

INFRARED SPECTRA OF NITROSAMINE AND ITS CATION TRAPPED IN SOLID NEON

MARILYN E. JACOX and WARREN E. THOMPSON, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD 20899.*

Photoionization and Penning ionization of dilute mixtures of nitrous oxide and hydrogen by neon atoms and their resonance radiation results in the formation of the nitrosamine cation (H_2NNO^+), which can be trapped in solid neon at 4.2 K. B3LYP/cc-pVTZ calculations provide estimates of the energy, structure, and vibrational fundamentals of that species and of the various isomers of the closely related HNNOH cation. Comparison of the observed infrared absorption patterns for several deuterium- and nitrogen-15 substituted isotopomers with the calculated patterns supports the identification of the nitrosamine cation. Electron recombination leads to the stabilization of uncharged nitrosamine, as well. The infrared absorption pattern for that species in the present neon-matrix study confirms and extends the previous argon-matrix identification. Infrared absorptions of the weakly bound ion-molecule complex of H_2O^+ with N_2 and of the van der Waals complex of H_2O with N_2 are also identified.