EXCITED BENDING STATES OF HeOCS

KELLY J. HIGGINS, ZHENHONG YU, and WILLIAM KLEMPERER, *Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA 02138*; CARL A. GOTTLIEB, *Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138 and Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138.*

A great deal of research in the area of helium nanodroplet spectroscopy has focused on OCS as the chromophore.[a] Detailed modeling of the behavior of OCS in a nanodroplet depends on an accurate He-OCS intermolecular potential covering the full range of the angular coordinate. Several potentials have recently been presented in the literature,[b,c,d] complemented by experimental work in the microwave[b] and infrared.[e] All three potentials are qualitatively similar, with the global minimum in a T-shaped configuration and two secondary wells at either end of the OCS. The ground state is predicted and observed to be T-shaped, the first excited bending state is predicted to be localized on the O end, and the second excited state is predicted to be localized on the S end. One of the main differences between the three potentials is the predicted energy difference between the ground state and the excited bending states, with the predictions ranging from 4.3 cm^{-1}(Ref. *c*) to 8.8 cm^{-1}(Ref. *b*) for the first bending state. This energy difference reflects both the difference in the relative well depths and the stiffness of the potential in the wells. Molecular beam electric resonance experiments in the mm-wave region are currently underway to determine the exact energy difference between the ground state and the first two excited bending states of HeOCS.

[a] S. Grebenev, J. P. Toennies, and A. F. Vilesov, Science **279**, 2083 (1998).
[b] K. Higgins and W. Klemperer, J. Chem. Phys. **110**, 1383 (1999).
[c] F. A. Gianturco and F. Paesani, J. Chem. Phys. **113**, 3011 (2000).
[d] J. M. M. Howson and J. M. Hutson, J. Chem. Phys. **115**, 5059, (2001).
[e] J. Tang and A. R. W. McKellar, J. Chem. Phys. **115**, 3053, (2001).