QUANTUM CASCADE LASER SPECTROSCOPY OF CARBONYL SULFIDE AND METHANOL ISOTOPOLOGUES IN HELIUM NANODROPLETS

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Superfluid helium nanodroplets present a unique environment for the investigation of the coupling of solvent density to the rotation of embedded molecules [1]. This coupling results in a reduction of the gas phase rotational constant, B_{gas}, by an amount that depends on both the gas phase rotational velocity and the anisotropy of the helium-rotor interaction potential [2]. We can gain insight into the dependence of B_{gas} on the coupling by investigating different isotopologues of a given molecule, such as HCN/DCN [3] (since the interaction potential is approximately the same between them). With this in mind, we recorded the high-resolution infrared spectra of carbonyl sulfide and methanol isotopologues from 4.7 to 5.0 μm, using a newly built spectrometer. This spectral region allows for coverage of the CO stretching and third overtone bending bands of carbonyl sulfide, and the symmetric CD_3 stretching band of methanol. For both systems, we find that the heavier isotopologues couple to more helium density, and explore the connection between the two molecules in terms of their dependence of B_{gas} on the amount of coupled helium density.

[1] S. Grebenev, J. P. Toennies, and A. F. Vilesov, Science 279, 2083 (1998).

[2] S. Paolini, S. Fantoni, S. Moroni, and S. Baroni, J. Chem. Phys. 123, 114306 (2005).

[3] A. Conjusteau, C. Callegari, I. Reinhard, K. K. Lehmann, and G. Scoles, J. Chem. Phys. 113, 4840 (2000).