

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

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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.