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METASTABLE RARE GAS COLLISIONS WITH MOLECULES. (U)
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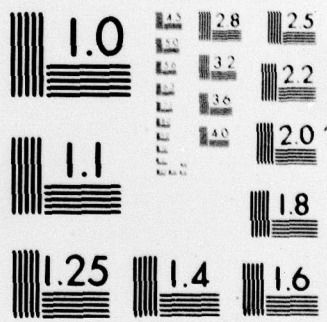
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Metastable Rare Gas Collisions with Molecules

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metastable rare gas collisions; metastable helium; metastable argon; excited state collisions; excited atom collisions; ion-pair formation; collisional excitation; Penning ionization.

This report summarizes recent progress in an experimental investigation of reactive and inelastic scattering of fast metastable rare gas atoms by various target molecules. Detailed investigations have been made of reactions between He*(2¹S), He*(2³S), and Ar* projectiles and O₂ target molecules. Collisional ion-pair formation differential cross sections and electronically and vibrationally inelastic cross sections have been emphasized. Classical trajectory calculations on diabatic potential surfaces have been used to model and interpret the experimental results.

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

Institution: SRI International

Contracting Agency: Office of Naval Research

Contract Number: N00014-76-C-0734

SRI Project FYU-5389

Metastable Rare Gas Collisions with Molecules

1. Contract Description

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

2. 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 model systems, comparisons and extrapolations should yield tremendous insight into the reaction

channels and mechanisms important in the most general case.

3. 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 systematically 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.

4. Progress October 1978 - October 1979

We have been investigating the interactions of $\text{He}^*(2^3\text{S})$, $\text{He}^*(2^1\text{S})$, and Ar^* with O_2 in the collision energy range from ~ 25 eV to 100 eV. For these collisions there are several major competing inelastic and reactive scattering processes. We have measured the detailed double differential cross sections for ion-pair formation in each of these

systems. $\text{He}^*(2^1\text{S}) + \text{O}_2$ is the first system where evidence exists for an ion-pair formation channel involving more than two coupled potential energy surfaces. We have also examined electronic and vibrational excitation in collisions of Ar^* with O_2 and NO targets. We have also made preliminary measurements of branching ratios into the various product channels important in collisional destruction of the fast metastable projectiles.

We have implemented a classical trajectory surface-hopping computer code (originally developed for fast collisions of alkali atoms with diatomic molecules) to model our ion-pair differential cross section data using diabatic potential surfaces. We have extended this code to treat collisions involving metastable rare gases by adding an absorption channel. The computer code has been generalized to three coupled potential surfaces to test and verify our understanding of the ion-pair production process in the $\text{He}^*(2^1\text{S}) + \text{O}_2$ system.

5. Publications

- a. "Ion-Pair Mediated Translational to Internal Energy Transfer in Fast Collisions of Metastable Ar with O_2 ", K. T. Gillen, and T. M. Miller, abstract of a paper presented at the American Chemical Society - Japanese Chemical Society Joint Congress, Honolulu, April 1979.
- b. "Mechanism of Electron Transfer in Fast Collisions of $\text{He}(1s2s^{1,3}\text{S})$ with O_2 ", A. P. Hickman, K. T. Gillen and T. M. Miller, abstract of paper to be presented at the 1979 meeting of the Division of Electron and Atomic Physics of the American Physical Society, Houston, December 1979.

6. Extenuating Circumstances

None

7. Unspent Funds Remaining

We do not expect to have any unspent funds remaining at the end of the current contract period.

8. Graduate Students and Postdoctoral Fellows

The only graduate student involved in this work was Aart Kleyn from the FOM Institute for Atomic and Molecular Physics in Amsterdam, who visited us for six weeks last spring and aided in implementing the classical trajectory program on our computer. Professor Tom M. Miller, from the Physics Department of the University of Oklahoma, also participated in this work as a visiting scientist.

9. Graduate Student Degrees

None

10. RESEARCH SUPPORT FOR K. T. GILLEN AND D. C. LORENTS

<u>Existing SRI Project No.</u>	<u>Title</u>	<u>Sponsor</u>	<u>Expiration</u>	<u>Annual Budget</u>	<u>% of Professional Time Per Project</u>
7155	Collision Processes In- volving Metastable Atoms and Molecules	NSF	5/30/80	\$ 78,000	Gilllen 30% Lorents 5%
4529	Inelastic Collisions of Excited Atoms	ONR	2/28/80*	\$ 55,000	Gilllen 20%
6158	Blue-Green XeF(C-A) Laser	DARPA	2/15/80	\$400,000	Lorents 25%
8916	Krf Fusion Laser Studies (subcontract on DOE Program)	Western Research Corporation	3/31/80	\$ 26,000	Lorents 10%
5389	Study of Metastable Rare Gas Collisions with Molecules	ONR	12/31/79	\$ 58,000	Gilllen 33% Lorents 5%
<u>PROPOSAL</u>					
PYU 78-074R	Electron Capture & Loss Cross Sections... Formation of D Beams ...	DOE		\$ 89,000	Gilllen 5%
PYU 79-065 (Ext. 8916)	Krf Fusion Laser Kinetics & Propagation (to be a sub- contract on a DOE program)	Western Research Corporation		\$500,000	Lorents 40%
PYU 79- (Ext. 6158)	New Blue-Green Laser Systems	DARPA		\$569,000	Lorents 40%
This Proposal (Ext. 5389)	Study of Metastable Rare Gas Collisions with Molecules	ONR		\$ 62,000	Gilllen 33% Lorents 6%

* Terminates