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13. ABSTRACT (Maximum 200 words) The <i>object</i> of this research is to characterize the energetics, spectroscopic properties, and elementary chemical reactions of molecular ions. The approach used will exploit recent developments in <i>ab initio</i> molecular quantum mechanics. Some of the systems to be studied include the species CF_n and $(n=1-3)$, SF_n and $(n=1-7)$, $(HNO_3)_n$, $(H_2O)_m$, $(ClNO_3)$, $(H_2SO_4)_m$, $(HNO_3)_n$, $(H_2O)_o$, and $+CH_4$.			
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"Fundamental Studies of Ions and Ionic Processes"

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I. Summary

The primary thrust of this research during the past three years has been toward the reliable prediction of the electron affinities of molecular species of atmospheric interest. The research has produced many important practical results, for example the electron affinities of all the simple fluorocarbons, chlorine fluorides, and bromine fluorides. Moreover, we have developed theoretical methods that can reliably predict the electron affinities of much larger molecules. Indeed, our computational proof that density functional theory is applicable to negative ions is one of the most surprising results to emerge from electronic structure theory in recent years.

II. Publications Supported by the Grant

(November 1, 1994 - October 31, 1997).

1. Y. Xie and H. F. Schaefer, "The Electron Affinity of CF", *J. Chem. Phys.* **101**, 10191 (1994).
2. C. M. B. Marsh and H. F. Schaefer, "Trimethylamine Alane and its Dissociation Products" *J. Phys. Chem.* **99**, 195 (1995).
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9. C. M. B. Marsh and H. F. Schaefer, "Bisammonia Alane Does Not Incorporate Dative Bonds," *J. Phys. Chem.* **99**, 14309 (1995).

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