

# REPORT DOCUMENTATION PAGE

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Christe, Karl (ERC) et al., "Polynitrogen Chemistry"

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Molecular Dynamics Conference

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## 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 polyazido compounds, such as  $\text{As}(\text{N}_3)_3$ ,  $\text{Sb}(\text{N}_3)_3$ ,  $\text{As}(\text{N}_3)_5$ ,  $\text{Sb}(\text{N}_3)_5$ ,  $\text{As}(\text{N}_3)_6^-$ ,  $\text{Sb}(\text{N}_3)_6^-$ ,  $\text{Te}(\text{N}_3)_4$ ,  $\text{Te}(\text{N}_3)_6^{2-}$ ,  $\text{P}(\text{N}_3)_6^-$ , and  $\text{B}(\text{N}_3)_4^-$ , and have studied the combination of  $\text{N}_5^+$  with some of these anions. Most of these compounds are extremely energetic and shock sensitive.

We have studied the reactions of the  $\text{NF}_4^+$  and  $\text{N}_2\text{F}_3^+$  cations with  $\text{HN}_3$  in HF solution. The synthesis of the  $\text{N}_7^-$  anion was also pursued by preparing and characterizing  $\text{R}_3\text{SiNCl}_2$  and  $(\text{R}_3\text{Si})_2\text{NCl}$  compounds. Although their chlorine atoms could not be replaced by azido groups, the reaction of the latter with HF/MF<sub>5</sub> resulted in the isolation of salts of the novel monochloroammonium cation.

Enthalpies of formation were calculated for gas phase  $\text{N}_3$ ,  $\text{N}_3^-$ ,  $\text{N}_5^+$ , and  $\text{N}_5^-$  from *ab initio* molecular orbital theory. Stability calculations were carried out for solid  $\text{N}_5^+\text{N}_3^-$  and  $\text{N}_5^+\text{N}_5^-$ , using these values and lattice energy estimates.

The possible existence of  $\text{FN}_5$  was studied both experimentally by FT-IR spectroscopy of the volatile decomposition products from the thermolysis of  $(\text{N}_5^+)_2\text{SnF}_6^{2-}$  and computationally using a RRKM analysis.