INFRARED SPECTRA OF HYDROGEN CLUSTERS CONTAINING CO, N_2O, OR OCS

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Infrared spectra of small hydrogen clusters containing a single CO, N_2O or OCS molecule have been studied in the 2050 - 2250 cm^{-1}region using a tunable diode laser spectrometer and pulsed supersonic jet source with cooled pinhole or slit nozzles and high backing pressures (< 40 atm). For N_2O and OCS, both $para$- and $ortho$-H_2 clusters were observed (plus HD clusters for OCS [1]). Simple symmetric rotor type spectra were observed and assigned for clusters containing up to N = 7 or 8 hydrogen molecules. There was no resolved K-structure, and Q-branch features were present for $ortho$-H_2 and HD but absent for $para$-H_2. These characteristics can be rationalized in terms of near symmetric rotor structures, very low effective rotational temperatures (0.15 to 0.6 K), and nuclear spin statistics. The observed vibrational shifts can be compared with those from recent observations on helium clusters. The observed rotational constants for $(para\text{-}H_2)_N$-OCS agree well with a recent quantum Monte Carlo simulation [2]. Various mixed clusters were also observed, such as HD-HD-He-OCS and $para$-H_2-$ortho$-H_2-N_2O.
In the case of CO, only $para$-H_2 clusters have been studied so far. With the help of reptation Monte Carlo simulations [3], $R(0)$ transitions have been assigned for clusters containing up to 9 hydrogens for a b-type series, and 14 hydrogens for an a-type series. Theory and experiment agree rather well, except that theory tends to overestimate the b-type energies. The $(para\text{-}H_2)_{12}$-CO cluster, which is calculated to be particularly stable and (relatively) rigid, corresponds to completion of the first solvation shell, and is observed to have the strongest a-type transition.

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[3] S. Moroni, M. Botti, S. De Palo, and A.R.W. McKellar, *J. Chem. Phys.*, in press (2005).