D_{6h} symmetry structure, where the rare gas atoms are positioned above and below the plane of the Benzene monomer. Although jet conditions have resulted in excellent signal to noise for the dimer and trimer spectra, we have not been able to identify any lines which might be due to tetramers or larger clusters. We intend to pursue the search for large clusters using a cooled nozzle.

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[a] S. M. Beck, M. G. Liverman, D. L. Monts and R. E. Smalley, J. Chem. Phys. 70, 232 (1979).

[b] M. Hayashi and Y. Ohshima , Chem. Phys. 419, 131 (2013).

[c] J. Pliva and A.S. Pine, J. Mol. Spectrosc. 126, 82 (1987).