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MECHANISMS OF MULTIPHOTON DISSOCIATION OF MOLECULAR IONS.(U)
NOV 79 M J COGGIOLA , J R PETERSON N00014-76-C-1035
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Multiphoton dissociation, polyatomic ions, infrared absorption, dissociation dynamics.

This report discusses

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The dissociation of molecular ions resulting from infrared photon absorption by highly vibrationally excited molecular ions ~~will be studied~~. Photfragments will be identified and their dissociative lifetime determined where possible. Measurements will also be made of the fragment translational energy distribution results to date on ions such as CF_3I^+, CF_3Br^+, and $C_3F_6^+$ show that a strong correlation exists between this single photon dissociation process and the final step of multiphoton dissociation. Preliminary analysis indicates that the dissociation dynamics follow a simple statistical mechanism.

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SUMMARY QUESTIONNAIRE

ONR Contract N00014-76-C-1035

Mechanisms of Multiphoton Dissociation of Molecular Ions

1. Contract Description

The dissociation of molecular ions resulting from infrared photon absorption will be studied. Photfragments will be identified and their dissociative lifetime determined where possible. Measurements will also be made of the fragment translational energy distributions.

2. Scientific Problem

In contrast to the well-characterized mechanisms of infrared multiphoton absorption and dissociation in neutral molecules, the MPD of molecular ions has only recently been demonstrated and its mechanism and dynamics remain largely unknown. The present study will provide valuable information on fundamental questions of the absorption spectra of molecular ions, the dissociative lifetime of highly excited ions, the dynamical details of the energy redistribution within such ions and the degree to which MPD in ions is a statistical thermodynamic process.

In general, this work will probe, in detail, the nature and properties of highly excited molecular ions, and their absorption of infrared radiation. This will result in a clearer characterization of the quasi-continuum of molecules and of the final step in MPD.

3. Scientific and Technical Approach

Highly vibrationally excited positive ions are formed in an electron impact source and focused into a highly collimated beam. This beam is merged over a distance of ~ 35 cm with the output from a line tunable CW CO_2 laser. Ion fragments resulting from the single photon photodissociation of ions whose initial internal energy was within $h\nu$ of the dissociation limit are identified. High resolution electrostatic energy analysis of the fragments yields the center of mass kinetic energy distribution. Dissociative lifetimes are determined by measuring the photofragment signal over two different path lengths. Photodissociation cross sections are measured as a function of CO_2 laser wavelength to obtain information on the vibrational frequencies of the ions.

4. Progress

The infrared single photodissociation cross section was measured for a wide variety of molecular ions, such as CF_3I^+, CF_3Br^+, $C_2F_5I^+$, $C_3F_6^+$ and $C_6F_6^+$. Many of the ions studied showed very strong resonant absorption behavior which has been identified with the ν_1 symmetric C-F stretch mode of the ion. The dissociation pathway has been confirmed in each case to follow the least endothermic channel, as found in neutral MPD. Dissociative lifetimes were also measured for several ions, and found to correlate qualitatively with molecular complexity. The absorption and subsequent dissociation process observed here is interpreted corresponding directly with the final step in MPD of ions, and hence provides new information on the details of that phenomenon. An estimation of the photodissociation cross section of CF_3I^+ indicates that approximately 0.4% of the ions in the beam have sufficient internal excitation to participate in the observed process. The measured lifetimes and kinetic energy distributions of the fragements correlate with a simple statistical picture of the redistribution of internal energy within an ion.

5. Publications

A paper entitled, "Infrared Photodissociation of Molecular Ions", by M. J. Coggiola, P. C. Cosby and J. R. Peterson has been submitted for publication in the Journal of Chemical Physics.

6. Extenuating Circumstances

None

7. Funds

We anticipate having no funds remaining at the end of the current contract period.

8. Graduate Students and Postdoctoral Personnel

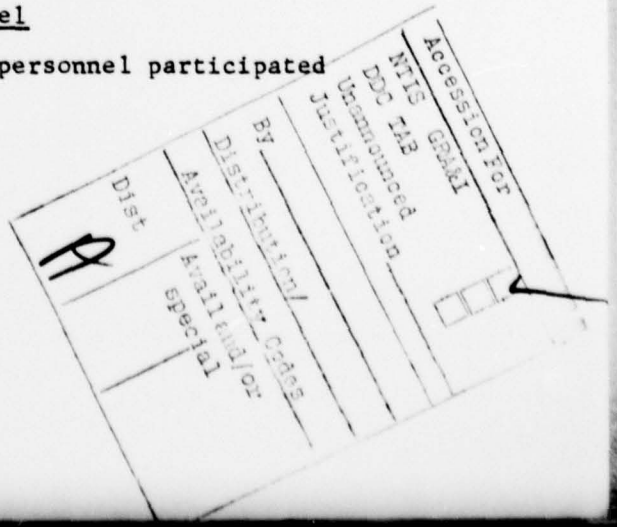
No graduate students or postdoctoral personnel participated in this work.

9. Graduate Student Degrees

None

10. Other Government Support

See accompanying Table.



CURRENT AND PROJECTED RESEARCH SUPPORT

SRI Project No.	Title	Sponsor	Expiration	Annual Budget	Percentage of Professional Time per Project	
7155	Collision Processes Involving Metastable Atoms and Molecules	NSF	5/30/80	$78,000	Peterson Coggiola Hodges	5% 25% 50%
-	Electron Capture and Loss Cross Sections and Angular Scattering of $D^{+,0,-}$ in Cs	DOE	11/1/80	$89,000	Peterson Coggiola Hodges	24% 25% 32%
6772	Properties of Excited States of Molecular Ions	ARO	9/11/80	$50,000	Peterson Cosby	6% 34%
7433/2	Ion Photofragment Spectroscopy	AFOSR	5/30/80	$60,000	Cosby	10%
This Proposal				$55,000	Coggiola Peterson Cosby Hodges	20% 8% 12% 15%