INFRARED SPECTRUM OF THE OCS - He COMPLEX NEAR 2062 cm^{-1}

JIAN TANG AND A.R.W. McKELLAR, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada*.

Remarkable results on rotationally resolved spectra of OCS molecules embedded in large helium droplets [1] have stimulated recent interest in the bimolecular complex, OCS - He [2,3]. Higgins and Klemperer [2] observed 10 microwave transitions of the complex with $J \leq 2$. They also carried out *ab initio* calculations of the interaction potential which showed the ground vibrational state to have a T-shaped configuration. The first two excited vibrational states were found to be loosely localized with the He atom at either end of the OCS molecule, though these were not experimentally observed.

Guided by the microwave results, we have observed the infrared spectrum of OCS-He in the region of the ν_1 fundamental of OCS, near 2062 cm^{-1}. The band origin is shifted only slightly (+0.11 cm^{-1}) from that of the OCS monomer, and the rotational energy level pattern is similar in the ground and excited OCS stretching states. We observe J values up to 5, and find that centrifugal distortion effects are large, as noted previously [2]. Unlike other OCS - rare gas complexes, parallel (a-type) transitions of OCS-He are observed to be much stronger than perpendicular (b-type) ones.

References

[1] S. Grebenev, M. Hartmann, M. Havenith, B. Sartakov, J.P. Toennies, and A.F. Vilesov, *J. Chem. Phys.* **112**, 4485 (2000).
[2] K. Higgins and W. Klemperer, *J. Chem. Phys.* **110**, 1383 (1999).
[3] F.A. Gianturco and F. Paesani, *J. Chem. Phys.* **113**, 3011 (2000).