MATRIX ISOLATION ELECTRON SPIN RESONANCE INVESTIGATION OF H_2^+ , H_4^+ , AND THEIR ISOTOPOMERS

KYLE P. DICKERT, MARK A. PITTMAN, JOHN J. BANISAUKAS, LON B. KNIGHT, JR., Department of Chemistry, Furman University, Greenville, S.C. 29613.

Hydrogen cluster ions are of interest as reactants in astrophysical processes and as simple models for theoretical calculations. In this work, H_4^+ and its deuterated isotopomers were isolated in a neon matrix and investigated by electron spin resonance spectroscopy. The various isotopomers were formed by mixing H_2 , D_2 , and HD gases with neon and depositing the mixtures onto a copper rod cooled to 2.6 K. The matrices were then x-irradiated at 60 keV for 30 minutes. Electron spin resonance spectra were recorded for H_4^+ , H_3D^+ , $H_2D_2^+$, HD_3^+ , and D_4^+ at temperatures ranging from 2.6 K to 9 K. These isotopomers could only be formed at 2.6 K, and were very sensitive to changes in temperature. Diatomic hydrogen ions (H_2^+ and HD^+) were also observed at 2.6 K at low sample gas concentrations. Experimental values for the hyperfine interactions were determined by fitting the observed hyperfine structure lines with those obtained from an exact diagonalization of the spin Hamiltonian.