MATRIX ISOLATION INFRARED OBSERVATION OF THE $HSiN_2$ AND H_2SiN_2 COMPLEXES USING A 121 NM VACUUM-ULTRAVIOLET PHOTOLYSIS SOURCE

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Matrix isolation infrared spectroscopy was used to characterize the complexes of H_2Si and HSi with N_2 that result from the vacuum-ultraviolet photolysis of silane (SiH_4) in cryogenic nitrogen (N_2) matrices. Experiments were performed by depositing mixtures of SiH_4 with N_2 onto a CsI window at 12 K while simultaneously photolyzing the mixture with 121 nm vacuum-ultraviolet radiation from a hydrogen resonance lamp. The infrared bands of the H_2SiN_2 complex observed in these experiments are the N-N stretching mode at 2274.2 cm^{-1} and the H_2Si asymmetric and symmetric stretching modes at 2013.6 and 2009.4 cm^{-1}, respectively. The infrared bands of the $HSiN_2$ complex observed in these experiments are the N-N stretching mode at 2023.9 cm^{-1}, the Si-H stretching mode at 2006.6 cm^{-1}, and the H-Si-N bending mode at 813.7 cm^{-1}. The assignment of these bands to the H_2SiN_2 and $HSiN_2$ complexes is established by performing experiments with isotopic reagents (SiD_4, $^{15}N_2$), by performing matrix annealing experiments (warming to 20 - 30 K and refreezing to 12 K), by performing mercury-xenon lamp matrix photolysis experiments, and by comparison to density functional theory calculations at the B3LYP/aug-cc-pVTZ level.