INFRARED SPECTRA OF He-, Ne-, AND Ar-C_2D_2 COMPLEXES

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Remarkably, there are no previously published experimental spectra of the helium-acetylene van der Waals complex. Apparently, infrared spectra of He-C_2H_2 were recorded around 1990 in Roger Miller's lab, but a detailed rotational assignment was not possible even with the help of two extensive sets of theoretical predictions.[a] Here, we study rare gas-C_2D_2 complexes in the ν_3 region ($\sim$2439 cm^{-1}) using a rapid-scan tuneable diode laser spectrometer to probe a pulsed supersonic slit-jet expansion. The He-C_2D_2 assignment problem is readily apparent: most of the absorption is piled-up in a very narrow region around 2440.85 cm^{-1}, close to the $R(0)$ line of the C_2D_2 monomer. This pile-up is a signature of very weak anisotropy in the helium-acetylene intermolecular potential, leading to almost free internal rotation of the C_2D_2. We are able to achieve a convincing rotational assignment with the help of theoretical energy level calculations based on the intermolecular potential surface of Munteanu and Fernández.[b] So far the results are limited to He-C_2D_2 transitions which correlate with the monomer $R(0)$ transition.

Ne-C_2D_2 also shows a free-rotation pile-up of lines near $R(0)$ which makes assignment tricky. In contrast, Ar-C_2D_2 exhibits more conventional behavior and a normal asymmetric rotor analysis is possible.

[a] T. Slee, R.J. Le Roy, and C.E. Chuaqui, *Mol. Phys.* **77**, 111 (1992); R. Moszynski, P.E.S. Wormer, and A. van der Avoird, *J. Chem. Phys.* **102**, 8385 (1995).

[b] R. Munteanu and B. Fernández, *J. Chem. Phys.* **123**, 014309 (2005).