REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	May 31, 1995	Annual Report 1 Jun 94 - 31 May 95

4. TITLE AND SUBTITLE

Reactions of atmospheric cluster ions

5. FUNDING NUMBERS

F49620-93-1-0372
61103D
3484/XS

6. AUTHOR(S)

Stephen R. Leone
Veronica M. Bierbaum

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

The Regents of the University of Colorado
Campus Box 19
Boulder, CO 80309-0019

8. PERFORMING ORGANIZATION REPORT NUMBER

AFOSR-TR- 95-0450

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFOSR/~~NC~~NL
Building 410, Bolling AFB, DC 20332-6448

Dr Michael R. Berman

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for Public Release; Distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

A flow-drift tube instrument has been employed to measure the mobilities of five cluster ion systems that have been detected in the earth's atmosphere. The mobilities of $NO^+(H_2O)_{0-2}$, $H_3O^+(H_2O)_{0-3}$, $NH_4^+(NH_3)_{0-3}$, $NH_4^+(CH_3CN)_{0-3}$, and $NO^+(CH_3CN)_{0-3}$ were determined as a function of field strength by the dual ion signal depletion method. For $H_3O^+(H_2O)_{0-3}$ cluster ions, the reduced zero-field mobility decreases by almost equal amounts as a function of n, whereas for the $NH_4^+(NH_3)_{0-3}$, $NH_4^+(CH_3CN)_{0-3}$, and $NO^+(CH_3CN)_{0-3}$ cluster ions, the decrease in mobility with cluster size is more gradual for higher n. A simple geometrical model based on the effective cross-sectional area of the cluster ions is consistent with the observed n-dependence of the mobilities.

14. SUBJECT TERMS

atmospheric cluster ions, flow-drift, mobility, hydronium ion, ammonium ion, nitric oxide ion, water, ammonia, acetonitrile

15. NUMBER OF PAGES 2

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	

AASERT Evaluation Report
F49620-93-1-0372
May 31, 1995

Stephen R. Leone
JILA, University of Colorado
Boulder, CO 80309-0440

Parent Award No.	FA9620-92-J-0072
Amount of parent award prior to AASERT award:	$520,192 (36 months)
Number of full time graduate students one year prior to AASERT award:	2.0
Amount of parent award after AASERT award:	$501,000 (36 months)
Number of full time graduate students one year after AASERT award on parent grant:	1.25
Number of full time graduate students two years after AASERT award on parent grant	0
Amount of funding of AASERT award F49620-93-1-0372:	$102,582 (36 months)
Continuous number of full time graduate students on AASERT award:	1.0

Stephen R. Leone

"REACTIONS OF ATMOSPHERIC CLUSTER IONS"

Annual Technical Report

June 1, 1994 - May 31, 1995

Cluster ions play an important role in the ion chemistry of the earth's atmosphere. For example, clusters with NO^+, H_3O^+ and NH_4^+ as core ions, and with H_2O, NH_3 or CH_3CN as solvating ligands, among many others, have been detected in the earth's troposphere, stratosphere and ionosphere. Although the association and dissociation processes forming these ions are in general well-understood, their mobilities are largely unknown. These values are essential, not only in modeling atmospheric phenomena, but also in providing direct information about the ion-buffer gas interaction potential.

Our selected ion flow tube apparatus has been modified to include a well-defined flow drift region and instrumentation for ion modulation and data acquisition. Core ions are generated in an ion source, mass-selected and injected into the flow tube where they associate with added solvent molecules before entering the drift region. Two drift rings, at known separation, are simultaneously pulsed; the resulting ion depletions are detected with a quadrupole mass filter in a time-resolved manner, as a function of E/N. The measured zero-field mobilities for five cluster systems in helium are summarized in Table 1.

Table 1. Reduced zero-field mobilities ($cm^2\ V^{-1}\ s^{-1}$) of cluster ions at 300K

$A^+(B)_n$	n=0	n=1	n=2	n=3
$NO^+(H_2O)_n$	22.4 ± 0.5	16.8 ± 0.5	12.9 ± 0.3	
$H_3O^+(H_2O)_n$	21.5 ± 0.5	17.6 ± 0.4	13.7 ± 0.3	10.4 ± 0.3
$NH_4^+(NH_3)_n$	22.1 ± 0.6	15.7 ± 0.3	11.4 ± 0.3	10.2 ± 0.3
$NH_4^+(CH_3CN)_n$	22.1 ± 0.6	12.3 ± 0.5	6.8 ± 0.2	6.7 ± 0.2
$NO^+(CH_3CN)_n$	22.4 ± 0.5	12.3 ± 0.3	7.9 ± 0.5	7.9 ± 0.6

The observed size dependence of the cluster ion mobilities can be divided into two classes. For $H_3O^+(H_2O)_n$ with n=0-3, the mobilities decrease uniformly as the cluster size increases; this behavior reflects the systematic increase in the ionic cross section as water molecules add to the planar ionic structure. In contrast, for three other systems, the mobility decreases less dramatically for higher n species, and ions with two and three solvent molecules have similar mobilities. This behavior reflects a "tetrahedral" geometry where the effective ionic cross section increases only slightly during the filling of the first solvation shell. These experimental findings are consistent with simple molecular modeling. We are currently studying the mobilities of clusters with other core ions and solvent molecules, mixed cluster systems and the effect of other buffer gases.