INFRARED ABSORPTION OF NH_3 ISOLATED IN SOLID PARA-HYDROGEN : ADDUCT FORMATION AND NUCLEAR SPIN RELAXATION

YUAN-PERN LEE, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.*

Infrared absorption spectra of NH_3 isolated in solid para-H_2 at various concentrations were recorded and compared with spectra of NH_3 isolated in solid inert gases. Several rotational lines were observed for each vibrational mode. Rotational assignments were made based on line positions relative to the R(0, 0) line of each vibrational mode, behavior upon annealing, and nuclear spin relaxation after a long period. The rotational pattern for the inversion mode (ν_2) of NH_3 isolated in solid para-H_2 is distinctly different from those reported for NH_3 isolated in solid argon or NH_3 in helium droplet; the variation is due to the formation of an adduct $NH_3{\cdot}H_2$. Several absorption bands near 4140 cm^{-1} region were observed and assigned to the H-H stretching modes of these adducts. Quantum-chemical calculations on the vibrational wave numbers and rotational parameters of the adduct further support the assignments. Nuclear spin relaxation of this system is also investigated.