INFRARED SPECTRA OF He–CS_2, Ne–CS_2, AND Ar–CS_2

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Infrared spectra of weakly bound Rg–CS_2 (Rg = He, Ne, and Ar) clusters formed in a pulsed supersonic slit-jet expansion have been recorded by exciting the CS_2 ν_3 fundamental band ($\sim$ 1535 cm^{-1}) using a tuneable diode laser. Spectra were well fitted to a conventional semi-rigid asymmetric rotor Hamiltonian. The He–CS_2 spectrum was assigned to an a-type band, while spectra of Ne–CS_2 and Ar–CS_2 were well described by b-type bands, indicating a/b axis switching in transition from the He–CS_2 complex to the Ne–CS_2 and Ar–CS_2 complexes. The results show that the complexes have vibrationally averged T-shaped structures. The determined structural parameters along with the observed vibrational shifts are $R = 3.81, 3.57$ and 3.71 Å, $\theta = 80.0, 86.9$ and 86.4° and $\Delta\nu = 0.171, 0.181$ and 0.067 cm^{-1} for He–CS_2, Ne–CS_2 and Ar–CS_2, respectively. Here, R is the distance between the rare gas and the carbon atom, θ is the the angle between R and and the CS_2 axis and $\Delta\nu$ is the vibrational shift with respect to the free CS_2 monomer.