UNCLASSIFIED

AD NUMBER
AD852793
LIMITATION CHANGES
TO: **Approved for public release; distribution is unlimited.**
FROM: **Distribution authorized to U.S. Gov't. agencies and their contractors; Critical Technology; JAN 1968. Other requests shall be referred to Air Force Armament Laboratory, Attn ATWT, Eglin Air Force Base, FL 32542. This document contains export-controlled technical data.**
AUTHORITY
AFATL ltr, 25 Feb 1977

THIS PAGE IS UNCLASSIFIED

AFATL-TR-68-3

AN INVESTIGATION OF ENERGY STORAGE SOLIDS

Dr. R. H. Davis
Dr. J. G. Skofronick
Recon, Inc.

TECHNICAL REPORT AFATL-TR-68-3

JANUARY 1968

This document is subject to special export controls and each transmittal to foreign governments or foreign nationals may be made only with prior approval of the Air Force Armament Laboratory (ATWT), Eglin AFB, Florida 32542.

AIR FORCE ARMAMENT LABORATORY
AIR FORCE SYSTEMS COMMAND • UNITED STATES AIR FORCE
EGLIN AIR FORCE BASE, FLORIDA

56

AN INVESTIGATION OF ENERGY STORAGE SOLIDS

Dr. R. H. Davis
Dr. J. G. Skofronick

FOREWORD

This final report covers work performed during the period October 12, 1966, through October 11, 1967, by Recon, Inc., 694 Industrial Drive, Tallahassee, Florida, 32304, under Air Force Contract F08635-67-C0028 with the Air Force Armament Laboratory, Air Force Systems Command, Eglin Air Force Base, Florida. First Lieutenant John Trossbach (ATWT) was program monitor for the Air Force.

Work was performed by Dr. R. H. Davis and Dr. J.G. Skofronick with occasional but important contributions by other members of the molecular collision physics group at the Florida State University: Dr. D. Robson, Dr. J. Aldridge, Dr. E. Desloge and Dr. J. Sheldon.

Information in this report is embargoed under the Department of State International Traffic in Arms Regulations. This report may be released to foreign governments by departments or agencies of the U.S. Government subject to approval of the Air Force Armament Laboratory (ATWT), Eglin Air Force Base, Florida, 32542, or higher authority within the Department of the Air Force. Private individuals or firms require a Department of State export license.

This report has been reviewed and is approved.

Noble E. Brown

for GEORGE P. BRENNER, Col, USAF
Chief, Weapons Division

ABSTRACT

A microscopic approach to aid further research and exploratory developments in understanding of explosives is discussed. This approach makes use of studies involving the interaction behavior between pairs of molecules. The technique of crossed molecular beam scattering is proposed as the best means to obtain the interaction information. It is argued that the technology of neutral particle beams is now sufficiently advanced that differential cross sections can now be measured. These in turn give very sensitive information about the intermolecular potential. Since the shape of the potential is vital to the understanding of energy storage, this approach is regarded as one involving the basic science of explosives and very likely will provide new avenues and answers to energy storage.

(The reverse of this page is blank)

TABLE OF CONTENTS

LIST OF FIGURES

SECTION I

INTRODUCTION

The subject of explosives can be divided into three parts:

A. Formation

B. Properties (density, elasticity, stability and energy density)

C. Detonation

The work performed under present and preceding contracts with the Air Force Armament Laboratory fits in the first two categories, namely the formation and properties of explosives. The detonation problem is not separate and important connections are made in the discussion of follow-on work.

The objective of this effort is the establishment of a relationship between modern atomic and molecular physics and exploratory development in the formation and properties of new explosives. This relationship is a specialization of the more general problem of understanding chemical reactions and their interplay with chemical structure. The problem is immense as illustrated by Tchoubar's[1] statement in a recent book: "although the electronic theory has led to remarkable progress in this domain, no reactions or mechanisms have been as yet fully elucidated." This statement does not reflect the promise of the new crossed-beam techniques. It is this approach which has been investigated here.

The recent development of high intensity molecular beams and the companion application of molecular collision theory have opened the problem of chemical reactions to definitive investigations. The steps between molecular collision physics studies and exploratory development of new explosives are emerging and a purpose of this report is to define this line of attack and report the progress made during the past year.

Because of the importance and generality of the reaction problem, a research program in molecular collision physics has been initiated at the Florida State University. This program encompasses elastic and reactive molecular collision effects examining both the experimental and theoretical approach. While not all of the Florida State University program is applicable to energy storage, there is considerable overlap. The regions of overlap of this program are interpreted in terms of their importance to explosives in this report.

In Section II the evolution of the problem as approached by Recon, Incorporated, is discussed. A statement of the problem in terms of the most recent developments is given in Section III. The development of a high intensity sonic nozzle beam source, its application in crossed beam scattering experiments, and a short review of elementary scattering theory will be reported in Section IV. An example of the applicability of molecular collision theory in the understanding of the interaction between atoms (or molecules) is given in Section V. The suggested follow-on steps and related topics are considered in Section VI. Section VII is the summary.

SECTION II

EVOLUTION OF THE PROBLEM

Early Work

An explosive may be defined as a material in which the atoms are arranged in states of high potential energy relative to the states formed by the explosion products. It differs from the more general problem of energy storage in that the structure and allowed reaction mechanisms will support a detonation. A practical material is one in which a compromise is struck between high energy storage density and stability against slow dissipative reactions or accidental detonation during ordinary handling procedures.

While mixtures, such as oxygen-rich chemicals with fuels, continue to find important applications as explosives, the emphasis of current development work is on new materials in which the energy storage is understood in terms of the molecular (or crystal) properties. Here the problem reduces to the understanding of a stable system of atoms which are held together by weak bonds but which can, through a rearrangement form strong bonds.

The formation process with respect to the "natural" forms of the atom is endothermic. With respect to the atoms involved, it is a process of entropy reduction. Of the many systems which may be considered on the basis of energetics alone, only a few are obtainable in practical quantities, and the chemical processes for the formation of these systems generally requires several steps.

The early work of Recon, Inc., in this area was primarily concerned with the application of molecular and solid state structure principles to determine the probability of weak-bond attachment of oxidizing and fuel components in a stable molecular or solid state system. The general conclusion arrived at in the early work was that chemical reaction mechanisms were too poorly understood to quantitatively design an explosive material which would take advantage of energy storage mechanisms known in molecular and solid state physics.

Study of Formation of Solids with High Energy Storage

In the next phase of the work, the formation of solids in which atoms with unsaturated strong bonds were arranged and separated by "spectator atomic layers" was considered. Two inherent advantages are apparent at the outset. First, the properties of an ordered array of atoms (a crystal) may be investigated by a number of well-established techniques. Second, reactant atoms or molecules may be delivered to the solid surface where the formation reactions take place with a well defined momentum. The selection of a momentum which is optimum with regard to the desired bond formation is possible. It is also true that a solid substrate possesses intrinsic excitation modes for the take-up of momentum and energy required in certain reactive collisions.

While the surface chemistry approach utilizing well resolved reactant beams remains attractive for several reasons, it was rather quickly found that insufficient information on the scattering of momentum controlled beams (not to mention reactions) is available at this time for even an exploratory development program in new explosive formulations.

A major difficulty has been the absence of beam sources of sufficient intensity and resolution to consider experiments which would lead to the determination of surface potentials and reactive cross sections. Intense molecular beam sources have become available only recently, and the work to date has been principally devoted to the study of engineering surfaces. The necessary vacuum techniques are now established.

Crossed Molecular Beams

To understand the collision mechanisms involved in chemical reactions even if one of the molecules is fixed at the surface of a solid, it appears essential to first understand molecular collisions as individual events. In principle, the necessary technique of crossed molecular beam experiments has been available for some time. In practice, however, progress in the use of crossed-molecular beams to study individual collision events has been slow because of beam intensity and resolution problems. Effusive sources with velocity selectors produce insufficient beams for a general attack on the problem. Supersonic sources are now available which lift the intensity handicap. This is so recent a development that a full utilization of it and signal averaging devices has not been realized.

The work of Recon, Inc. prior to this year carried the investigation up to this point. The problem is cast in terms of recent technological and theoretical developments in the next section.

SECTION III

STATEMENT OF THE PROBLEM

Elastic Scattering and Intermolecular Potentials

As a result of the work reviewed in Section II, a starting point of a research and development program which will lead to exploratory development in new explosive formulations has been defined. It is the measurement of differential elastic scattering cross sections for various collision partners. Potentials extracted from these results determine whether or not bound states exist between collision partners. This is of crucial importance in the determination of whether or not a molecule made up of a given pair of collision partners is long lived and provides a means for estimating the stability. For example, the attachment of an NO_2 group to a given carbon ring may be investigated by this technique. These potentials are also necessary inputs for certain types of reaction cross section calculations.

While the means for measuring a variety of the elastic scattering cross sections is now at hand, few measurements have been made with the precision required to determine intermolecular potentials. Consequently, the experimental work must be initiated at a point rather distance from the applied goal in order to lay the necessary foundation of reliable experimental technique. At the Florida State University a supersonic nozzle has been constructed and a chamber is being designed for molecular collision physics investigations.

Parts of the existing and proposed programs are of importance to the question of energy storage.

The experimental problem may be divided into the following steps:

1. Elastic scattering differential cross section measurements for noble gas collision partners.

2. Differential cross section measurements of simple exchange reaction events.

3. Differential cross section measurements for elastic scattering and reaction where the collision partners are important to energy storage mechanisms.

4. Reactive scattering of molecules from the surface of energy storage solids.

It must be emphasized that point one above is the present state of the art with the exceptions cited in Reactions, Section IV. Not even intermolecular potential between helium atoms is well defined, and the study of such systems is essential to the understanding of collisions between molecular partners. Theoretical and experimental work on the intermolecular potential between helium atoms is under way as part of the more general molecular collision physics program at the Florida State University.

Theory

1. Current Reaction Rate Theories

A reaction rate theory for the formation of weak bonds is needed which will at least explain simple reaction mechanisms and provide a guide for an experimental program in new formulations.

Two theories for reaction rates have been widely discussed and utilized. These are the "collision theory" with which are associated the names Hinshelwood[2], Kassel, Rice, and Ramsperger, and the "activated complex theory" of Eyring[3]. The expressions given for the reaction rate G by these two theories may be written for a pair of particles

$$G = \sigma \left[\frac{8kT}{\pi m^*}\right]^{1/2} \exp\left[-E_o/(kT)\right] \qquad \text{Collision Theory} \tag{1}$$

$$G = \pi r_o^2 \left[\frac{8kT}{\pi m^*}\right]^{1/2} \exp\left[-U(r_o)/(kT)\right] \qquad \text{Activated Complex Theory} \tag{2}$$

where

r_o = separation of particles in transition complex

k = Boltzmann's constant

T = absolute temperature

m^* = reduced mass

$U(r_o)$ = potential characterizing the interaction between the two particles as a function of the separation r_o

E_o = activation energy

σ = collision cross section

An identification of E_o with $U(r_o)$ is apparent in the equations. The reaction is of the general form

$$A + B \longrightarrow C + D \tag{3}$$

where the entrance channel is made up of particles A and B with products C and D, and the potential $U(r_o)$ is related to the potentials for the reactants and the products, respectively, by the equation

$$U(r_o) \approx U_{AB}(r_o) \approx U_{CD}(r_o') \ . \qquad (4)$$

In this sense the potential for the activated complex $U(r_o)$ is the cross over of the two channel potentials. This is of course not true in detail since at least the rearrangement implicit in a reaction will change the radius characterizing the activated complex as suggested by the prime value r_o'. Also penetration effects reduce the value of $U(r_o)$ below the interaction of U_{AB} and U_{CD} as by the solid line, curve 1 of Figure 1. Obviously a necessary input for this analysis is a specification of the potentials $U_{AB}(r)$ and $U_{CD}(r')$. Information about these may be obtained from elastic scattering as well as by other means.

For a given choice of reactants (A,B) and products (C,D), a basin or potential well may be forced as illustrated by curve 2 of Figure 1. Long-lived compound systems may result from the multiple reflections within the basin before a decay into either the entrance or exit channel.

While these theories have been most useful in the discussion of chemical reactions where the collision conditions are specified only in terms of temperature, they do not provide a satisfactory framework for a discussion of reactions in which the momenta (and in the ultimate resolution case, the polarization and the exact quantum states) of the collision partners are controlled. All of the entrance

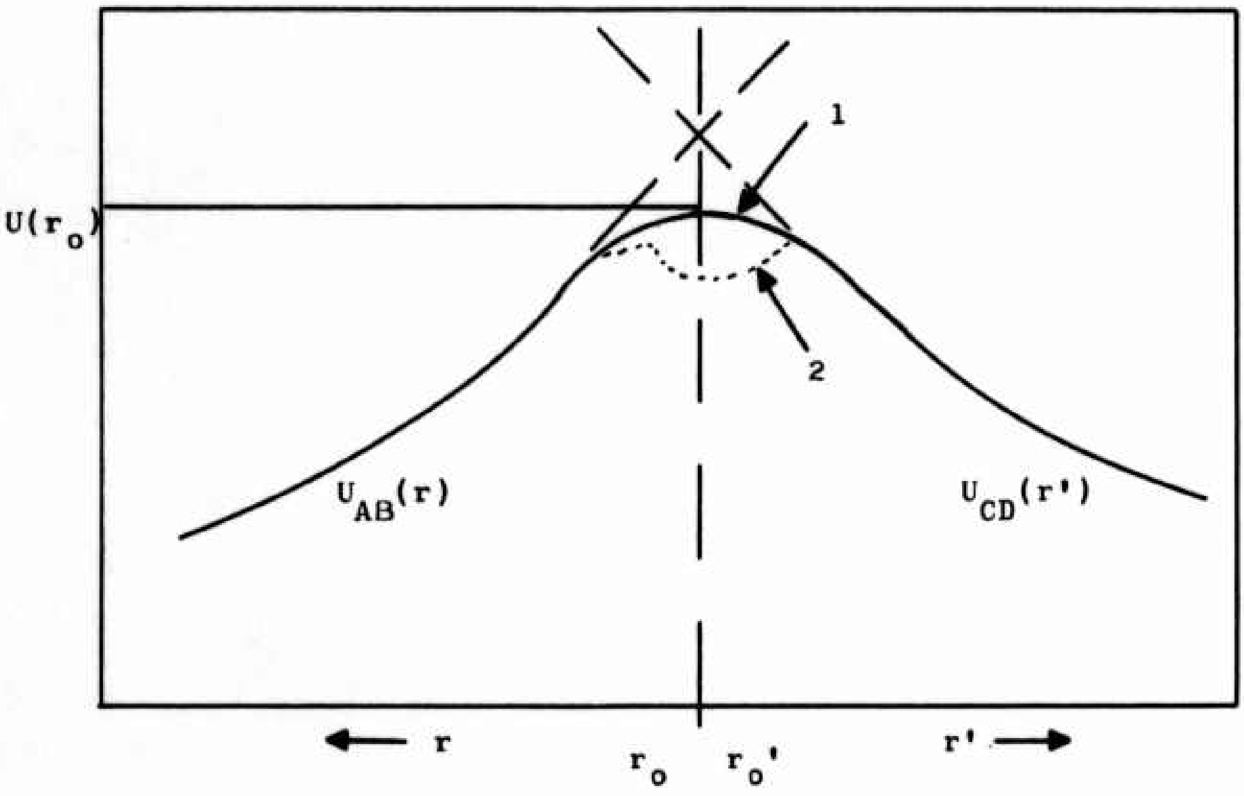


Figure 1. A Pictorial View of the Interaction Potential U (r) vs Intermolecular Distance for a General Chemical Reaction of the Form A+B → C+D, where A and B are the Reactants and C and D are the Products.

channels present in the state distributions for a given temperature are included in these theories. No attempt is made to preferentially form by means of entrance channel selection those collision complex states which are most likely to yield the desired product states. From a molecular collision point of view, the previous two theories are too limited and other approaches should be explored. Several of these are discussed in the next two sections.

2. R-Matrix Theory: Guidelines and Possible Importance

To permit experimental tests, the appropriate theory for the description of formation mechanisms should express in terms of experimentally controllable parameters, the quantum mechanical effects which may be advantageously utilized in the formation of an explosive molecule or solid. The nature of the problem is schematically represented in Figure 2. Here the potential energy for a system of n atoms (n_i of each type) is shown as a function of a parameter S representing the configuration or state of the atoms. The parameter S is not to be interpreted as a separation distance; it depends not only upon the separation distances but also on the type of interaction or coupling among the n atoms. The state S_0 is a state of high potential energy storage, the stability of which is governed by the lowest point of the potential rim about S_0. In this cut through the potential surface the lowest barrier height is labeled B.

By means of a rearrangement or change of state, possibly by an explosion the n atoms making up the system may arrive at states S_1 or S_2. As shown in Figure 2 the largest energy release results from a transition from state S_0 to state S_1. It should be emphasized that this potential is distinct from the potentials discussed in connection with the equation (4) in that this is the system potential energy for a large number of atoms rather than a potential energy for two particles.

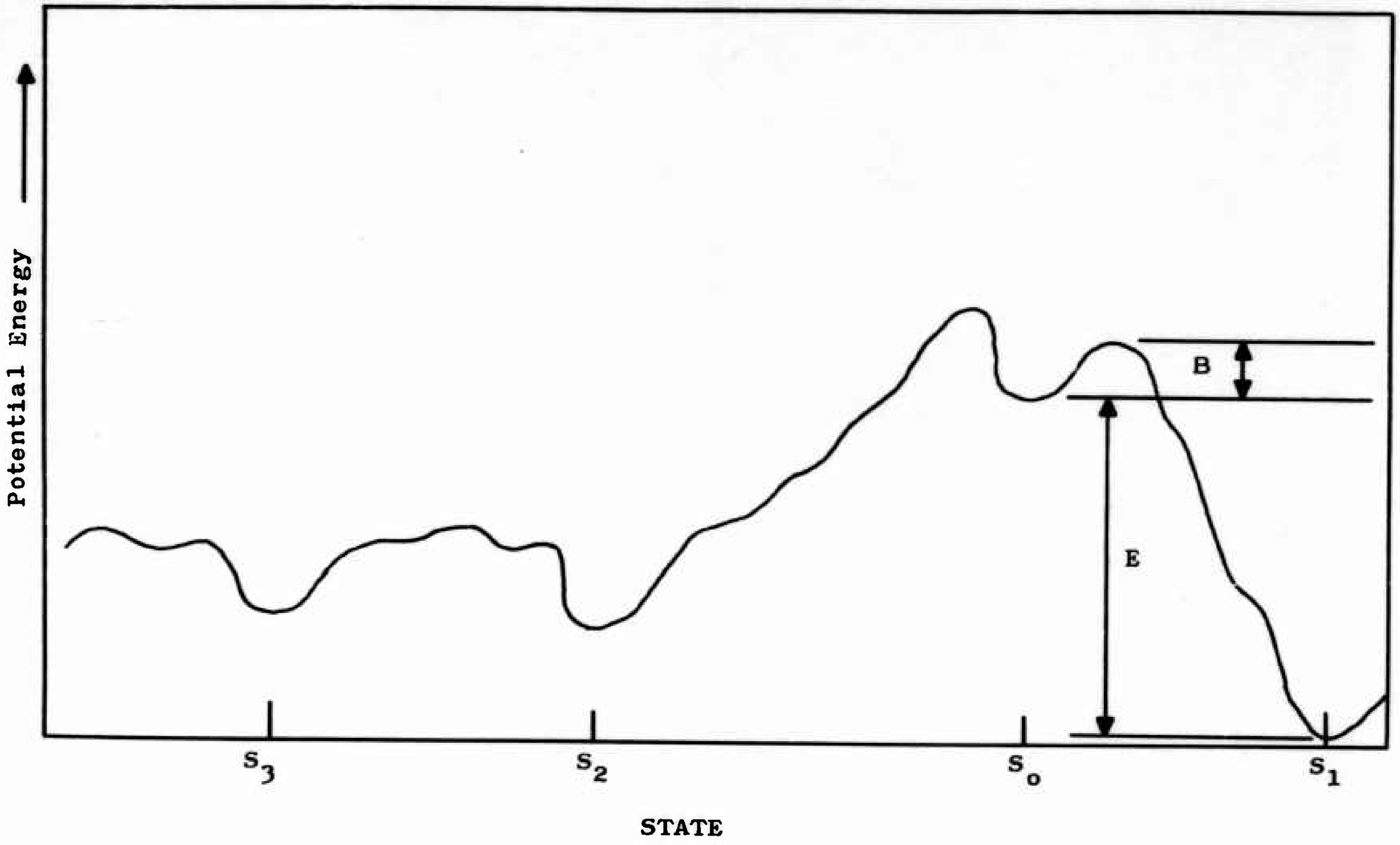


Figure 2. A Representation of the Potential Energy for a System of n atoms as a Function of a General Parameter S which Represents Both Separation and coupling Between the Atoms.

While the system potential energy concept is useful in fixing the objectives of the discussion here, its practical value is restricted to statistical analysis. One general approach to the problem of resonant collision mechanisms is that of R-matrix theory. Several authors have applied the R-matrix theory to chemical problems[4], but to date the most extensive application and development of the R-matrix theory has been to nuclear physics problems, for example the recent comprehensive papers both by Lane and Robson[5].

An objective of this theory is the separation of the energy dependent parts of the cross section from energy independent (or nearly so) parameters which characterize the reaction mechanism. Mathematically, the essential feature of the analysis is the separation of space into an "internal volume" in which the interaction forces are turned on and an "external volume" in which the forces between the particles are assumed to vanish. A variety of reaction mechanisms may be parameterized, such as long-lived intermediate systems (in the nuclear case the compound nucleus), direct reactions, and stepwise reactions which involve more than one identifiable intermediate stage. The theory is especially well suited for resonance reactions whether the resonances occur singly and well isolated (such as the Breit-Wigner resonances theory for nuclear reactions) or in situations where average resonance affects must be taken into account, such as is the case for isobaric analogue resonances.

One disadvantage of the R-Matrix theory, the seriousness of which has not been adequately investigated for the chemical reaction case, is that long range forces are operating in molecular interactions. Additional theoretical study and application to specific data is necessary to define the conditions for validity in terms of molecular collision parameters.

Certain guidelines for the design of experimental equipment are available based on the most general considerations. These are important in the determination of the experimental conditions under which parameters important to the further development of reaction theories may be observed. Inter-molecular potentials are only approximately known at present and it is necessary to assume penetration or transmission factors in order to extract parameters which will guide the experiment. The results of such estimates[6] are shown in Figure 3. These results may be compared with those given by Pauly and Toennies[7].

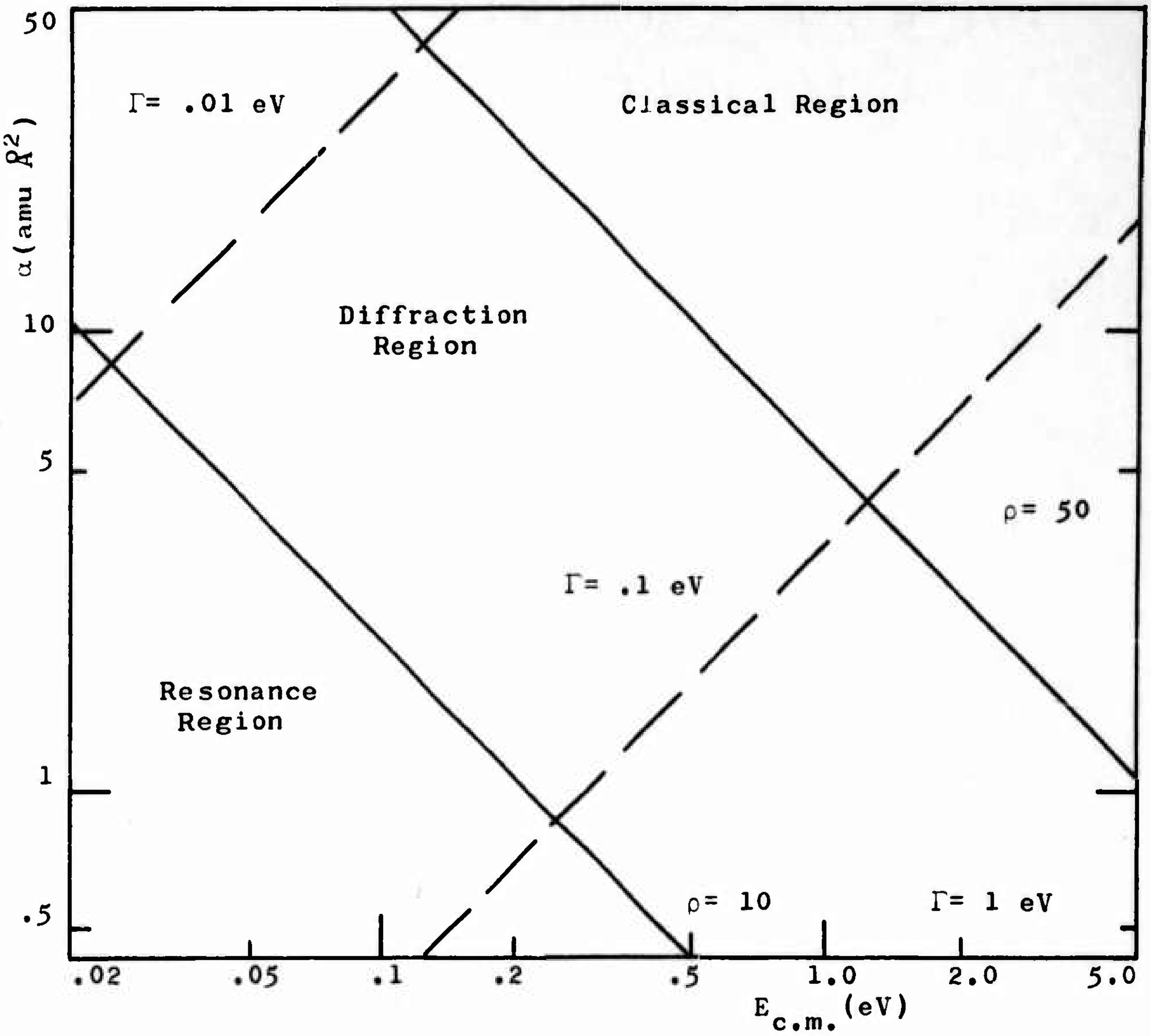
The results given in Figure 3 may be understood as follows:

Each collision can be characterized in terms of a parameter given by

$$\alpha=\mu R^2 \tag{5}$$

where R is the impact parameter and μ the reduced mass given by the expression

$$\mu = M_p M_t (M_p+M_t)^{-1} \tag{6}$$



$$\alpha = \frac{M_p M_t}{(M_p + M_t)} (M_p^{1/3} + M_t^{1/3})^2 \times 10^{-1} \ (\text{Å}^2 \times \text{hydrogen mass units})$$

$\alpha = .209\ E^{-1}$ ($\rho = 10$) $\qquad \alpha = 30E/\Gamma^2$

$\alpha = 20.9\ E^{-1}$ ($\rho = 100$) $\qquad \Gamma = 2\rho\delta^2$

Figure 3. A Plot of Effective Moment of Inertia α vs the Relative Energy Ec.m. This Plot Aids in Identifying the Phenomena to be Expected at the Various α and Ec.m. Combinations. The values of α are determined in Figure 4.

where the collision partners are the projectile with mass M_p and a target with mass M_t. Clearly α represents an effective moment of inertia for the system under consideration, and for the sake of convenience it is assumed to be a simple function of M_p and M_t. To do this, an approximate (but sufficiently accurate for these purposes) expression for the impact parameter R given by

$$R \;=\; 10^{-1/2}(M_p^{\,1/3} + M_t^{\,1/3})\ (\mathrm{\AA}). \qquad (7)$$

This expression yields the distance at which the two molecules just touch, if each molecule (or atom) is assumed to have a radius of $10^{-1/2} \times M^{1/3}$. This approximation gives a reasonable estimate of the size of the molecular atom provided M is in units of the mass of hydrogen atom.

The values of α to be used in Figure 3 may be obtained from Figure 4 where it is plotted against M_t for various projectile masses M_p. Having determined the value of α for a given pair of particles , the type of phenomena expected can be directly read off Figure 3 which indicates the various regions as a function of relative energy E and the parameter α.

In Figure 3, regions bounded by specific values of the parameter ρ are shown. This parameter is simply given by the equation

$$\rho \;=\; kR = \sqrt{\frac{2\mu E}{\hbar^2}} \times R \approx \ell_{max} \qquad (8)$$

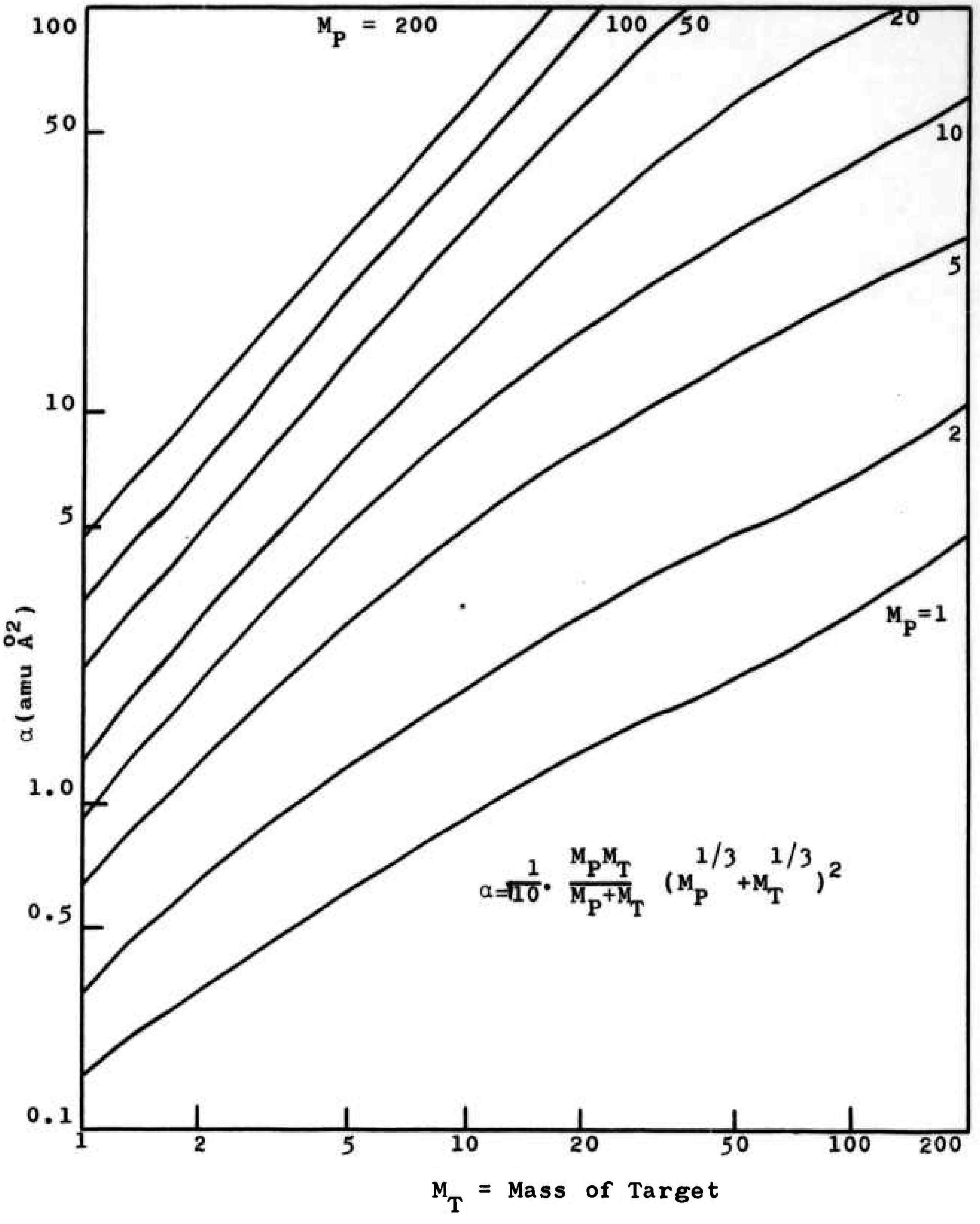


Figure 4. A plot of Effective Moment of Inertia vs the Mass of the Target, M_T, for Different Projectile Masses, M_P.

and it corresponds to the maximum angular momentum ℓ_{max} contributing to the cross section.

The E, α plane is approximately divided by the $\rho = 10$ and $\rho = 50$ lines into three physical regions:

1. $0 \leq \rho \leq 10$. In this "resonance" regions, the cross section should exhibit rapidly varying values as a function of the energy E due to the expected quantum mechanical phenomena of "compound states" in the continuum. High resolution is needed to study such behavior which is vital to an understanding of the nature of chemical reactions.
2. $10 \leq \rho \leq 50$. This is the "diffraction region" in which the cross section will tend to be smoother but the angular distributions of reaction products will still show quantum effects such as are well known in electron diffraction. Such angular distributions will be strongly angle dependent and indicative of the reaction mechanism.
3. $50 \leq \rho \leq \infty$. The "classical region" is a less interesting region where molecules tend to behave more like billiard balls so that the intrinsic structure becomes relatively unimportant.

Finally the E,α plane is divided by values for the "width" parameter Γ which is given by the equation

$$\Gamma = 2\rho \frac{\hbar^2}{\mu R^2} = \frac{4E}{\rho} \qquad (9)$$

The parameter Γ is an estimate of the width of the state in the compound system which exists during the collision process. It is a criteria for establishing the maximum energy resolution which can be allowed if atomic single particle states are to be experimentally detectable. The value of Γ immediately shows the necessity for high energy resolution. Clearly a resolution of $\Gamma/10$ is desirable at all energies. Resolutions of 10^{-2} to 10^{-3} eV would be adequate for all energies of $E = 1$ eV.

Precision elastic scattering studies are needed to determine potentials with sufficient accuracy such that experimental widths may be extracted and from these the intrinsic interaction parameters called reduced widths. Such studies will guide the development of R-matrix applications to chemical reactions.

3. Other Theoretical Approaches

Recently Micha[8] has discussed compound state resonances in atom-diatomic-molecule collisions. His work reinforces the approach developed here in two ways. First, as a result of a detailed discussion of the collision mechanism, resonance states are computed for the system Xe + H_2 and the system Xe + D_2. Second in order to precisely fix the parameters of this collision analysis, experimentally determined potentials for the elastic scattering are needed. The theory is essentially a form of the Feshbach theory, which has been commonly used in nuclear physics for many years.

Another extreme type of reaction has been discussed by Karplus, Porter, and Sharma[9]. For the collision of a hydrogen atom with a hydrogen molecule, their analysis indicates that a direct reaction mechanism is dominant. That is, the collision time is comparable to the transit time of the projectile across the diameter of the target. Such extreme situations are well known in nuclear physics, and it is only a careful measurement of the differential cross section as a function of both angle and energy which generally provides a proper estimate of the relative contributions of resonance mechanisms and direct reaction mechanisms. Here again the need for precision scattering data is a principle requirement for the next step towards understanding the interaction mechanism.

4. General Comments

It is first of all clear that measurements and analyses of elastic scattering, differential cross sections are essential to the formulation of a detailed theory for molecular collisions. Second, several theoretical approaches have already emerged. The one with the greatest generality and computability is that of R-matrix theory, although its applicability to chemical problems is subject to further test. Third, a remark should be made concerning the relationship between structure and reaction mechanism. The two are intimately connected and a better understanding of reaction mechanisms is expected to improve the knowledge of molecular structure. In particular it should shed light on those properties which are of special interest in explosives, that of energy storage, stability, and detonation. It is also clear that present day knowledge of structure is inadequate to explain the radical difference in performance characteristics for systems which are otherwise quite similar in structure. For example, see the discussion by Suzuki[10].

SECTION IV

CROSSED-MOLECULAR BEAM TECHNIQUES

Sonic Nozzle Source Development at F.S.U.

During the past year a sonic nozzle source for the production of high intensity neutral particle beams has been developed and tested by J. G. Skofronick[11]. It is discussed here to illustrate the recent and crucial advance of crossed-molecular beams techniques which are important to the problem of measuring cross sections for explosives research.

The essential point is that neutral beam sources of high intensity and good resolution are now available. With a suitable system comprising two sources, a chamber, and two (or more) detection systems, differential cross sections for a variety of collision partners may be measured and information about the interaction potentials extracted.

Skofronick's source produces N_2, H_2 and He beams with measured intensities of $4x10^{18}$, $3.0x10^{19}$ and $1.5x10^{19}$ particles per (sr-sec) respectively. The velocity resolution is 40%, 14%, and 10% FWHM for N_2, H_2, and He, respectively. Further improvements in velocity can be made by use of velocity selectors with a corresponding loss in intensity.

In a feasibility study of a system utilizing such sources and modern detection techniques the overall sensitivity was estimated to be 10^{-19} cm^2/sr for differential cross section measurements. (This system has not bee constructed yet for lack of funds).

In the remainder of this section, several of the concepts involved in crossed-molecular beam studies are reviewed.

Discussion of Previous Work

As far back as 1925, the possibilities of examining chemical reactions as molecular collision events was considered. Early work on chemical reactions was not successful primarily due to the lack of sophisticated experimental apparatus. A summary of this work along with the scattering experiments of Stern and his colleagues was given by R. Fraser[12].

Since the early work, there has been considerably more attention given to scattering experiments of various types: elastic, inelastic and reactive scattering. Most of the work in reactive scattering has been concerned with reactions of alkali metal atoms with halogen compounds which in turn produce alkali halides[13]. These latter reactions have been examined in the greatest detail for two reasons: 1) the beams may be produced with effusive beam sources and 2) the products can be easily detected by surface ionization techniques.

Elastic Scattering

A collision event is said to be elastic when there is no change in internal energy and when the products remain the same as the reactants. Generally atom-atom scattering at thermal energies is elastic.

The total cross section can be easily defined by considering a beam of particles of velocity g incident opon a chamber of length L which has within it a stationary vapor of density n. Then for an intensity I incident upon a differential volume AdL, a fraction dI of the particles will be scattered according to the relation

$$\frac{dI}{I} = \frac{\sigma^{u}_{tot}(g)\ n\ A\ dL}{A} \tag{10}$$

where $\sigma^{u}_{tot}(g)$ is the total cross section, which is the sum of the elastic, inelastic and reactive cross section and the u represents the possible quantum states of the reactants. (The notation of Pauly and Toennies[7] is used throughout this work).

If equation (10) is integrated from initial beam I_o at the entrance of the chamber to intensity I at the exit end then

$$I = I_o \exp -(\sigma^{u}_{tot}(g)nL) \tag{11}$$

is obtained. Thus if one experimentally measures the decrease in intensity of a steady beam of particles incident upon various densities of scattering particles then a semi log plot of intensity versus density should be a straight line and the slope divided by the chamber length yields the cross section.

In the realistic experimental situation the target particles have motion and this motion must be averaged out. This averaging is usually expressed as

$$\sigma^u_{tot\ eff}(v_1) = \sigma_{tot}(v_1)\ F(x), \tag{12}$$

where the previous cross section defined in equation (11) becomes an effective cross section and v_1 represents the velocity of the monoenergetic incoming beam. The right hand side has two terms: 1) the total cross section dependent only on v_1 and 2) a term F(x) which accounts for the averaging[14]. The variable x is the ratio of the velocity of the incoming particles to the most probable velocity of the scattering gas. Tables have been computed for these functions for velocity dependent cross sections which behave as

$$\sigma^u_{tot}(g) \propto g^{-2/s-1}, \tag{13}$$

where s is a parameter[14]. The s=6 corresponds to a van der Waal interaction potential while $s=\infty$ is that obtained for hard spheres. The case of a velocity distribution in the incoming beam has also been considered but is not necessary for this discussion.

If instead of a scattering chamber a second beam of particles is used as the scatterer, then the intensity over all possible scattering angles Θ and Φ is defined as the differential cross section $I^u_\nu(\Theta,\Phi,g)$ where the ν indicates the type of collision being observed. The integral of the differential cross section over all possible angles is the total integral cross section for the particular type of collision.

This can be expressed as

$$\sigma^{u}_{\nu,tot}(g) = \int I^{u}_{\nu}(\Theta,\Phi,g)d\Omega \ , \tag{14}$$

The total integral cross section is then the sum of the $\sigma^{u}_{\nu,tot}(g)$ over ν.

In any scattering experiment the differential and integral cross sections for the particular type of interaction are the two quantities that are desired.

Since this section is concerned with elastic scattering, further discussions of the inelastic and reaction quantities will be considered in a later section. The elastic cross sections will be discussed briefly from both a classical and quantum point of view. It will be observed that considerable information can be obtained from just a classical approach, but eventually quantum effects necessitate the quantum mechanical approach.

1. Classical Elastic Scattering

While the correct theoretical approach involves the quantum mechanical solution of Schrodinger's equation, there is still reason for examining the classical analog for it gives similar results as the quantum case for large angle scattering. However, this approach fails at small scattering angles and an exact approach is necessary. The full quantum mechanical treatment does give the correct results but this is hard to illustrate in a closed mathematical form. To circumvent this problem, a semi-classical approach which gives considerable information will also be discussed.

If we consider a classical central force situation between two bodies of mass m_1 and m_2, then conservation of energy stated in polar coordinates r and θ gives

$$\frac{\mu}{2}\,(\dot{r}^2+r^2\dot{\theta}^2) + V(r) = E\ , \qquad (15)$$

where the reduced mass $\mu=\frac{m_1m_2}{m_1+m_2}$, r is the relative coordinate between m_1 and m_2, V(r) is the potential energy and E is the total energy. This reduced mass case means that the motion of particle 1 as observed from particle 2 appears as if particle 2 were fixed and particle 1 had a mass μ. By using conservation of angular momentum and the impact parameter b, the following expression for the angle of deflection θ results

$$\theta = \pi - 2\int_{r_{min}}^{\infty} \frac{dr}{r\sqrt{\frac{r^2}{b^2}\,(1-\frac{V}{E})-1}}\ , \qquad (16)$$

where r is integrated from the apsidal distance r_{min} to r = ∞. It is conventional to use reduced parameters as follows:

a) $\beta = \frac{b}{r_m}$ (reduced impact parameter),

b) $\rho = \frac{r}{r_m}$ (reduced distance between particles),

c) $K = \frac{E}{\epsilon}$ (reduced energy), and

d) $U(\rho) = \frac{V(\rho)}{\epsilon}$ (reduced potential energy),

where the newly introduced parameters are defined in Figure 5.

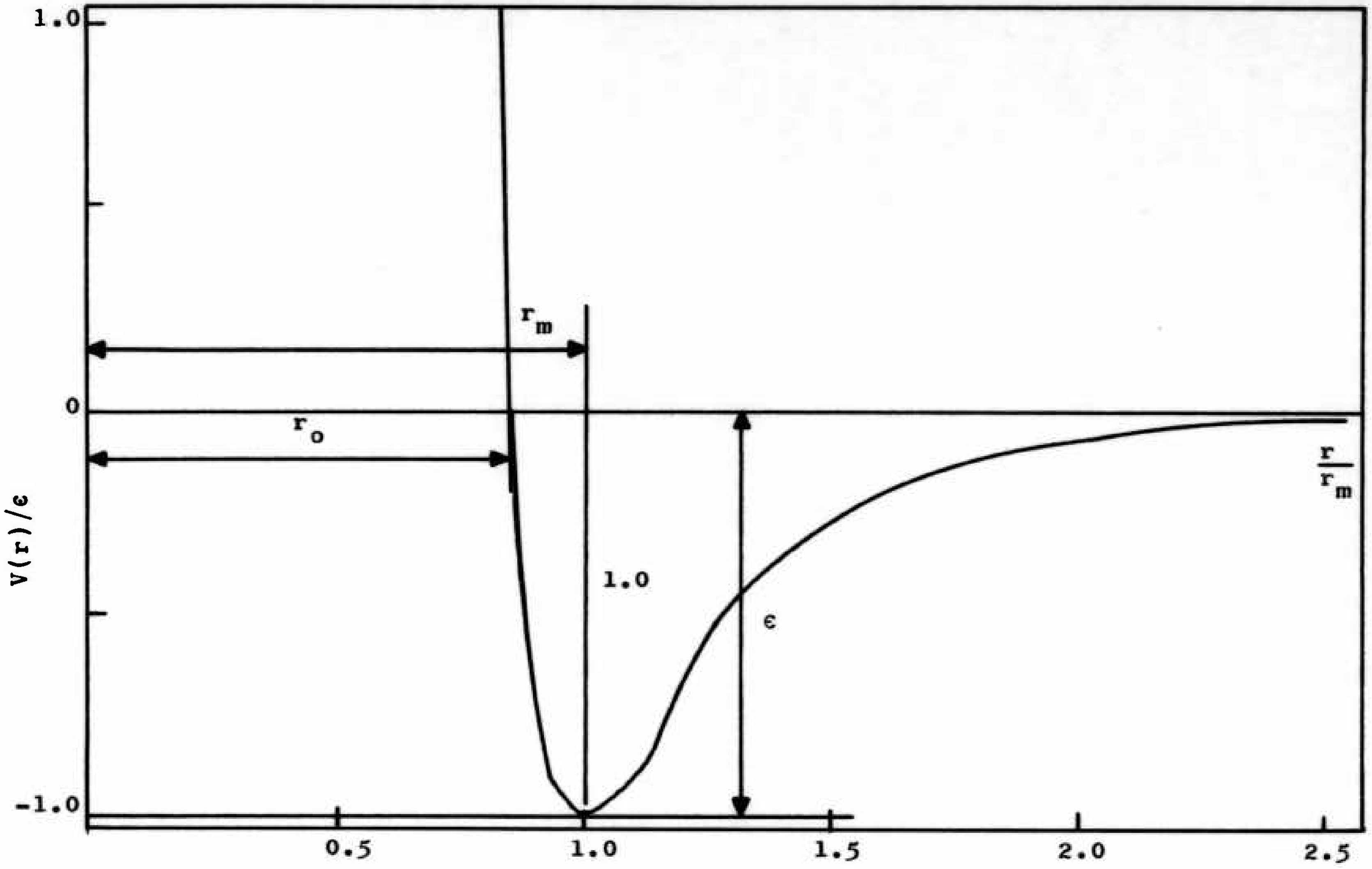


Figure 5. Schematic of Intermolecular Potential Between Atomic Pairs.

With these, equation (16) becomes

$$\theta = \pi - 2\beta \int_{\rho_{min}}^{\infty} \frac{d\rho}{\rho^2\sqrt{1 - \frac{U(\rho)}{K} - \frac{\beta^2}{\rho^2}}} , \qquad (17)$$

where θ is positive when the incoming particle is deflected away from the scatterer and negative when deflected toward it.

For any realistic potential $U(\rho)$, the deflection function θ cannot be solved in closed form. Several numerical calculations have been done with various potentials and the deflections function tabulated as a function of impact parameter for different values of reduced energy $K^{7,15}$. Figure 6 is a schematic sketch of the deflection function for the case where the Lennard-Jones 10,6 potential is used for $V(\rho)$, thus

$$V(\rho) = \frac{3\varepsilon}{2}\left[\frac{1}{\rho^{10}} - \frac{5}{3}\left(\frac{1}{\rho^6}\right)\right] , \qquad (18)$$

and where the ρ^{-10} term represents the repulsive core, while ρ^{-6} is the attractive long range Van der Waals contribution[7].

The information of Figure 6 is related to the differential cross section $I(\Omega)$ by recalling that in the simplest case all the particles with impact parameters b are deflected into the solid angle $d\Omega$. This defines $I(\Omega)$ as

$$I(\Omega)d\Omega = \frac{\text{number of particles scattered in } d\Omega/\text{unit time}}{\text{incident intensity}}$$

$$= \frac{I\ b\ db\ 2\pi}{I} , \qquad (19)$$

where I is the incident intensity and the azimuthal dependence

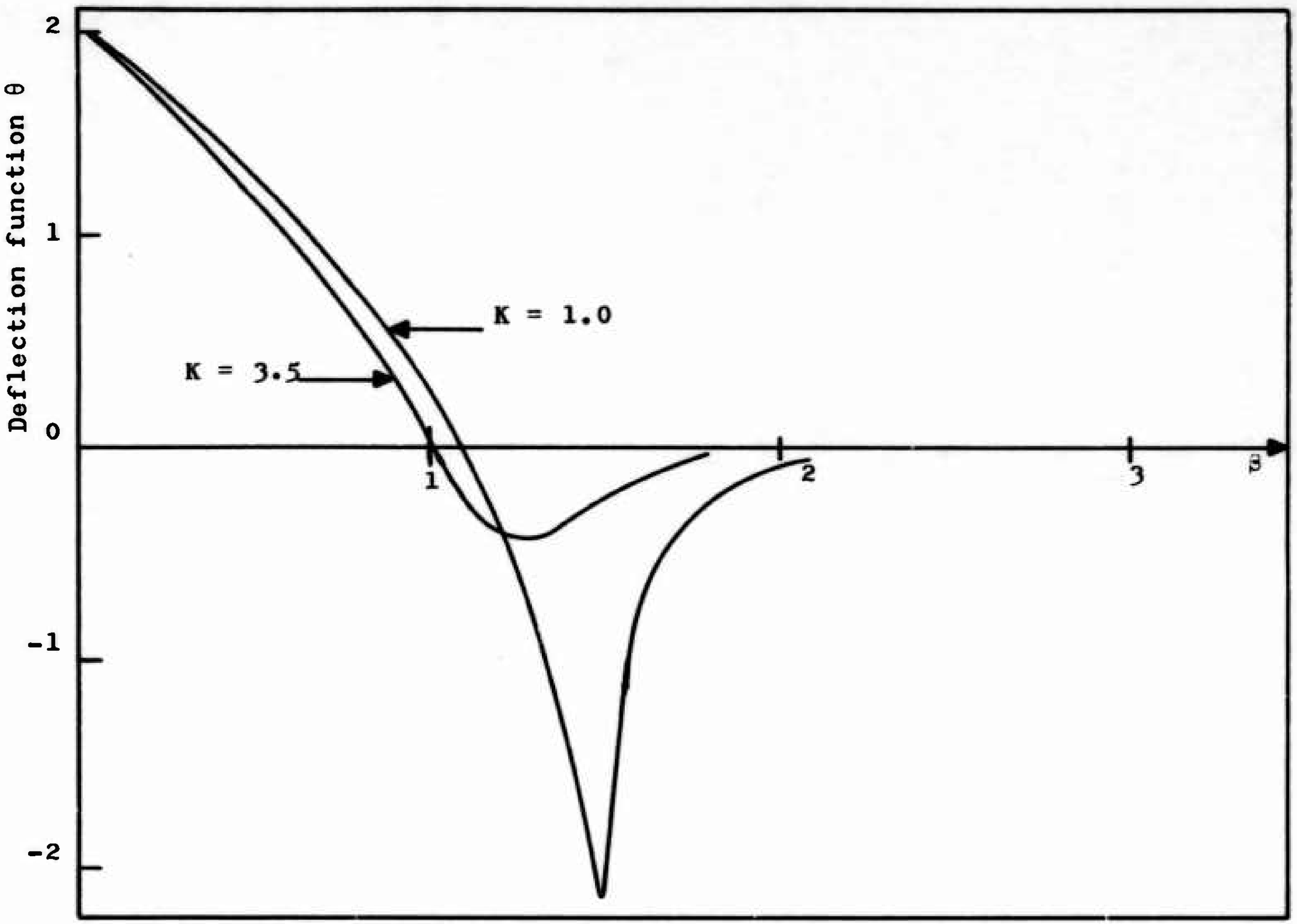


Figure 6. Approximate Behavior of Classical Deflection Function $\theta(\beta)$ for the Lennard-Jones Potential of Equation 18 for two Different Energies K.

has been integrated out and is indicated by the 2π. Since $d\Omega = 2\pi \sin\theta \, d\theta$, the differential cross section becomes

$$I(\Omega) = I(\theta,\varphi) = I(\theta) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| . \qquad (20)$$

For a more complex potential there may be several impact parameters which scatter into $d\Omega$ thus expression (20) must be summed over these. Further, the absolute value of the derivative insures all positive contributions to the differential cross section. Thus in reduced coordinates,

$$I(\theta) = \frac{r_m^2}{\sin\theta} \Sigma_j \beta_j \left|\frac{d\beta_j}{d\theta}\right| . \qquad (21)$$

The results of Figure 6 can be used directly to obtain $I(\theta)$. However, there are three singularities: 1) At large impact parameters, 2) At points where $\theta = 0$ and 3) Positions where $\frac{d\theta}{d\beta} \longrightarrow 0$. The first type occurs at large impact parameters where $\frac{d\beta}{d\theta} \longrightarrow \infty$, hence $I(\theta)$ increases without bound as $\theta \longrightarrow$ zero. Here classical mechanics fail and a quantum approach is necessary to account for small angle scattering. At the point where the deflection angle goes to zero another singularity occurs because $\frac{1}{\sin\theta} \longrightarrow \infty$. This type of singularity is called the "glory effect" and also occurs whenever $\theta(\beta)$ passes through integer values of π (as indicated in $K = 1.0$ case for negative angles). The last singularity occurs at an impact parameter corresponding to the minimum in the deflection function as indicated in the $K = 3.5$ case where $\frac{d\beta}{d\theta} \longrightarrow \infty$. This latter singularity leads to rainbow scattering[7].

The differential cross section is shown in Figure 7. The singularities at $\theta = 0$ contains (1) and (2) above while the other which occurs at larger θ is that due to rainbow scattering.

The "rainbow effect" can be observed experimentally[16] and the data agrees with classical theory. However, experimentally the small angle scattering is not infinite as predicted by equation (21). Thus classical mechanics must be replaced by the quantum approach to explain the behavior in the small angle scattering region.

2. Quantum Approach

This method has been discussed in many standard tests[17,18] thus this presentation will be brief. A general form of the Schrodinger equation is given by the equation.

$$-\frac{\hbar^2}{2\mu} \nabla^2 \psi(\vec{r}) + V(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r}) , \tag{22}$$

In this case, the time independent and non-relativistic form is required. The quantity $\hbar$ is Planck's constant divided by 2π, μ is the reduced mass, $V(r)$ is the potential, E the energy and $\psi(r)$ the wave function. This can be rewritten as

$$(\nabla^2 + k^2) \psi(\vec{r}) = \frac{2\mu}{\hbar^2} V(\vec{r}) \psi(\vec{r}), \tag{23}$$

where $k^2 = \frac{2\mu E}{\hbar^2}$. Using Fourier transforms, the following solution for the asymptotic region is obtained in terms of partial waves with angular momentum ℓ,

$$\psi = e^{ikz} + \frac{e^{ikr}}{r} \left[\frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell+1)(e^{i2\delta_\ell} -1)P_\ell(\cos) \right]. \tag{24}$$

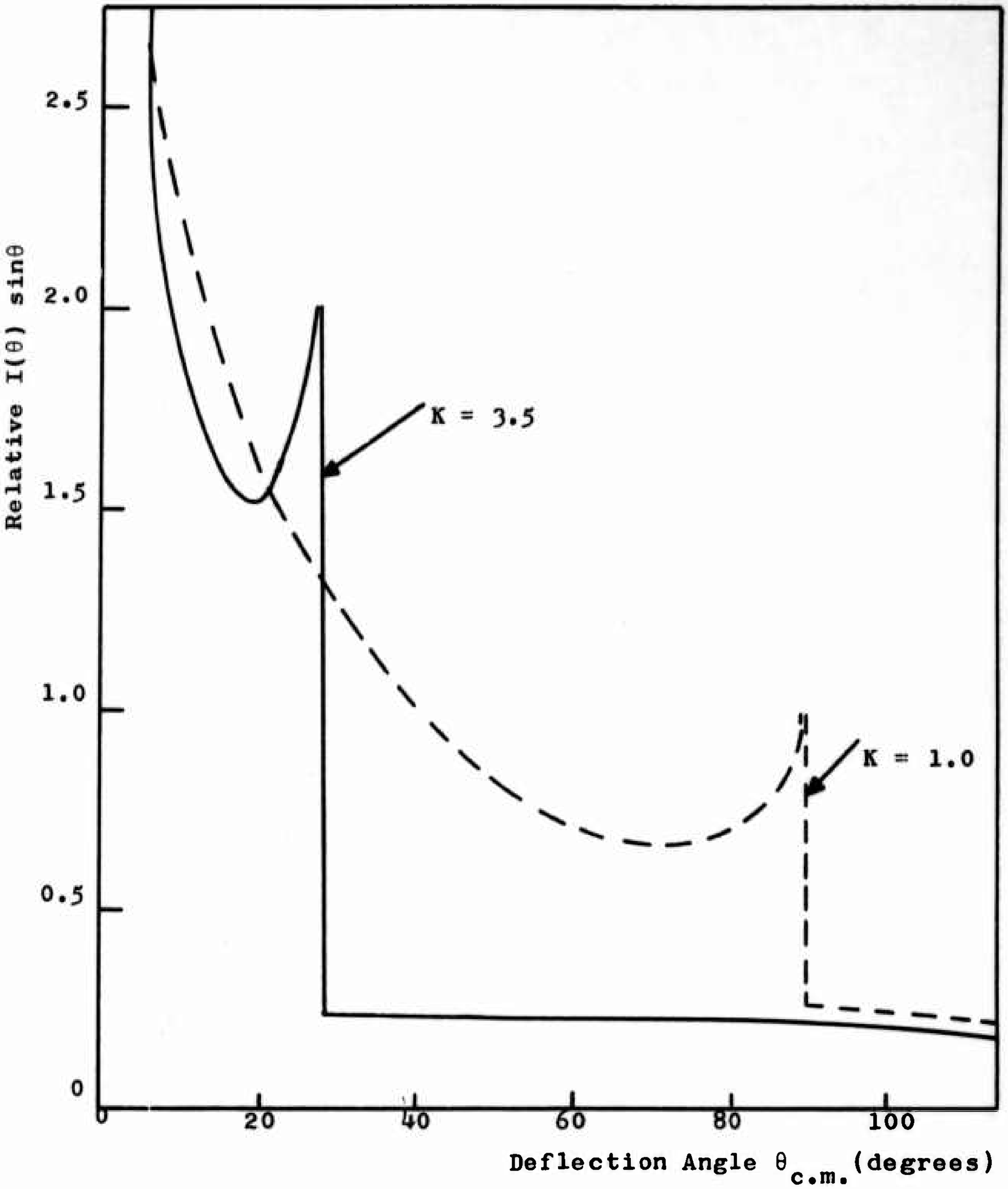


Figure 7. Schematic Behavior of Classical Differential Cross Section I (θ) weighted by sinθ versus the deflection angle θ for two Energies K.

where the first term on the right hand side of the equation is the incident wave assumed along the Z axis, and the second term corresponds to the outgoing spherically scattered wave. The term in brackets contains the θ dependence and has the Legendre polynomials $P_\ell(\cos\theta)$ and phase shift δ_ℓ for the ℓ^{th} angular momentum. This bracketed term is called the scattered amplitude $f(\theta)$ and is related to the differential elastic scattering cross section $\sigma(\theta)$ by $\sigma(\theta) = |f(\theta)|^2$. The total integral cross section can be expressed as the integral over all possible angles. This gives, by using the orthogonality properties of the Legendre functions,

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2\delta_\ell \ . \tag{25}$$

The object is to take the scattering amplitude in the brackets of equation (24) and equate it to the scattering amplitude as obtained in the exact solution of (23). In this latter case

$$f(\theta) = -\frac{1}{4\pi}\int e^{-i\vec{k}_f\cdot\vec{r}\,'} \frac{2\mu}{\hbar^2} V(\vec{r}\,') (\vec{r}\,')d\vec{r}\,' \ , \tag{26}$$

where $\vec{k}_f = k\hat{r}$, the $\hat{r}$ being the direction of the outgoing wave.

Usually the $f(\theta)$ of equation (26) is reduced further and put into a form of a sum over ℓ values with r' replaced by r:

$$f(\theta) = -\sum_{\ell=0}^{\infty} (2\ell+1)P_\ell(\cos\theta) \int_0^{\infty} j_\ell(kr) \frac{2\mu}{\hbar^2} .V(r)v_\ell(r)r^2dr, \tag{27}$$

where the only new term appearing is $v_\ell(r)$ which is the exact ℓth radial wave function. Thus equation (27) and the bracketed term in equation (24) gives the connection between the phase shift and the potential,

$$e^{2i\delta_\ell} - 1 = \frac{2k}{i} \int_0^\infty j_\ell(kr) \frac{2\mu}{\hbar^2} V(r) v_\ell(r) r^2 dr \quad . \tag{29}$$

This expression can be rearranged into various forms and sometimes reduced with suitable approximations (semi classical form). Thus in general if a potential is known or assumed, the $v_\ell(r)$ is obtained and equation (28) is evaluated for each value of ℓ. The resulting δ_ℓ then is used to obtain both the total and differential elastic cross section.

3. Information Obtained From Elastic Scattering

The primary information as obtained from the integral cross section versus velocity and the differential cross section versus scattering angle in elastic scattering concerns the intermolecular potential. In particular, for heavy atoms, absolute measurements of elastic integral cross sections gives directly the potential constant for the attractive potential. If the velocity dependence is known then the power dependence of the distance between the two particles can be determined. For the case of low mass atoms, oscillations are expected in the velocity dependence. This gives information about the product of the well depth times the radius of the minimum in the potential $(\epsilon r_m)^7$.

The differential cross section is very sensitive to the potential and the r_m (Figure 5) can be extracted from the oscillatory behavior.

Reactions

A reactive collision is defined to take place when the products are different than the reactants. At present almost all experimental work with reactions has involved the combination of alkali metal atoms with halogen conpounds[7,13]. The reaction products include the resulting alkali halide. Some additional work involving hydrogen on other molecules/atoms has also been performed[7,19].

Reactions have been limited to these types mainly because c.m. energies of order of a few kcal/mole are needed for these reactions to go. Almost all other types of reactions that might be considered are excluded because the energy considerations usually are between 1-10ev which at present is an experimentally untouchable region. However, some of the reactions that can be considered are the most fundamental, particularly those involving hydrogen as one of the reactants.

Of the two categories, the alkali-halogen type have received the most attention because the experimental problem of detection are easier since surface ionization techniques can be used. There have been about twenty reactions studied in this category and these have been classified according to the angular distribution of the alkali halide products[7,13]. In one extreme case the product recoils forward with respect to the incoming alkali beam. This has been called a "stripping process" and seems to occur with the reactions that have a large cross section $\gtrsim 100 \mathring{A}^2$. The reaction $K + Br_2 \rightarrow KB_r + B_r$ is an example of a reaction that obeys a stripping process. The other extreme occurs when the alkali halide product recoils backward in the center of mass and appear at an angle in the lab which is considerably different than that of the incoming alkali beam. This process has been called a "rebound mechanism" and appears to dominate in reactions with cross sections $\lesssim 10 \mathring{A}^2$. The classical example of rebound is the $K + CH_3I \rightarrow KI + CH_3$ reaction. Many of the alkali-halogen compound reactions fall between these two limits and cannot be so readily classified.

The reactions involving hydrogen $H + H_2 \rightarrow H_2 + H$, $H + D_2 \rightarrow HD + H$, etc., have received less attention than those discussed above mainly because of experimental difficulties. However, they are of fundamental importance in understanding of chemical kinetics and should be reconsidered.

1. Theoretical Approaches

One approach to the understandings of reactions involves Monte Carlo methods[20, 21]. Generally a potential is assumed and a classical mechanics approach is used to obtain the necessary equations of motion. The initial values of the internal and relative motion of the reactants are picked from suitably weighted random distributions. These are used in the equations of motion to determine the trajectory. The distance of approach determines whether a reaction or scattering has taken place. At the end of the trajectory, the internal and relative motion are computed for each case. By suitable averaging, the differential and total cross section for reactive scattering can be obtained along with the final conditions of the products. These in turn can be compared to experiment. Many of the calculations have been concerned with $K + CH_3I$ and (H, H_2) and the results appear promising, however, additional experimental evidence is still needed[9,20,21].

The understanding of the simplest chemical kinetic system would provide a most appropriate starting point for the consideration of energy storage problems because it should answer questions about possible relative minima on the potential surface generated by the reactants.

2. Inelastic Scattering

In this section a schematic presentation for inelastic cross section will be given. Up to the present, the phase shift δ_ℓ has been considered to be real. If δ_ℓ is considered to have a real and an imaginary part then the imaginary part can be used to describe inelastic scattering. This imaginary term reduces the amplitude of the outgoing wave i.e. fewer particles leave the interaction region than are incident.

The total cross section is then the sum of two terms, the elastic and inelastic contribution. The elastic part is obtained by integrating the absolute value of the square of the scattering amplitude over all possible scattering angles. This yields

$$\sigma_{el} = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \left| 1 - e^{2i\delta_\ell} \right|^2 . \qquad (29)$$

The inelastic term is obtained by integrating over all space the difference in incoming flux from outgoing flux. This gives

$$\sigma_{inel} = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \left(1 - \left| e^{2i\delta_\ell} \right|^2\right) . \qquad (30)$$

While it is relatively straight forward to obtain equation (30), it is much more difficult to compare it to experiment. There have been several experiments involving inelastic scattering of neutral molecules where internal energy states have been changed. One of the most interesting was that done by Toennies with $T\ell F$ on several other gases[22]. This work involved changes in rotational states of the $T\ell F$ upon colliding with the other molecules.

Schematic Presentation of a Research Apparatus

As can be seen in the brief presentation of this section, the theoretical background is already available, but the information lacking is precise experimental results. Prior to the recent development of the nozzle source, very few experiments could be considered for possible crossed beam experiments. These almost always involve the alkali metals because the detection efficiency was nearly one, while almost all other combinations of molecules or atoms had to be rejected because of intensity limitations. The nozzle source gives 10^2 to 10^3 more beam, which in crossed beam work means 10^4 to 10^6 more events and thus lifts the previous limitations on precise experiments. The experiments that now can be considered range from exchange reactions of a very simple nature to those which involve complex organic molecules.

In order to consider many different scattering combinations, it is necessary to have a scattering chamber with sufficient versatility built into it so that it can be easily adapted for many purposes. Figure 8 is a schematic view of such a scattering chamber. It consists of a 125cm stainless steel chamber which has: 1) two nozzle beam sources, 2) adequate vacuum pumps, and 3) a state-of-the-art detection system.

Initially the source will follow the proven design of Skofronick[11]. This design, which makes use of an isentropic expansion of a gas through a noxzle, has been shown to have particle intensities in the range of 5×10^{18} to 4×10^{19} particles/sr sec for various gases. These intensities range from 100 to 1,000 times that expected from an effusive source. Besides the very favorable intensity associated with this nozzle source, the expansion reduces the thermal spread in the beam thus yielding a beam with a velocity spread of approximately ± 5% for Argon and slightly greater for the lower mass gases.

Most work with nozzle sources has been concerned with

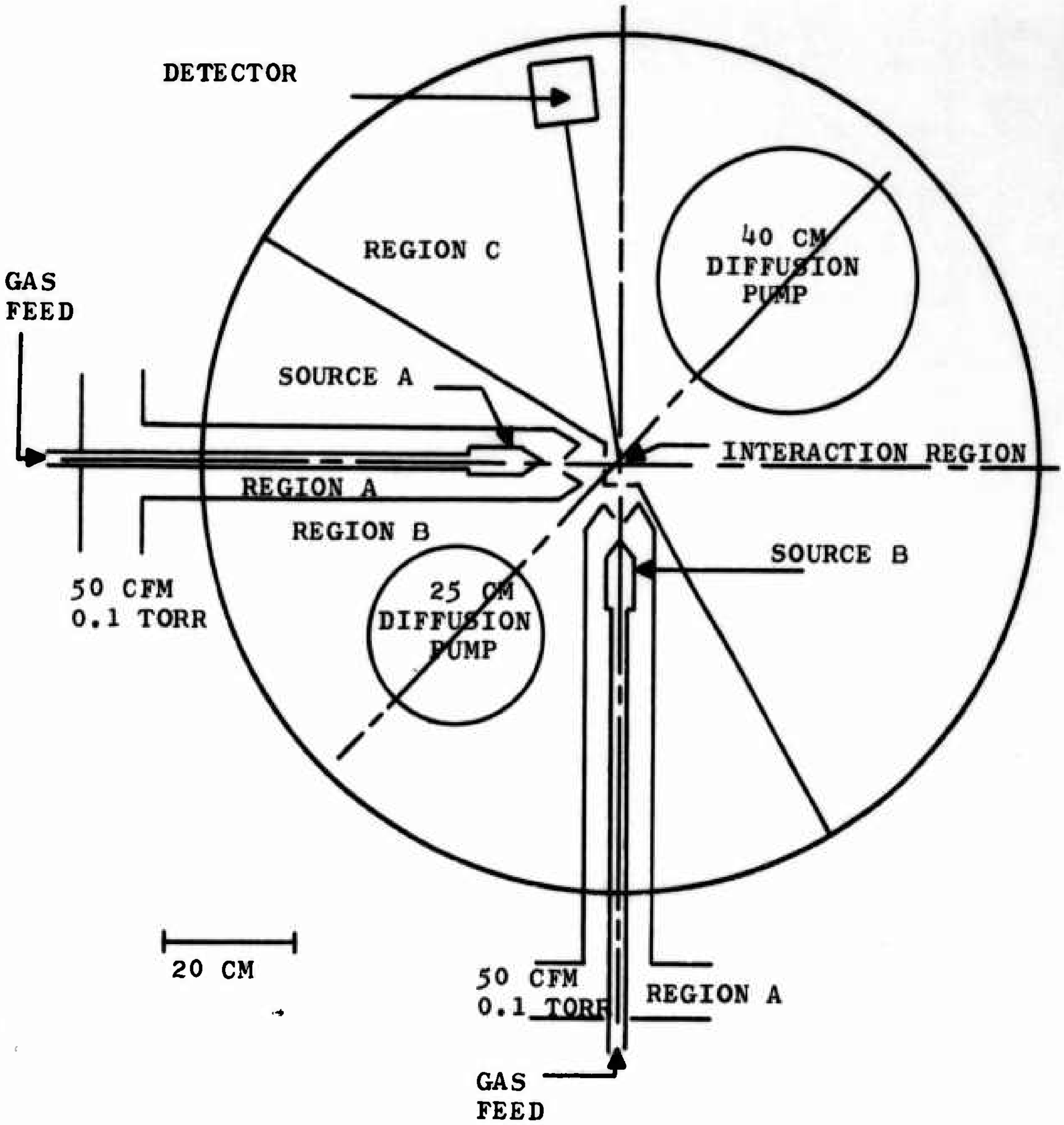


Figure 8. Scattering Chamber for Crossed Neutral Particle Molecular Beams.

the properties of thermal beams at room temperature. However, by varying the temperature of the nozzle source it is possible to change the energy of the beam, thus the energy range of 15 meV to 80 meV should be easily obtainable simply by changing the temperature of the nozzle. This feature is extremely useful for studies of excitation yields as well as differential cross section behavior.

For particle detections, mass selection is the obvious means. Fortunately a state-of-the-art detector is commercially available which can measure as few as 10^{+6} particles/sec of Nitrogen. This corresponds to a pressure of 10^{-15} torr.

For maximum detection sensitivity, the beams can be chopped so that synchronous detection and signal averaging techniques can be used. In this regard both techniques involve commercially available apparatus which should provide a detection sensitivity sufficient to detect scattered particle intensities as are expected in molecular beam experiments.

A very adequate apparatus for detection could be made of: 1) a Ultek Quad 250 Residual Gas Analyser[23], 2) a Princeton Applied Research HR8 Lock-in Amplifier[24], and 3) a Fabri-Tek Signal Averager[25].

The apparatus of Figure 8 thus has the essential components to make it a useful starting piece of apparatus for crossed-beam work.

SECTION V

IMPORTANCE OF DIFFERENTIAL CROSS SECTION MEASUREMENTS: AN EXAMPLE

Recently Aldridge and Davis[26] reported results on the scattering of He by He in which a Ramsauer-Townsend effect[18] was predicted for He-He collisions. This work illustrates two points which are of interest in connection with the work here.

First, the interaction potentials for systems as simple as two helium atoms are not well know. Second, total cross sections are not very informative compared with differential cross sections as a means of fixing the interaction potential.

Indeed it is the relative insensitivity of the total cross sections to the precise form of the interaction potential which made the Ramsauer-Townsend analysis possible. The prediction of a Ramsauer-Townsend phenomena for atoms is of interest itself. In the cited calculation it occurs provocatively close to the λ point for liquid helium II.

SECTION VI

FOLLOW-ON AND RELATED TOPICS

It is clear from the preceding discussion that the first steps toward understanding the efficient formulation of new explosives, their properties and their detonation mechanisms is part of the larger question of understanding chemical reactions in detail. The research program in molecular collision physics at the Florida State University represents a generalization of the applied problem in explosives and several connections to the specialized problem have been pointed out. The next step is to study both experimentally and theoretically the collisions between molecules starting with the simplest systems. The specialized follow-on is to then consider collisions between particles which are constituents of explosive materials. The object is to obtain information about the interactions potentials. Such an experiment program will require the construction of a suitable reaction chamber with proper neutral beam sources for the various types of particles to be studied as collision partners.

Several aspects of the problem have not been touched upon because of limitations on effort rather than importance. A critical point is the relationship between formation and detonation of an explosive. To the extent that the mechanisms of formation are understood, the potentials and mechanisms for some of the breakup channels will be understood.

In one sense, the formation and detonation of an explosive may be regarded as one reaction which proceeds through two distinct stages well separated in time.

Other follow-on topics involve questions of polarized beams, utilization of radiation baths for the pertubation of initial state population, and the study of the breakup of energy storing molecules event by event.

SECTION VII

SUMMARY

It is argued in this report that the study of differential elastic scattering cross sections for various atoms and molecules is the starting point for research and development in the field of new explosive material. Such data is needed for computations with the existing reaction theories and experimental results will offer guidance in the development of new reaction theories.

The next major step of the experimental program outlined here is the design and construction of a large chamber for the study of molecular collisions which includes state of the art beam sources and detection systems. Funds are being sought for this purpose.

Several throretical models for chemical reactions have been discussed here. Further development of these models, especially the R-matrix analysis, will be continued and their applications to reactions leading to energy storage investigated.

REFERENCES

1. Blanca Tchoubar, Reaction Mechanisms in Organic Chemistry, (American Elsevier Publishing Company, New York, 1966), p. 45.

2. C. N. Hinshelwood, The Kinetics of Chemical Change in Gasious Systems, Third Edition: (Oxford: Clarendon Press, 1933).

3. S. G. Glasstone, K. J. Laidler, and H. Eyring, The Theory of Rate Process, (McGraw-Hill Book Company, New York, 1933).

4. B. C. Eu and J. Ross, J. Chem. Phys., 44, 2467, (1966).

5. A. M. Lane and D. Robson, Phys. Rev., 151, 774, (1966).
   D. Robson and A. M. Lane, Phys. Rev., 161, 982, (1967).

6. Private communication with D. Robson.

7. H. Pauly and J. P. Toennies, Advances in Atomic and Molecular Physics, Vol. I., ed. by D. R. Bates, (Academic Press, New York, 1965), pp. 195-344.

8. D. A. Micha, Phys. Rev., 162, 88, (1967).

9. M. Karplus, N. R. Porter, R. D. Sharma, J. Chem. Phys., 43, 3259, (1965).

10. A. Suzuki, "Explosive Properties of Initial Explosives, Crystallographic, Molecular and Quantum-Chemical Considerations", Clearinghouse for Federal Scientific and Technical Information, U. S. Dept. of Commerce, AD 620-222, August 1965.

11. J. G. Skofronick, to appear in Rev. Sci. Inst.

12. R. Fraser, Molecular Rays, (MacMilliam Company, Cambridge, England 1931).

13. D. R. Herschbach, Adv. in Chemical Physics, Vol. I., ed. by J. Ross, (John Wiley, New York 1966), pp. 319-391.

14. K. Berkling, R. Helbing, K. Kramer, H. Pauly, Ch. Schlier and P. Toschek, Z. Physik 166, 406, (1962).

15. R. B. Bernstein, Adv. in Chemical Physics, Vol. X, Ed. by J. Ross, (John Wiley and Sons, Inc., New York 1966), pp. 75-134.

16. K. W. Ford and J. A. Wheeler, Ann Phys. (New York) 7, 259-287, (1959).

17. E. Merzbacher, *Quantum Mechanics*, (John Wiley and Sons, Inc., New York, 1961) pp. 213-247.

18. L. I. Schiff, *Quantum Mechanics*, (McGraw-Hill Book Company, New York, 1955), pp. 92-121.

19. S. Datz and E. H. Taylor, J. Chem. Phys., **39**, 1896,(1963).

20. D. L. Bunker and N. C. Blais, J. Chem. Phys., **41**, 2377, (1964).

21. M. Karplus and L. Raff, J. Chem. Phys., **41**, 1267, (1964).

22. J. P. Toennies, Disc Faraday Soc., **33**, 96, (1962).

23. Ultek-EAI/QUAD, 250 Residual Gas Analyzer, Ultek Corp., Box 10920, Palo Alto, California.

24. Princeton Applied Research, Lock In Amplifier Model HR-8, Princeton Applied Research Corp., Box 565, Princeton, New Jersey 08540.

25. Fabri-Tek Model FT-952, High Speed Digitizer and FT-1052, Signal Averager, Fabri-Tek, Inc., P. O. Box 4218, Madison, Wisconsin 53711.

26. J. P. Aldridge and R. H. Davis, Phys. Rev., Letters **19**, 1001, (1967).

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)*
Recon, Inc.
694 Industrial Drive
Tallahassee, Florida 32304

2a. REPORT SECURITY CLASSIFICATION
UNCLASSIFIED

2b. GROUP

3. REPORT TITLE
AN INVESTIGATION OF ENERGY STORAGE SOLIDS

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*
Final Report - 12 October 1966 through 11 October 1967

5. AUTHOR(S) *(First name, middle initial, last name)*
Dr. R. H. Davis
Dr. J. G. Skofronick

6. REPORT DATE
January 1968

7a. TOTAL NO. OF PAGES
59

7b. NO. OF REFS
26

8a. CONTRACT OR GRANT NO.
F08635-67-C-0028

b. PROJECT NO.

c.

d.

9a. ORIGINATOR'S REPORT NUMBER(S)
Recon Technical Report No. 30F

9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*
AFATL-TR-68-3

10. DISTRIBUTION STATEMENT This document is subject to special export controls and each transmittal to foreign governments or foreign nationals may be made only with prior approval of the Air Force Armament Laboratory (ATWT), Eglin AFB, Florida 32542

11. SUPPLEMENTARY NOTES
Available in DDC

12. SPONSORING MILITARY ACTIVITY
Air Force Armament Laboratory
Air Force Systems Command
Eglin Air Force Base, Florida 32542

13. ABSTRACT

A microscopic approach to aid further research and exploratory developments in understanding of explosives is discussed. This approach makes use of studies involving the interaction behavior between pairs of molecules. The technique of crossed molecular beam scattering is proposed as the best means to obtain the interaction information. It is argued that the technology of neutral particle beams is now sufficiently advanced that differential cross sections can now be measured. These in turn give very sensitive information about the intermolecular potential. Since the shape of the potential is vital to the understanding of energy storage, this approach is regarded as one involving the basic science of explosives and very likely will provide new avenues and answers to energy storage.

DD FORM 1 NOV 65 **1473**

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
FORMATION OF EXPLOSIVES						
PROPERTIES OF EXPLOSIVES						
DETONATION OF EXPLOSIVES						
HIGH INTENSITY MOLECULAR BEAMS						
MOLECULAR COLLISION THEORY						
ENERGY STORAGE						
CROSSED MOLECULAR BEAMS						