INFRARED SPECTRA OF OCS-C_6H_6, OCS-C_6H_6-HE AND OCS-C_6H_6-NE VAN DER WAALS COMPLEXES

M. DEHGHANY, J. NOROOZ OLIAEE, MAHIN AFSHARI, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada*; A.R.W. McKELLAR, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada.*

The infrared spectrum of weakly-bound OCS-C_6H_6 is studied in the region of the ν_1 fundamental band of OCS ($\sim$2060 cm^{-1}) using a tunable diode laser spectrometer to probe a pulsed supersonic jet expansion. A very simple band is observed, corresponding to a parallel transition of a symmetric top. It is shifted by -11.1 cm^{-1} with respect to the free OCS monomer. The resulting structure has OCS located along the benzene C_6 symmetry axis in an S-bonded configuration with a center of mass separation of 4.42 Å, in good agreement with previous microwave spectra.[a] The isotopomers OCS-$^{13}C^{12}C_5H_6$ and $OC^{34}S$-C_6H_6 are also observed. Similar bands are observed for the OCS-C_6H_6-He and OCS-C_6H_6-Ne trimers, whose structure is obtained by adding an on-axis rare gas atom to the other side of the benzene. However, the analogous band for OCS-C_6H_6-Ar was not detected, raising the possibility that the stable form of this trimer may not have the same symmetrical structure.

---

[a] U. Dahmen, H. Dreizler, and W. Stahl, *Ber. Bunsenges. Phys. Chem.* **99**, 434 (1995).