INFRARED SPECTROSCOPIC EVIDENCE FOR $NeHF^+$ AND $HFFH^+$ TRAPPED IN SOLID NEON

CATHERINE L. LUGEZ, MARILYN E. JACOX, and RUSSELL D. JOHNSON III, *National Institute of Standards and Technology, Gaithersburg, MD 20899-8441*.

When a Ne:HF mixture is subjected to Penning ionization and/or photoionization by neon atoms in their first excited states, between 16.6 eV and 16.85 eV, and the products are rapidly frozen at approximately 5 K, the infrared spectrum of the resulting deposit includes absorptions assigned to $NeHF^+$ and $HFFH^+$. Evidence is presented suggesting that neon-matrix shifts may be anomalously large for protonated molecules which are derived from species with proton affinities near or below 550 kJ/mol. The results of earlier *ab initio* studies, as well as those of the present experimental and *ab initio* studies, indicate that the $NeHF^+$ complex is quite strongly bound. The ν_3 absorptions of $NeHF^+$ and $NeDF^+$ are identified, and the $\nu_1 + \nu_3$ absorption of $NeHF^+$ is tentatively identified. An absorption at 3064.7 cm^{-1} has isotopic substitution behavior appropriate for its assignment to $HFFH^+$. Density functional and more elaborate *ab initio* calculations support this assignment.