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METASTABLE RARE GAS COLLISIONS WITH MOLECULES.(U)
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Metastable rare gas collisions; metastable helium; excited atom collisions; metastable argon; excited state collisions; ion-pair formation; inelastic scattering; collisional excitation; Penning ionization

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

This report summarizes recent progress in an experimental and computer-modeling investigation of reactive and inelastic scattering of fast metastable rare gas atoms [~~He (2 ^{1}S), He (2 ^{3}S), and Ar $^*_2$~~] Metastable Helium and argon by various target molecules ~~(O_2, I_2, and NO)~~ oxygen, iodine, and nitrogen oxide.

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November, 1980

Metastable Rare Gas Collisions with Molecules

Institution: SRI International

Contracting Agency: Office of Naval Research

Contract Number: N00014-76-C-0734

SRI Project PYU-5389

1. Principal Investigators: K. T. Gillen and D. C. Lorents

2. Contract Description

~~We are investigating~~ the elastic, inelastic, and reactive scattering of fast metastable rare gas atoms by various target molecules properties are being investigated. ~~We are attempting~~ to elucidate the factors important in determining competition between various alternative reaction pathways in these relatively complex systems. Attempts are being made → to Form 1473

3. Scientific Problem

Recent experimental and theoretical progress in two important areas of gas phase collision physics--electronically inelastic atom-atom scattering and reactive scattering on a single electronic potential energy surface--suggests that we are now able to examine seriously the more general system of three or more atoms interacting on several potential surfaces. These most general collisional interactions (usually with one of the reactants electronically excited) have enough complexity, both experimentally and theoretically, that they challenge the most sophisticated tools currently available. Yet these interactions are important in so many areas of gas phase physics (e.g., discharges, lasers, excited atmospheres) that we are required to improve our understanding of the physics involved. If detailed reaction rate information can be generated and understood for a few relatively simple and carefully chosen models systems, comparisons and extrapolations should yield tremendous insight into the reaction channels and mechanisms important in the most general case.

4. Scientific and Technical Approach

Over the past several years, we have developed an atomic beam scattering apparatus capable of detailed differential cross section measurements for interactions involving excited (metastable) rare gas atom beams. In this

particular investigation, we have chosen to apply our advanced experimental beam techniques to the study of collisions involving metastable rare gas atoms and various target molecules. By proper systematic variation of the rare gas projectile and the target molecule, we can explore a wide range of possible interactions and the competition between product channels whose relative importance will vary considerably from one system to another. We can investigate energy-dependent total destruction cross sections (reaction rates), ion-pair formation, Penning ionization, excitation transfer, and the competition between the various channels, often using double-differential cross section measurements to extract the detailed information needed for an understanding of the dynamical processes involved. In addition, we are supplementing our experimental measurements and analysis with a modest theoretical effort designed to explore the same basic phenomena using classical trajectory calculations. The long-range goals of this work are to understand model reactive systems and to use this understanding to gain insight into the most general collision systems involving multiple potential energy surfaces.

5. Progress Nov. 1979 - Nov. 1980

We have used classical trajectory surface-hopping calculations of diabatic surfaces with the inclusion of a competing continuum or pseudo-continuum channel to model and compare the ion-pair formation differential cross section results for Ar^* and K projectiles with I_2 and O_2 target gases. We have demonstrated the relative insensitivity of the product ion distributions to the competing channel in the $Ar^* + O_2$ system. Using analytic formulas for a model two state system, we have explained the origin of the low angle shoulder associated with the main ionic rainbow in many ion-pair reactions. We have also discovered and explained a novel and potentially important mechanism for collisional excitation that is mediated by temporary ion-pair formation and has an energy dependence related to the vibrational period of the transient negative ion.

We have developed a technique for simultaneously and independently investigating ion-pair formation for the projectiles $He^*(2^1S)$ and $He^*(2^3S)$. This neutralization-reionization technique has been applied to the study of $He^*(2^1S)$ and $He^*(2^3S)$ with O_2 over a wide energy range. Work is continuing on reactions of $He^*(2^1S)$ and $He^*(2^3S)$ with NO. The experimental apparatus has

now been interfaced to a computer, which will allow convenient measurements over a wider energy range and faster data processing for both time-of-flight and angular distribution measurements.

6. Publications

a. "Ion-Beam Neutralization-Reionization Spectroscopy of Ion-Pair Formation in Reactions of $He^*(2^3S)$ and $He^*(2^1S)$ with O_2," T. M. Miller and K. T. Gillen, Phys. Rev. Lett. 44, 776 (1980).

b. "Collisional Excitation of $Ar^* + O_2$ Mediated by Ion-Pair Formation," K. T. Gillen and T. M. Miller, Phys. Rev. Lett. 45, 624 (1980).

c. "Comparison of Ion Pair Formation in the Systems $Ar^* + I_2$ and $K + I_2$," A. P. Hickman and K. T. Gillen, J. Chem. Phys. 73, 3672 (1980).

d. "Schematic Model for the Differential Cross Section in Ion-Pair Formation," K. T. Gillen and A. P. Hickman, Chem. Phys. (in press 1980).

7. Extenuating Circumstances

None.

8. Unspent Funds Remaining?

No.

9. Graduate Students

There were no graduate students associated with this work during this contract period.

10. Research Support for K. T. Gillen and D. C. Lorents

Existing SRI Project No.	Title	Sponsor	Expiration	Annual Budget	% of Professional Time Per Project	
7155	Collision Processes Involving Metastable Atoms and Molecules	NSF	6/30/81	$ 78,000	Gillen	30%
1522	Blue-Green XeF(C-A) Laser	DARPA	12/31/81	$ 450,000	Lorents	25%
5389	Study of Metastable Rare Gas Collisions with Molecules	ONR	3/31/81	$ 62,000	Gillen Lorents	33% 5%
1341	Kinetics Processes of High Power Switches	AFOSR/ Texas Tech	10/31/81	$ 85,000	Lorents	12%
Proposals						
80-237R	Electron Capture & Loss Cross Sections... Formation of D^- Beams...	DOE		$130,000	Gillen	5%
80-349 (Ext. 5389)	Study of Metastable Rare Gas Collisions with Molecules	ONR		$ 60,000	Gillen Lorents	25% 3%
80-189	Air Chemistry	ONR/DARPA		$275,000	Lorents	13%