The H+ and Ho sbombardment of O2 in the 10-120 kev range
by Edward Andrew Teppo

A thesis submitted to the Graduate Faculty in partial fulfillment of the requirements for the degree of MASTER OF SCIENCE in Physics
Montana State University

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ABSTRACT

A study has been made of the relative emission cross sections of hydrogen atoms and protons incident on oxygen in the 10-120 kev range. The results for Lyman alpha emission were compared to those of nitrogen. At 1304 A, the hydrogen atom and proton were shown to have nearly the same excitation cross section. Numerous atomic oxygen lines were seen indicating excitation was present to some dissociative states of the molecule.

Theoretical calculations were limited to the Born approximation largely because of the uncertainty in the wave function of the electronic energy levels.

INTRODUCTION

In the past thirty years great progress has been made in particle accelerators and, hence, in ion-atom collisions. As a result, scientists have learned a great deal about the colliding particles and their interaction in a collision. The evaluation of collision cross sections is a valuable aid in this interpretation. Experimental methods are the most feasible means of studying these cross sections.

The study of the physics of the upper atmosphere has increased rapidly since 1958. Cosmic radiation, which consists largely of energetic protons, is constantly incident upon our upper atmosphere. Fortunately this radiation is largely absorbed there. But such absorption processes are not well understood. Research is being done toward this interpretation through analysis of the aurora.

Since the major components of the atmosphere are nitrogen and oxygen and the proton accelerator is readily available, scientists can do the equivalent of space physics in the laboratory. Their capabilities are limited by their apparatus. Commonly, general studies of collision processes are not possible; only particular processes are studied in great detail.

Several cross section studies have been made in oxygen which show some similarities to results obtained in this study. The similarities lie in the shape of the cross section curves obtained.

Unfortunately the theoretical calculations of such cross sections are unreliable. In general, they have been "re-done" until they agree appropriately with experimental results. Many of the theoretical calculations made have originated from consistencies found in experimental results. As a result, such calculations done in this study are unavoidably minimal.

THEORY

Atomic Collisions

The encounter of a projectile with a target gas may lead to elastic, inelastic and radiative collisions. In an elastic collision, there is no change in the internal energy of the colliding particles; in an inelastic collision some of the translational energy of the projectile is transferred to internal energy of the molecule. Inelastic collisions may lead to the emission of electromagnetic radiation. In extreme cases, the projectile may be captured by the molecule and an ion or excited state is produced.

Collisions are normally described by the following notation:[1] "1" refers to a singly charged positive ion; "0" refers to a neutral atom or molecule; "'" refers to an excited state; "e" refers to an electron; a "/" separates the initial and final products of the collision; and "()" refers to two or more particles bound to a system. Using this notation, the most pertinent collisions in this study include

i)	10/01	Charge transfer
ii)	10/10'	Excitation
iii)	00/0'0	Excitation
iv)	10/1'0	Excitation

Other processes include

v)	10/11e	Ionization
vi)	1(00)/100	Dissociation

Ionizing collisions where an electron is taken from the projectile are referred to as stripping, e.g.,

$$H^{0} + O_2 \longrightarrow H^{+} + O_2 + e$$

The measurement of Lyman alpha radiation (1216 A) by a similar interaction implies only the excitation process

$$H^{o} + O_2 \longrightarrow H^{o}(2p) + O_2$$

which requires less energy.

The charge transfer cross section implies the evaluation of interactions like

$$H^{+} + O_2 \longrightarrow H^{o} + O_2^{+}$$

The measurement of Lyman alpha radiation demands an interaction such as

$$H^{+} + O_2 \longrightarrow H^{o}(2p) + O_2^{+}$$

i.e., besides the transfer of an electron from an oxygen molecule to a proton, the electron must be excited to the lowest-lying excited state of the atom. This process then requires more energy than the charge transfer process. Therefore an attempt at making exact comparisons in the results found at 1216 A and those of stripping and charge transfer should be avoided.

If, during a collision between two systems of particles, one or more particles are exchanged between them, the process is known as a rearrangement collision. It is energetically possible that 10/20e (ionization) and 00/10e (ionization by rearrangement) occur. Double excitation becomes quite probable at high energies.

Cross Sections

Let n_i denote the number of atoms excited to the state i. Then[2]

$$\frac{dn_i}{dt} = NIQ_i + \sum_{k>i} A_{ki} n_k - \sum_{j<i} A_{ij} n_j$$

is the time rate of change of the number of atoms excited to state i. The terms contribute as direct excitation to state i, cascading from upper k to state i, and the decay of state i to the state j, respectively.

Assuming only direct excitation, then

$$Q_i = n_{ij}(L)/NIL$$

denotes the excitation cross section to the state i, where $n_{ij}(L)$ represents a number density of photons emitted from such a transition, I is a measure of the incident beam flux, N is the gas density (proportional to the pressure), and L is the observed path length of interaction.

To enable the experimenter to do absolute cross section measurements, the quantum yield (current of the detector per incoming photon per second) and the value of L must be calculable. Such measurements have been done by several experimenters for ion-atom and atom-atom collisions.[3,4] These calculations enable others to do relative cross section measurements by comparative techniques.

Some emission cross sections have recently been shown to have several maxima as function of energy.[5] The oscillatory behavior in the cross sections extend almost to the threshold energy. This result contradicts the adiabatic approximation which assumes a gradual decrease in the cross section below a maximum characteristic of the relative velocity of the projectile and the interacting electron-orbital. Since threshold energies are normally in the ev range, the present study did not reveal this characteristic.

The Massey criterion predicts a characteristic interaction distance a at a maximum in the cross section given by the equation

$$\frac{a}{v} \; \frac{\Delta E}{h} \cong 1$$

where ΔE is the difference in internal energy between the two states of the system and v is the relative velocity of the colliding particles. Recent studies indicate that the levels involved in the collision approach each other in energy as R, the internuclear separation, decreases, i.e., they approach a pseudo-crossing. Only if the optically allowed excited states are widely separated from the initial state of the compound system are the molecular interactions negligible and hence, the probability of excitation small at low energies.[6]

Experimental results imply a strong velocity dependence of the projectile and the interacting electron at high energies. Such analogies may then be applied to an equivalent velocity electron in proton cross section measurements.

Theoretical Calculations

The study of cross sections of atomic and molecular processes are of great value in providing information about how constituents in an interaction behave. The experimental work in all but the simplest atoms and molecules forms the basis of our understanding in collision processes. Since the many-body problem cannot be solved exactly, theoreticians can make only approximate calculations in the interpretation of such processes. These approximations are indeed necessary to make these calculations feasible. Yet the numerical values obtained are at the expense of unreliability of results.

In molecular physics or quantum chemistry, numerous methods of estimating wave functions have been introduced since the advent of quantum mechanics. At present, the best wave functions (those which agree best with experiment) have been found by using self-consistent field theory. Other interpretations have produced the Hartree-Fock calculations, the method of Roothaan, the distorted wave approximation, the Heitler-London theory, molecular orbital theory, and the valence bond theory by the chemist. These methods have met with varying degrees of success. Computer programs have been written for the approximate interpretation of atomic and molecular collisions incorporating the above theories, occasionally in concert. The calculation of electronic energy levels by such methods have yielded some very satisfactory results. However, these methods have not necessarily given reliable matrix elements as needed in the evaluation of transition probabilities.

Theoretical calculations for atomic collisions have been carried out using the impact parameter method[7] and by the wave treatment.[8] Such calculations have been largely restricted to H, H^+, He and He^+.

Theoretical Born cross sections have been done using an ion as the incident projectile. These calculations have shown that a typical cross section at high energies should vary as $E^{-1} \ln E$ for optically allowed transitions. Its validity for protons has been questioned below 200 kev.

Recently Born cross sections have been done for atom-atom collisions[9] due to Ochkur's contribution.[10] Unreliable wave functions do not allow such an evaluation in this experiment. The Born cross sections for electrons for optically allowed transitions is given to a first approximation by

$$Q = \frac{4\pi m^2 e^4}{k^2 h^4} |Z_{on}|^2 \ln \frac{2mv^2}{E_n - E_o}$$

The interaction between ions (or atoms) and molecules does not allow such a calculation.[1] It is not expected then that the Born approximation is reliable in the evaluation of cross sections for atom-molecule collisions.

The Oxygen Molecule

See Table I.[11]

The $^3\Sigma_g^-$ ground state of the oxygen molecule is paramagnetic. Unlike most ions, the O_2^+ ion has a larger dissociation energy and more bonding electrons than does O_2.

The electronic configuration of the oxygen molecule in atomic orbital theory is

$$1s^2 2s^2 2p_x^2 2p_y 2p_z$$

or equivalently in molecular orbital theory.

$$KK(\sigma_g 2s)^2(\sigma_u 2s)^2(\sigma_g 2p)^2(\pi_u 2p)^4(\pi_g 2p)^2$$

Both atomic orbital and molecular orbital theory have been used with limited success in the molecular interpretation of oxygen.

Since the oxygen molecule does not have a closed-shell configuration, its theoretical description is extremely difficult. Some unique contributions to the atomic orbital description have simplified electronic energy level designations a great deal. Yet the complexities in large part still remain.(12,13)

THE EXPERIMENT AND APPARATUS

Apparatus Description

See Figure 1. The protons were produced in a rf-driven ion cell(14) by introducing hydrogen gas into the system by means of a palladium leak. Initial pumping of the polyethylene line and trapping with liquid air reduced the possibility of water vapor entering the system.

Once ions were produced, the extraction, focusing and solenoid voltages were adjusted in unison with the high voltage to accelerate the ions down the accelerator. Additional focusing by an electrostatic quadrupole lens reduced the beam divergence prior to its entrance into the mass-analyzing magnet.

The beam contained approximately 10% undesirable ions; the mass analyzer allowed their removal by their smaller e/m ratio. The production of hydrogen atoms was also present in the beam and corrections due to their presence were necessary.

The composite beam, after passing through an aperture at A, entered the exchange cell which was used to produce a much higher density of hydrogen atoms in the beam. This was done by introducing hydrogen gas into the cell by means of a variable leak. At 50 Kev, approximately one-half of the particles coming out of the exchange cell were neutral.

With the high density of hydrogen atoms in the beam, the charged particles were then removed by electrostatic deflection. To insure that no charged particles were entering the interaction region, varying the deflection potential produced no noticeable change in the current at the Faraday cage.