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(Statement A)
Polynitrogen Chemistry

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Under combined DARPA, AFOSR, NSF, and DOE sponsorship, we have continued our work in polynitrogen chemistry. We have successfully prepared and characterized numerous polyzido compounds, such as As(N₃)₃, Sb(N₃)₃, As(N₃)₅, Sb(N₃)₅, As(N₃)₆⁻, Sb(N₃)₆⁻, Te(N₃)₄, Te(N₃)₆²⁻, P(N₃)₅⁻, and B(N₃)₄⁻, and have studied the combination of N₅⁺ with some of these anions. Most of these compounds are extremely energetic and shock sensitive.

We have studied the reactions of the NF₄⁺ and N₂F₃⁺ cations with HN₃ in HF solution. The synthesis of the N₇⁻ anion was also pursued by preparing and characterizing R₃SiNCl₂ and (R₃Si)₂NCl compounds. Although their chlorine atoms could not be replaced by azido groups, the reaction of the latter with HF/MF₅ resulted in the isolation of salts of the novel monochloroammonium cation.

Enthalpies of formation were calculated for gas phase N₃, N₅⁻, N₅⁺, and N₅⁻ from ab initio molecular orbital theory. Stability calculations were carried out for solid N₅⁺N₅⁻ and N₅⁺N₅⁺, using these values and lattice energy estimates.

The possible existence of FN₅ was studied both experimentally by FT-IR spectroscopy of the volatile decomposition products from the thermolysis of (N₅⁺)₂SnF₆²⁻ and computationally using a RRKM analysis.

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