

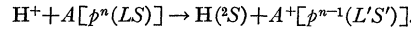
## Electron Capture from Atomic Nitrogen and Oxygen by Protons. I

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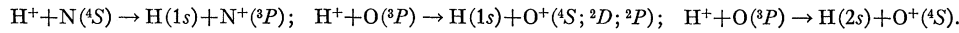
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(Received 16 January 1963)

The BK approximation (Born approximation using only the proton-active electron interaction,  $ne$ ) is used to derive the cross sections for  $p$ -orbital capture from atomic nitrogen and atomic oxygen by protons. These processes are represented symbolically as follows:



Russell-Saunders ( $LS$ ) coupling is assumed for the description of the atoms and ions, and only terms of the ground configurations are considered. Cross sections are derived for the set of processes for which the multiplicity is conserved between the initial state,  $H^+ + A[p^n(LS)]$ , and the final state,  $H(^2S) + A^+[p^{n-1}(L'S')]$ . Approximate cross sections for the inverse processes are expressed in terms of the cross sections for the corresponding direct processes. Furthermore, it is shown that all these cross sections are approximately related to one another for each atom. From this same analysis it is found that the cross sections for the direct processes are proportional to each of the following quantities:  $(2L+1)^{-1}$ ;  $n$ , the number of  $p$  orbitals in the target atom; the square of a coefficient of fractional parentage; a sum of squares of vector coupling coefficients. Detailed numerical calculations are presented for the following processes:



The cross sections for the last process are approximately  $\frac{1}{3}$  of the cross sections for the second process, and thus they obey the  $n^{-3}$  law of Oppenheimer. This fact supports the use of this rule for estimating the cross sections for capture into all  $s$  states of hydrogen for each residual ion. Estimates of  $(2s)$  and  $(1s)$  orbital capture are also obtained; the cross sections for  $(2s)$  orbital capture from  $N(^4S)$  and  $O(^2P)$  are compared, and it is found that the process becomes significant relative to  $p$ -orbital capture for an impact energy somewhat below 1 MeV for nitrogen, and somewhat above 1 MeV for oxygen; however,  $(2s)$  orbital capture dominates  $(2p)$  orbital capture from both atoms for impact energies above 8 MeV. Estimates of the Born cross sections (Born approximation using the proton-nucleus interaction together with all proton-electron interactions, " $nm+ne$ ") are obtained from the relation,  $Q_{Be}(A) = R(H; He)Q_{BK}(A)$ .  $R$  is the ratio,  $Q_B/Q_{BK}$ , previously calculated for atomic hydrogen and helium, and  $Q_{BK}(A)$  are the calculated BK cross sections of this paper. These Born estimates,  $Q_{Be}$ , do not differ a great deal from the experimental cross sections per gas atom for capture from the corresponding diatomic molecule.

**I**N a previous paper<sup>1</sup> this author proposed a method for estimating the Born electron capture cross section for protons passing through an atomic gas. This method is used in the present paper to estimate the Born cross sections for capture from the ground state of atomic nitrogen and atomic oxygen. As was discussed in I, this method consists of calculating the Brinkman-Kramers cross section for the atom of interest, and multiplying this result by the ratio,

$$R(A) = Q_B(A)/Q_{BK}(A),$$

which has been calculated for atomic hydrogen and helium at the same impact energy. ( $A$  represents the atom, hydrogen or helium, and the subscripts, B and BK, refer to Born and Brinkman-Kramers, respectively.) Although this program of calculation has some basis for successfully predicting the electron capture cross sections for a restricted energy range, there are questionable assumptions implicit which will be discussed later in the paper. (By BK approximation is meant the Born approximation with only the proton-active electron interactions,  $ne$  terms, whereas the Born approximation is reserved to mean the same approximation but with the inclusion of the proton-nucleus inter-

action and all of the proton-electron interactions, " $nm+ne$ " terms.)

The unsymmetrized BK amplitude for the capture of electron one (1) from an oxygen atom by a proton is given by Eq. (1).<sup>2</sup> [In the integral of Eq. (1) and all subsequent calculations of this paper, integration over spin coordinates is always understood, and is not written.]

$$g(\theta) = \frac{\mu a_0}{2\pi m} \int^3 [H(\mathbf{x}_{91})O^+(\mathbf{x}_2 \cdots \mathbf{x}_8)] O(\mathbf{x}_1 \cdots \mathbf{x}_8) |\mathbf{x}_{91}|^{-1} \\ \times \exp[i(\mathbf{A}_9 \cdot \mathbf{x}_{91} - \mathbf{A}_1 \cdot \mathbf{x}_1 + \sum_{j=2}^8 \mathbf{A}_j \cdot \mathbf{x}_j)] \\ \times d\mathbf{x}_{91} d\mathbf{x}_1 \cdots d\mathbf{x}_8. \quad (1)$$

For the present, some of the identifying subscripts are omitted from  $g(\theta)$ , and the notation,  $^3[HO^+]$ , is explained later in the text. The other notation used in Eq. (1) is now explained. The laboratory coordinates of the particles are the following:  $\mathbf{r}_j (j=1 \cdots 8)$  = electron;  $\mathbf{r}_n$  = oxygen nucleus;  $\mathbf{r}_p$  = proton. In the center-of-mass system, the set of independent relative coordinates used are

$$\mathbf{x}_j = \mathbf{r}_j - \mathbf{r}_n (j=1 \cdots 8); \quad \mathbf{x}_{91} = \mathbf{r}_1 - \mathbf{r}_p.$$

<sup>1</sup> Robert A. Mapleton, Phys. Rev. **126**, 1477 (1962). This paper is denoted by I.

<sup>2</sup> N. F. Mott and H. S. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1949), 2nd ed., Chapter XII, p. 273.

The masses on the  $O^{16}=16$  mass scale are:  $M$ =proton;  $m$ =electron;  $M_{n8}$ =oxygen atom;  $M_1=M+m$ ;  $M_{n7}=M_{n8}-m$ ;  $M_T=M_{n8}+M$ ;  $\mu=M_1M_{n7}/M_T$ . The magnitudes of the initial and final wave vectors of relative motion are denoted by  $\mathbf{K}_0$  and  $\mathbf{K}$ , respectively, and other derived quantities are  $A_9=\mathbf{K}M/M_1-\mathbf{K}_0$ ;  $\mathbf{A}_1=\mathbf{K}-\mathbf{K}_0M_{n7}/M_{n8}$ ;  $\mathbf{A}_j=\mathbf{A}_1m/M_{n7}$ . The wave functions that represent the hydrogen atom, the oxygen ion, and the oxygen atom are denoted by  $H$ ,  $O^+$ , and  $O$ , respectively. Dimensionless units are used with  $a_0=\hbar^2/me^2$ , the unit of length, and  $\epsilon_0=me^4/2\hbar^2$ , the unit of energy. In the subsequent calculations the momentum change vectors of the passive electrons,  $\mathbf{A}_j$  ( $j=2\cdots 8$ ), are neglected, since their omission does not affect the accuracy of this calculation.<sup>3</sup> Before proceeding with the calculation it is necessary to determine the wave functions.

The Russell-Saunders, or  $LS$ , coupling scheme is assumed, and the  $LSM_LM_S$  representation is used. Now the wave functions for the ground states of the oxygen atom and ion contain equivalent  $p$  electrons, and Racah has developed methods for the construction of such wave functions<sup>4</sup>; moreover, these wave functions not only are antisymmetrical in the electron coordinates, but they are orthogonal for the different terms of a given configuration. The wave functions for the  ${}^4S$ ,  ${}^2D$ , and  ${}^2P$  terms of the configuration  $p^3$ , written below, are taken from Table I of R.

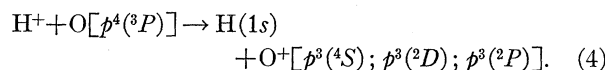
$$\begin{aligned}\psi[p^3({}^4S)] &= \psi[p^2({}^3P)p; {}^4S], \\ \psi[p^3({}^2D)] &= (1/\sqrt{2})\{\psi[p^2({}^3P)p; {}^2D] \\ &\quad - \psi[p^2({}^1D)p; {}^2D]\}, \\ \psi[p^3({}^2P)] &= [1/(18)^{1/2}]\{2\psi[p^2({}^1S)p; {}^2P] \\ &\quad - 3\psi[p^2({}^3P)p; {}^2P] \\ &\quad - 5^{1/2}\psi[p^2({}^1D)p; {}^2P]\}.\end{aligned}\quad (2)$$

The notation used here is fairly standard, and it is described elsewhere.<sup>5</sup> These relations are diagonal in  $M_L$  and  $M_S$ , and the vector coupling formulas for the addition of two angular momenta are used to get the various components ( $M_L$  and  $M_S$  values) of the different terms.<sup>6</sup> The numerical coefficients appearing in these relations are called the coefficients of fractional parentage, abbreviated cfp's.<sup>4</sup> These cfp's and Eqs. (19R) and (65R) (with  $n=2$ ) can be used to obtain the cfp's required for the construction of  $\psi[p^4({}^3P)]$ . Alternatively, one can use Eqs. (9R) and (11R) and solve for the cfp's, but, as discussed in R, this latter method leaves a phase

factor undetermined. These cfp's and  $\psi[p^4({}^3P)]$  are given by

$$\begin{aligned}(\psi^3 {}^4S \parallel p^4 {}^3P) &= -(4/12)^{1/2}, & (\psi^3 {}^2D \parallel p^4 {}^3P) &= (5/12)^{1/2}, \\ (\psi^3 {}^2P \parallel p^4 {}^3P) &= -(3/12)^{1/2}; \\ \psi[p^4({}^3P)] &= -(4/12)^{1/2}\psi[p^3({}^4S)p; {}^3P] \\ &\quad + (5/12)^{1/2}\psi[p^3({}^2D)p; {}^3P] \\ &\quad - (3/12)^{1/2}\psi[p^3({}^2P)p; {}^3P].\end{aligned}\quad (3)$$

The normalized antisymmetric wave functions are now easily constructed by coupling the two  ${}^1S$  subshells to the wave functions given in Eqs. (2) and (3). These wave functions can be expressed as linear combinations of determinants, and they are listed in Appendix II. The calculations for the processes of Eq. (4) are described next.



Since spin-dependent forces are neglected, the final state, hydrogen atom, and oxygen ion, must be a triplet. This condition is fulfilled by vector coupling the spin of the hydrogen doublet to the oxygen ion in question so that the coupled state forms a triplet. The  $M_S$  components of the coupled state,  ${}^3[H({}^2S)O^+({}^{2S+1}L)]$ , are given in Eq. (5) for the case that electron one (1) is captured (T. A. S.). The customary notation,  $\alpha$  and  $\beta$ , is used to denote the spin functions.

$$\begin{aligned}&{}^3[H({}^2S)O^+({}^4S)]: \\ &\quad M_S=1, \\ &H(\mathbf{x}_{91})\left[\frac{1}{2}\alpha(1)O^+({}^4S; \frac{1}{2}) - \frac{\sqrt{3}}{2}\beta(1)O^+({}^4S; \frac{3}{2})\right]; \\ &\quad M_S=0, \\ &\frac{H(\mathbf{x}_{91})}{\sqrt{2}}\left[\alpha(1)O^+({}^4S; -\frac{1}{2}) - \beta(1)O^+({}^4S; \frac{1}{2})\right]; \\ &\quad M_S=-1, \\ &H(\mathbf{x}_{91})\left[\frac{\sqrt{3}}{2}\alpha(1)O^+({}^4S; -\frac{3}{2}) - \frac{1}{2}\beta(1)O^+({}^4S; -\frac{1}{2})\right]. \\ &{}^3[H({}^2S)O^+({}^2L)]: \\ &\quad M_S=1, \\ &H(\mathbf{x}_{91})\alpha(1)O^+({}^2L; M_L, \frac{1}{2}); \\ &\quad M_S=0, \\ &\frac{H(\mathbf{x}_{91})}{\sqrt{2}}\left[\alpha(1)O^+({}^2L; M_L, -\frac{1}{2}) + \beta(1)O^+({}^2L; M_L, \frac{1}{2})\right]; \\ &\quad M_S=-1, \\ &H(\mathbf{x}_{91})\beta(1)O^+({}^2L; M_L, -\frac{1}{2}).\end{aligned}\quad (5)$$

<sup>3</sup> Robert A. Mapleton, Phys. Rev. **122**, 528 (1961). This paper is denoted by II.

<sup>4</sup> Giulio Racah, Phys. Rev. **63**, 367 (1943). This paper is denoted by R.

<sup>5</sup> D. R. Bates, *Quantum Theory* (Academic Press Inc., New York, 1962), Vol. II, Chapter I, pp. 66-67.

<sup>6</sup> E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, New York, 1953), Chapter III. This reference is denoted by T. A. S.

The relations in Eq. (5) are diagonal in  $M_L$  of the ion. These relations are not antisymmetrical in all electron coordinates, but this detail is treated at a later stage of the calculation. At this point of the calculation an interesting fact is mentioned. Since the independent relative coordinate,  $\mathbf{x}_{91}$ , of the electrostatic interaction is not contained among the coordinates of O and  $O^+$ , and remembering the approximation,  $\mathbf{A}_j=0$  ( $j=2\cdots 8$ ), it is evident from Eqs. (1), (3), (4), and (5) that non-vanishing matrix elements occur only for the case that coordinate one (1) of O is occupied by a  $p$  orbital; i.e., only a  $p$  orbital is captured. For example, if the approximation,  $\mathbf{A}_j=0$ , is not invoked, then matrix elements exist for  $s$  orbitals of O occupying coordinate one. This approximation is excellent and it simplifies the calculation immensely.

For the calculations of this paper, the wave functions derived by Tubis are used.<sup>7</sup> The one-electron orbitals are written for convenient reference:

$$S_1(\mathbf{x}) = (\gamma_1^3/\pi)^{1/2} e^{-\gamma_1 x},$$

$$S_2(\mathbf{x}) = \left( \frac{\gamma_2^5}{3\pi N(A)} \right)^{1/2} \left[ x e^{-\gamma_2 x} - \frac{3A(A)}{\gamma_2} e^{-\gamma_3 x} \right],$$

$$A(A) = \frac{(a+b)^3}{(1+a)^4}, \quad N(A) = 1 - \frac{48A(A)}{(1+b)^4} + \frac{3A(A)^2}{b^3}, \quad (6)$$

$$P_{\pm 1,0}(\mathbf{x}) = \left( \frac{\alpha^5}{\pi} \right)^{1/2} x e^{-\alpha x} \left[ \frac{\sin\theta}{\sqrt{2}} e^{\pm i\phi}, \cos\theta \right],$$

$$\gamma_1 = ua, \quad \gamma_2 = u, \quad \gamma_3 = ub, \quad \alpha = uc.$$

The functions of Eq. (6) are the one electron orbitals for O and N written in the notation of this paper.  $S_{1,2}$  denote the orbitals of the subshells  $(1s)^2$  and  $(2s)^2$ , respectively, and the notation for the  $p$  orbitals is self-evident. This notation is replaced by the following notation for the  $O^+$  and  $N^+$  orbitals.  $T_{1,2}$  are the  $(1s)^2$  and  $(2s)^2$  orbitals;  $\gamma_{1,2,3}$  are replaced by  $\beta_{1,2,3}$ ;  $P_m$  is replaced by  $P_m^*$ , and  $\alpha$  is replaced by  $\beta$ . [The value of  $(ub)$  is misprinted in the table of the  $O(^3P)$  parameters,<sup>7</sup> and the corrected value,  $ub=7.11$ , has been supplied by a separate calculation.<sup>8</sup>] An important property of the orbitals,  $T_{1,2}$ , of the ion is their approximate orthogonality to the orbitals,  $S_{2,1}$ , of the parent atom, and in the subsequent calculations, the following very good approximation is used:

$$\int d\mathbf{x} T_{1,2}(\mathbf{x}) S_{2,1}(\mathbf{x}) \ll \int d\mathbf{x} T_{1,2}(\mathbf{x}) S_{1,2}(\mathbf{x}) = (T_{1,2}, S_{1,2}).$$

With this stock of information, it is not difficult to evaluate the BK matrix element. That capture process

of Eq. (4) which leaves the ion in the  $^4S$  state is described first. With the use of the relations in Eq. (5) that define  $^3[\text{HO}^+(^4S)]$ , and Eq. (1), the BK amplitude can be reduced to the form

$$g_{M_L, M_S}(\theta) = \frac{2\mu a_0}{2\pi m (24)^{1/2}} (T_2, S_2)^2 (T_1, S_1)^2 (\beta\alpha)^{15/2} \\ \times \left( \frac{2}{\beta+\alpha} \right)^{15} \int d\mathbf{x}_1 d\mathbf{x}_{91} |\mathbf{x}_{91}|^{-1} H(\mathbf{x}_{91}) \\ \times P_{M_L}(\mathbf{x}_1) \exp[i(\mathbf{A}_9 \cdot \mathbf{x}_{91} - \mathbf{A}_1 \cdot \mathbf{x}_1)]. \quad (7a)$$

In Eq. (7a), both  $M_L$  and  $M_S$  assume the values,  $\pm 1, 0$ , corresponding to the three orbitals,  $P_{\pm 1,0}$ , and the triplet state of the atom,  $O(^3P)$ ; however, this amplitude is the same for all three  $M_S$  values. The integrals in Eq. (7a), called  $I_{\pm 1,0}$  are easily evaluated, and are given by

$$I_{\pm 1,0} = \frac{-i128\pi\alpha^{7/2}}{[1+A_9^2][\alpha^2+A_1^2]^3} \left[ \frac{A_{1x} \pm iA_{1y}}{\sqrt{2}}, A_{1z} \right]. \quad (7b)$$

In Eq. (7b),  $(A_{1x}, A_{1y}, A_{1z})$  are the rectangular components of  $\mathbf{A}_1$ . At this stage of the calculation a normalized antisymmetric state is constructed from the quantity,

$$^3[\text{H}(\mathbf{x}_{91}) O^+(^4S; \mathbf{x}_2 \cdots \mathbf{x}_8)],$$

in the usual manner. As discussed in II, this operation requires the use of a different relative coordinate,  $\mathbf{x}_{9j}$  ( $j=1\cdots 8$ ), for each permutation of the electron coordinates. However, the relabeling of  $\mathbf{x}_{9j}$  does not change the value of Eq. (1), and thus, using the antisymmetric property of  $O(^3P)$  it follows straightforwardly that the net effect of calculating the amplitude with the antisymmetric final state is to multiply the amplitude of Eq. (7a) by the factor,  $8^{1/2}$ .

The cross section is defined by<sup>2,9</sup>

$$Q = 2\pi \int_0^\pi d\theta \sin\theta \left( \frac{v_f}{g_i v_i} \right) \\ \times \sum_{M_L'=-L'}^{L'} \sum_{M_L=-L}^L \sum_{M_S=-S}^S |g_{M_L M_S}^{M_L'}(\theta)|^2. \quad (8a)$$

In Eq. (8a),  $v_i$  and  $v_f$  are the initial and final velocities of the incident particle, respectively;  $g_i$  is the degeneracy of the target atom;  $L'$  and  $L$  are the  $L$  values of the ion and its parent atom, respectively, and  $(2S+1)$  is the multiplicity of the atom. In the present example these values are  $g_i=9$ ,  $L'=0$ , and  $L=1$ . Conservation of energy is applied and momentum change variables are introduced. The final result for the process of interest is

<sup>7</sup> Arnold Tubis, Phys. Rev. **102**, 1049 (1956).

<sup>8</sup> Professor John C. Slater (private communication).

<sup>9</sup> Gerhard Herzberg, *Spectra of Diatomic Molecules* (D. Van Nostrand Company, Inc., New York, 1951), Chapter I, p. 21.

given by

$$Q(^4S) = -\frac{4 v_f C(^4S)}{9 v_i K_0 K} \pi a_0^2 \int_x^\infty \frac{dA_1 A_1^3}{[1 + A_0^2]^2 [\alpha^2 + A_1^2]^6}$$

$$= \frac{4}{9} Q(x), \quad x = A_1(\text{min}),$$

$$C(^4S) = \frac{2M_{n8}}{M_{n7}} \left[ \frac{64\mu\alpha^{7/2}}{m} (T_2 S_2)^2 \right. \\ \left. \times (T_1 S_1)^2 (\beta\alpha)^{15/2} \left( \frac{2}{\beta + \alpha} \right)^{15-2} \right]. \quad (8b)$$

In Eq. (8b),  $x$  is the minimum value of the momentum change variable, and the notation,  $Q(x)$ , is introduced for later use. Since  $(K_0 K)$ ,  $A_0^2$ , and  $A_1^2$  are all proportional to the impact energy  $E$ , the cross section decreases as  $E^{-7}$  for sufficiently high energies.<sup>10</sup> It is a relatively simple exercise to derive the cross sections for the other two processes of Eq. (4), and the results of this calculation are given by

$$Q(^2D) = (5/9) Q[x(^2D)],$$

$$Q(^2P) = (3/9) Q[x(^2P)]. \quad (8c)$$

The quantities,  $Q[x(^2D)]$  and  $Q[x(^2P)]$ , differ only slightly from  $Q(x)$  of Eq. (8b), and these differences result from the small internal energy changes together with the small changes in the atomic orbitals of the different terms of the ions. Mention is made of the fact that the internal energy associated with the center of gravity of the multiplet of a given term is the energy that is used in the calculations [(T.A.S.), p. 195]. Each of these cross sections exhibits the same energy dependence at high energies; however, the onset of the  $E^{-7}$  dependence occurs at a higher impact energy than it does for the corresponding cross section for capture of an  $s$  orbital from atomic hydrogen and helium into a  $p$  state of hydrogen.<sup>1,3</sup> This difference in the onset of the  $E^{-7}$  dependence is readily explained in terms of the difference in the exponential terms of the relevant orbitals for these three cases. Perhaps more interesting is the fact that the cross sections of Eqs. (8b) and (8c) are proportional to the squares of the cfp's [see Eq. (3)]. Thus, approximately  $\frac{2}{3}$  of the  $O^+$  ions are left in the metastable  $^2D$  and  $^2P$  states. From a consideration of the degeneracies associated with the final states, ion, and hydrogen atom, and  $O(^3P)$ —or by a direct calculation—it is rather easy to derive the approximate cross sections for the processes inverse to those of Eq. (4).<sup>11,12</sup> These

cross sections are labeled by the term values of the ion and the atom.

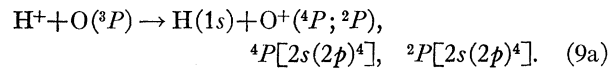
$$Q[^4S \rightarrow ^3P] \approx (9/8) Q[^3P \rightarrow ^4S] = \frac{1}{2} Q[x(^4S)],$$

$$Q[^2D \rightarrow ^3P] \approx (9/20) Q[^3P \rightarrow ^2D] = \frac{1}{4} Q[x(^2D)],$$

$$Q[^2P \rightarrow ^3P] \approx (9/12) Q[^3P \rightarrow ^2P] = \frac{1}{4} Q[x(^2P)].$$

From these relations it is seen that the sum of the cross sections for the inverse processes is approximately equal to  $\frac{3}{4}$  the sum of the cross sections for the direct processes.

An investigation of electron capture from  $O(^3P)$  leaving the  $O^+$  ion in excited configurations is treated next. The first cases considered are the processes given by



This example of the capture of a  $2s$  orbital is of particular interest since the cross section for this process obeys an  $E^{-6}$  law at high energies in contrast to the  $E^{-7}$  law for  $p$  orbital capture. Thus, the problem is to determine the energy region where this process becomes important. The procedure for deriving the BK cross sections is described briefly. From considerations of coupling two angular momenta, it is clear that the ion wave functions are obtained by vector coupling a  $(2s)$  orbital to  $p^4(^3P)$ , and with this task accomplished, one forms the antisymmetrical states,  $^3[H(\mathbf{x}_{0j})O^+(^4P)]$  and  $^3[H(\mathbf{x}_{0j})O^+(^2P)]$ , as outlined previously. The cross sections for the two processes have been estimated by using the  $O(^3P)$  radial functions for  $O^+(^4P; ^2P)$ . These cross sections are given by

$$Q(^2P) = \frac{2}{3} \pi a_0^2 \frac{v_f C(^2P)}{v_i K_0 K} I[x(^2P)],$$

$$Q(^4P) = \frac{4}{3} \pi a_0^2 \frac{v_f C(^4P)}{v_i K_0 K} I[x(^4P)], \quad (9b)$$

$$I(x) = \int_x^\infty \frac{dA_1 A_1}{[1 + A_0^2]^2} \left[ \frac{1}{(\gamma_2^2 + A_1^2)^2} \right. \\ \left. - \frac{4\gamma_2^2}{(\gamma_2^2 + A_1^2)^3} + \frac{3A(0)\gamma_3}{\gamma_2(\gamma_3^2 + A_1^2)^2} \right].$$

These formulas were evaluated for two values of  $E$ , and the results are expressed in terms of the sum of the cross sections,  $\Sigma(E)$ , of Eq. (4).

$$E = 1 \text{ MeV}, \quad Q(^4P) + Q(^2P) = 0.05 \Sigma(1),$$

$$E = 10 \text{ MeV}, \quad Q(^4P) + Q(^2P) = 24 \Sigma(10).$$

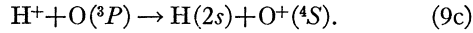
These results show the predominance of  $(2s)$  orbital capture at high energies.<sup>2</sup> For sufficiently large impact energies  $(1s)$  capture likewise becomes important, and for this case the ion configuration is  $1s(2p)^4$ . In fact,  $(1s)$

<sup>10</sup> D. R. Bates and R. McCarroll, *Phil. Mag. Suppl.* **11**, 39 (1962).

<sup>11</sup> H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Oxford University Press, London, 1952), Chapter VII, p. 417.

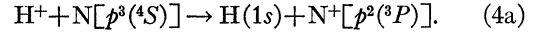
<sup>12</sup> Donald Rapp and Irene B. Ortenburger, *J. Chem. Phys.* **33**, 1230 (1960).

capture dominates ( $2s$ ) capture for a sufficiently high energy since the ( $1s$ ) electron is more tightly bound, and consequently, has the larger spread in momentum space.<sup>10</sup> The cross sections for the process given by Eq. (9c) have also been computed, but a discussion of these results is deferred for the present.



The calculation of cross sections for capture from atomic nitrogen is described next.

The first process considered is the one given by



The unsymmetrized BK amplitude for the preceding process is given by Eq. (1a).

$$g(\theta) = \frac{\mu a_0}{2\pi m} \int^4 [\text{H}(\mathbf{x}_{81}) \text{N}^+(\mathbf{x}_2 \cdots \mathbf{x}_7)] \text{N}(\mathbf{x}_1 \cdots \mathbf{x}_7) |\mathbf{x}_{81}|^{-1} \exp[i(\mathbf{A}_8 \cdot \mathbf{x}_{81} - \mathbf{A}_1 \cdot \mathbf{x}_1 + \sum_{j=2}^7 \mathbf{A}_j \cdot \mathbf{x}_j)] d\mathbf{x}_{81} d\mathbf{x}_1 \cdots d\mathbf{x}_7, \quad (1a)$$

$$\begin{aligned} \mathbf{A}_1 &= \mathbf{K} - \mathbf{K}_0 M_{n6} / M_{n7}, & \mathbf{A}_8 &= \mathbf{K} M / M_1 - \mathbf{K}_0, \\ \mathbf{A}_j &= \mathbf{A}_1 m / M_{n6}, & M_{n6} &= M_{n7} - m, \\ M_T &= M + M_{n7}, & \mu &= M_1 M_{n6} / M_T. \end{aligned}$$

In Eq. (1a)  $M_{n7}$  represents the mass of the nitrogen atom, and the other notation has been explained. Exactly the same procedure as described under the oxygen calculations is repeated, and with the omission of these details, the results of this calculation are

$$\begin{aligned} Q(^3P) &= \frac{v_f C(^3P)}{v_i K_0 K} \pi a_0^2 \int_x^\infty \frac{dA_1 A_1^3}{[1 + A_8^2]^2 [\alpha^2 + A_1^2]^6} = Q[x(^3P)], \\ C(^3P) &= \frac{2M_{n7}}{M_{n6}} \left[ \frac{64\mu\alpha^{7/2}}{m} (T_2 S_2)^2 (T_1 S_1)^2 (\beta\alpha)^5 \left( \frac{2}{\beta + \alpha} \right)^{10-2} \right], \\ Q[^3P \rightarrow ^4S] &\approx (2/9) Q[^4S \rightarrow ^3P] = (2/9) Q[x(^3P)]. \end{aligned} \quad (10a)$$

Also included in Eq. (10a) is the approximate relation between the inverse and direct processes. All the notation was described under the oxygen calculations. Attention is directed to the absence of the numerical factor that defines the cross section [see Eqs. (8b), (8c)]; the origin of such factors is explained in Appendix I. With use of the same type of approximation that led to the relations of Eq. (9b), several cross sections for capture of ( $2s$ ) and ( $1s$ ) orbitals were calculated. The nitrogen ions in this case are the  $^5S$  and  $^3S$  terms of the configurations  $2s(2p)^3$  and  $1s(2p)^3$ . The cross sections are written in the notation of Eq. (9b), and are given in Eq. (10b) for ( $2s$ ) capture—of course,  $\gamma_2, \gamma_3$ , etc., are the constants appropriate to nitrogen.

$$\begin{aligned} Q(^5S) &= -\frac{5 v_f C(^5S)}{4 v_i K_0 K} \pi a_0^2 I[x(^5S)], \\ Q(^3S) &= -\frac{3 v_f C(^3S)}{4 v_i K_0 K} \pi a_0^2 I[x(^3S)]. \end{aligned} \quad (10b)$$

These cross sections were calculated for two energies, and the cross section for ( $1s$ ) capture was evaluated only

for one energy. The results are expressed in terms of  $Q(^3P)$  of Eq. (10a).

$$\begin{aligned} Q &= Q(^5S) + Q(^3S); \\ 1 \text{ MeV, } & Q(1) = 0.25 Q(^3P)(1), \quad (1s)^2(2s)(2p)^3; \\ 10 \text{ MeV, } & Q(10) = 49 Q(^3P)(10), \quad (1s)^2(2s)(2p)^3; \\ 1 \text{ MeV, } & Q(1) = 0.03 Q(^3P)(1), \quad (1s)(2s)^2(2p)^3. \end{aligned}$$

A comparison of these results with  $s$ -orbital capture from oxygen suggests that this capture process starts to dominate  $p$ -orbital capture at a somewhat lower energy. However, this comparison should be accepted with reservation until it is supported, or rejected, by a calculation with improved wave functions, a task the author hopes to accomplish. It is instructive to notice that the numerical factors in Eqs. (9b) and (10b) are equal to  $(2S'+1)(2L'+1)/(2S+1)(2L+1)$ , and this factor is the ratio of the degeneracy of the ion to that of its parent atom.

The numerical values of the cross sections are presented in Tables I and II. The notation used in Table I is explained first.  $R(\text{H})$  and  $R(\text{He})$  denote the ratios that were described at the beginning of this paper.

TABLE I. Cross section for capture from atomic oxygen in units of  $\pi a_0^2 = 8.79 \times 10^{-17}$  cm<sup>2</sup>.  $E =$  incident energy of the proton in keV—laboratory system. (See text for explanation of notation.)

$E =$	39.5	70.3	100	125	150	200	222.3	300	395.3	600	703	1000	10 000
$R(H)$	0.147	0.167		0.196		0.228	0.236	0.260	0.284	0.322	0.337	0.370	
$R(He)$	0.194	0.203		0.218			0.236	0.245	0.254	0.266	0.271	0.284	
$Q_1(^1S)$	3.02	1.27		$4.16 \times 10^{-1}$		$1.28 \times 10^{-1}$	$9.42 \times 10^{-2}$	$3.64 \times 10^{-2}$	$1.35 \times 10^{-2}$	$2.41 \times 10^{-3}$	$1.17 \times 10^{-3}$	$2.08 \times 10^{-4}$	$1.47 \times 10^{-10}$
$Q_1(^2D)$	3.36	1.49		$5.07 \times 10^{-1}$		$1.60 \times 10^{-1}$	$1.18 \times 10^{-1}$	$4.62 \times 10^{-2}$	$1.72 \times 10^{-2}$	$3.10 \times 10^{-3}$	$1.51 \times 10^{-3}$	$2.67 \times 10^{-4}$	$1.87 \times 10^{-10}$
$Q_1(^2P)$	1.86	$8.47 \times 10^{-1}$		$2.96 \times 10^{-1}$		$9.46 \times 10^{-2}$	$7.02 \times 10^{-2}$	$2.76 \times 10^{-2}$	$1.03 \times 10^{-2}$	$1.86 \times 10^{-3}$	$9.04 \times 10^{-4}$	$1.60 \times 10^{-4}$	$1.12 \times 10^{-10}$
$Q_2(^1S)$	$2.55 \times 10^{-1}$	$1.28 \times 10^{-1}$		$4.90 \times 10^{-2}$		$1.65 \times 10^{-2}$	$1.23 \times 10^{-2}$		$1.84 \times 10^{-3}$		$1.60 \times 10^{-4}$	$2.80 \times 10^{-5}$	$1.87 \times 10^{-11}$
$Q_3$	9.90	4.34		1.47		$4.60 \times 10^{-1}$	$3.39 \times 10^{-1}$	$1.32 \times 10^{-1}$	$4.93 \times 10^{-2}$	$8.86 \times 10^{-3}$	$4.30 \times 10^{-3}$	$7.63 \times 10^{-4}$	$5.36 \times 10^{-10}$
$Q_{B_e}(H)$	1.45	$7.23 \times 10^{-1}$		$2.86 \times 10^{-1}$		$1.05 \times 10^{-1}$	$7.98 \times 10^{-2}$	$3.43 \times 10^{-2}$	$1.40 \times 10^{-2}$	$2.85 \times 10^{-3}$	$1.45 \times 10^{-3}$	$2.96 \times 10^{-4}$	
$Q_{B_e}(He)$	1.92	$8.79 \times 10^{-1}$		$3.18 \times 10^{-1}$			$7.98 \times 10^{-2}$	$3.23 \times 10^{-2}$	$1.25 \times 10^{-2}$	$2.35 \times 10^{-3}$	$1.17 \times 10^{-3}$	$2.27 \times 10^{-4}$	
	(40) <sup>a</sup>	(70) <sup>a</sup>											
$Q_B$	2.13	1.08	$6.26 \times 10^{-1}$		$3.07 \times 10^{-1}$	$1.17 \times 10^{-1}$							

<sup>a</sup> The numbers in parentheses refer to the energies appropriate to the values of  $Q_B$ .

TABLE II. Cross section for capture from atomic nitrogen in units of  $\pi a_0^2 = 8.79 \times 10^{-17}$  cm<sup>2</sup>.  $E =$  incident energy of the proton in keV—laboratory system. (See text for explanation of notation.)

$E =$	39.5	70.3	100	125	150	200	222.3	300	395.3	600	703	1000	10 000
$Q_1(^2P)$	9.46	3.75		1.10		$2.95 \times 10^{-1}$	$2.10 \times 10^{-1}$	$7.26 \times 10^{-2}$	$2.44 \times 10^{-2}$	$3.72 \times 10^{-3}$	$1.71 \times 10^{-3}$	$2.68 \times 10^{-4}$	$1.28 \times 10^{-10}$
$Q_3$	11.4	4.51		1.32		$3.54 \times 10^{-1}$	$2.52 \times 10^{-1}$	$8.72 \times 10^{-2}$	$2.93 \times 10^{-2}$	$4.48 \times 10^{-3}$	$2.05 \times 10^{-3}$	$4.03 \times 10^{-4}$	$1.54 \times 10^{-10}$
$Q_{B_e}(H)$	1.67	$7.53 \times 10^{-1}$		$2.58 \times 10^{-1}$		$8.08 \times 10^{-2}$	$5.95 \times 10^{-2}$	$2.27 \times 10^{-2}$	$8.33 \times 10^{-3}$	$1.44 \times 10^{-3}$	$6.92 \times 10^{-4}$	$1.49 \times 10^{-4}$	
$Q_{B_e}(He)$	2.21	$9.16 \times 10^{-1}$		$2.87 \times 10^{-1}$			$5.95 \times 10^{-2}$	$2.14 \times 10^{-2}$	$7.45 \times 10^{-3}$	$1.19 \times 10^{-3}$	$5.57 \times 10^{-4}$	$1.14 \times 10^{-4}$	
	(40) <sup>a</sup>	(70) <sup>a</sup>							(400) <sup>a</sup>		(700) <sup>a</sup>		
$Q_B$	2.56	1.25	$5.7 \times 10^{-1}$		$2.5 \times 10^{-1}$	$8.5 \times 10^{-2}$	$1.8 \times 10^{-2}$	$5.7 \times 10^{-3}$	$1.3 \times 10^{-3}$	$1.3 \times 10^{-3}$	$7.6 \times 10^{-4}$	$2.3 \times 10^{-4}$	

<sup>a</sup> The numbers in parentheses refer to the energies appropriate to the values of  $Q_B$ .

$R(\text{He})$  is obtained from the cross sections that were calculated using the six-parameter helium wave function of Hylleras.<sup>13</sup>  $Q_1(^{2S+1}L)$  signifies the BK cross section for capture from  $O(^3P)$  into the final state,  $H(1s)+O^+(^2S+1L)$  [see Eq. (4)];  $Q_2(^4S)$  denotes the BK cross section for capture from  $O(^3P)$  into the final state,  $H(2s)+O^+(^4S)$ ;  $Q_3$  is the sum of the BK cross sections for capture into all  $s$  states of hydrogen and the same three states of the ion,  $^4S$ ,  $^2D$ , and  $^2P$ .  $Q_{B_e}(\text{H})$  and  $Q_{B_e}(\text{He})$  are estimates of the Born cross sections, and are equal to  $Q_3R(\text{H})$  and  $Q_3R(\text{He})$ , respectively. In both tables the Born estimates contain allowance for ( $2s$ ) orbital capture at the energy, 1 MeV. This notation, interpreted through Eq. (4a) instead of Eq. (4), is used for the analogous cross sections for capture from atomic nitrogen that are presented in Table II. The notation,  $Q_E$ , appearing in both tables, denotes the cross sections per gas atom for electron capture by protons from the corresponding diatomic molecule.<sup>14</sup> Some interesting properties of the numerical values of Table I are now discussed. It has already been suggested following Eq. (8c) that the ratios of the cross sections,  $Q_1$ , are nearly proportional to the ratios of the corresponding squares of the cfp's, and the numerical values of  $Q_1$ , support this remark. The second interesting feature is the nearly constant ratio,  $Q_2(^4S)/Q_1(^4S)$ . Except at the lowest value of  $E$ , this ratio is approximately equal to  $\frac{1}{3}$ , and this is the first term of the  $n^{-3}$  relation for capture into  $s$ -states of atomic hydrogen.<sup>1,3,15</sup> Since this relation is obeyed so well for capture into  $H(2s)$ , this  $n^{-3}$  law is assumed to hold for capture into all  $s$  states of hydrogen (for each of the three  $O^+$  ions), and thus, one obtains the cross sections,  $Q_3$ . The two Born estimates are not in serious disagreement with the cross sections per gas atom of the molecule; nevertheless, the experimental values for capture from  $O_2$  do not cover a sufficient energy range to allow much of a comparison. However, in the case of capture from  $N_2$ , the energy range of the measured values is much larger.

The cross sections,  $Q_E$ , for  $N_2$  are larger than those for  $O_2$  at the low energy part of Tables I and II, but the  $O_2$  cross sections start to dominate those for  $N_2$  in the vicinity of 100 keV. This same behavior is exhibited by the corresponding two calculated sets  $Q_3$ , and  $Q_{B_e}(\text{H or He})$ . The  $Q_{B_e}$  are smaller than the corresponding  $Q_E$  near both ends of the energy range, but some of this apparent discrepancy can be explained. First, the study made of BK and Born cross sections for electron capture from atomic and molecular hydrogen showed that the cross section per gas atom for capture from  $H_2$  exceeds the corresponding cross section for capture from H for energies above 400 keV.<sup>16</sup> Moreover, the preceding

analysis also showed that agreement between these two cross sections at any energy was accidental. Since it is reasonable to expect similar relations to exist between the cross sections for capture from N and  $N_2$ , the aforementioned high-energy discrepancy is less disturbing. But quite separate from these molecular effects, there are other contributions to the total capture cross section that require mention. No allowance has been made for capture into  $p$  and  $d$  states of atomic hydrogen, and the calculations of I and II show that these contributions are significant in the low-energy range of Tables I and II; furthermore, contributions from simultaneous capture and excitation have been omitted, but again using the results of II as an example, the author does not believe that these latter omissions would significantly alter the present values. However, it does appear that the calculated cross sections are probably too small at (Table II) energies in excess of 700 keV, and this may be due to the inadequacy of the present estimates, but perhaps more likely, to the failure of the Born approximation itself, and an example of this sort of failure is found in the helium capture calculations.<sup>3,13</sup> Additional evidence that the Born approximation underestimates the cross sections for impact energies exceeding (roughly) 800 keV is supplied by comparisons of the Born approximation with recent calculations using an improved perturbation procedure.<sup>17,18</sup>

The author believes that the relative simplicity of Born capture calculations together with the apparent success of this method in predicting reasonably good cross sections for capture from helium and the atoms of this paper justifies the use of this method in the intermediate energy range of 40 keV to 1 MeV.

#### APPENDIX I

A different approach to the calculation of BK cross sections for  $p$ -orbital capture is described in this Appendix. It is recalled that the  $p$ -orbital part of the wave functions for the terms of the configuration  $p^n$  are expressed as linear combinations of terms of the configuration  $p^{n-1}$  each coupled to  $p(^2P)$ . The normalized antisymmetrical wave function for  $(n+4)$  electrons can now be written in terms of the  $(n+4)!/n!4!$  products of the antisymmetrical  $p^n$  ( $p$  orbital) part and the antisymmetrical  $(1s)^2(2s)^2$  part. Thus, in the calculation of a BK amplitude for  $p$ -orbital capture, one can antisymmetrize the captured electron with respect to the  $p$  orbital (configuration  $p^{n-1}$ ) part of the ion, and then antisymmetrize this group of electrons with respect to the  $(1s)^2(2s)^2$  group as was just described. Since it is readily verified that there are  $(n+4)!/n!4!$  nonvanishing integrals of the type implicit in Eqs. (1) and (1a), and, that the values of these integrals are all equal, the result for  $n=4$  is the same as given in Eq. (7a) except that the

<sup>13</sup> R. A. Mapleton, following paper [Phys. Rev. **130**, 1839 (1963)].

<sup>14</sup> S. K. Allison, Rev. Mod. Phys. **30**, 1137 (1958).

<sup>15</sup> J. R. Oppenheimer, Phys. Rev. **31**, 349 (1928); J. D. Jackson and H. Schiff, *ibid.* **89**, 359 (1953).

<sup>16</sup> T. F. Tuan and E. Gerjuoy, Phys. Rev. **117**, 756 (1960).

<sup>17</sup> R. McCarroll, Proc. Roy. Soc. (London) **A264**, 547 (1961).

<sup>18</sup> R. McCarroll and M. B. McElroy, Proc. Roy. Soc. (London) **A266**, 422 (1962).

numerical factor  $2(24)^{-1/2}$  is replaced by the product of several numerical factors.

Attention is now focused on the numerical factors, and the origin of these factors is what motivated this separate investigation. The number,  $n^{1/2}$ , originates from antisymmetrizing the captured electron [now part of  $H(^2S)$ ] with respect to the configuration  $p^{n-1}$  of the ion; i.e., the normalizing factor of the  $p$  orbital part of the ion,  $[(n-1)!]^{-1/2}$ , has to be changed to  $[n!]^{-1/2}$  to allow for the inclusion of the hydrogen atom coordinate in this group, and since  $n$  permutations are involved, the origin of this number is clear. (It will be recalled that the factor,  $(n+4)^{1/2}$ , was required using the methods in the main body of the text.) The next modification introduced is the decomposition of the triple sum of Eq. (8a) into the following three triple sums:

$$\sum_{M_S=-S}^S \sum_{M_L=-L}^L \left[ \sum_{M_L'=M_L} + \sum_{M_L'=M_L+1} + \sum_{M_L'=M_L-1} \right].$$

This expression represents the nonvanishing contributions to the sums of Eq. (8a). The result becomes self-evident when one considers the fact that coupling the components,  $m_l = \pm 1, 0$  of  $p(^2P)$  to the components,  $M_L'$  of a given term of the ion can change these  $M_L'$  values only by  $\pm 1, 0$ . From these considerations and the correspondence between the components of the momentum change variable,  $\mathbf{A}_1$ , ( $\mathbf{A}$  in this discussion) and the  $p$  orbitals,  $P_{\pm 1,0}(\mathbf{x}_1)$ , [see Eqs. (7a), (7b)] it is readily verified that the contribution from the sums of Eq. (8a) can be written as in Eq. (A1).

$$\begin{aligned} & (2S+1)n | \langle p^{n-1}(^2S'+1L') || p^n(^2S+1L) \rangle |^2 \\ & \times \sum_{M_L=-L}^L [A_z^2 \sum_{|M_L| \leq L'} |C(M_L, M_L)|^2 + |A_{-1}|^2 \\ & \times \sum_{|M_L+1| \leq L'} |C(M_L+1, M_L)|^2 \\ & + |A_1|^2 \sum_{|M_L-1| \leq L'} |C(M_L-1, M_L)|^2] g(\theta)^2. \quad (\text{A1}) \end{aligned}$$

The notation used here corresponds to the notation employed for the process defined by Eq. (A2).

$$\begin{aligned} & H^+ + A [p^n(^2S+1L)] \rightarrow H(1s) \\ & + A^+ [p^{n-1}(^2S'+1L')]; \quad n=3, 4. \quad (\text{A2}) \end{aligned}$$

In Eq. (A2),  $A$  denotes the atom and  $A^+$ , the ion. Much of the notation used in Eq. (A1) has been explained previously;  $g(\theta)$  is that part of the unsymmetrized amplitude that is independent of  $L$  and  $L'$ ; the quantities  $C(M_L', M_L)$  are the vector coupling coefficients, orbital and spin parts combined, that enter into the construction of  $\psi[p^n(LS M_L M_S)]$  from the various components of  $\psi[p^{n-1}(L'S' M_L' M_S')] p(M_L'' M_S'')$ ;  $p^n(LS M_L M_S)$ . For any of the  $p$ -orbital capture processes considered in this paper, the three sums in Eq. (A1) are equal,

TABLE III. Nitrogen cross sections,  $n=3$ .

Direct	Inverse
$Q(^4S \rightarrow ^3P) = Q(x)$	$Q(^3P \rightarrow ^4S) \approx (2, 9)Q(x)$
$Q(^2P \rightarrow ^1S) = (2/9)Q(x)$	$Q(^1S \rightarrow ^2P) \approx \frac{2}{3}Q(x)$
$Q(^2P \rightarrow ^1D) = (5/18)Q(x)$	$Q(^1D \rightarrow ^2P) \approx \frac{5}{6}Q(x)$
$Q(^2P \rightarrow ^3P) = \frac{1}{2}Q(x)$	$Q(^3P \rightarrow ^2P) \approx \frac{1}{2}Q(x)$
$Q(^2D \rightarrow ^1D) = \frac{1}{2}Q(x)$	$Q(^1D \rightarrow ^2D) \approx \frac{1}{2}Q(x)$
$Q(^2D \rightarrow ^3P) = \frac{1}{2}Q(x)$	$Q(^3P \rightarrow ^2D) \approx (5/18)Q(x)$

although the value of the sum is usually different for each process. (More will be said about this in a future publication.) Consequently, the sums appear as a common factor, denoted by  $\sum(L \rightarrow L')$ , and the desired numerical coefficient can now be identified in terms of its separate factors. The factor,  $(g_i)^{-1} = [(2S+1)(2L+1)]^{-1}$ , is taken from Eq. (8a), and it is combined with the other factors of Eq. (A1) to give the final result.

$$\begin{aligned} F(L \rightarrow L') &= (2L+1)^{-1} n \sum(L \rightarrow L') \\ & \times | \langle p^{n-1}(^2S'+1L') || p^n(^2S+1L) \rangle |^2. \quad (\text{A3}) \end{aligned}$$

This number,  $F(L \rightarrow L')$ , is the factor by which the quantity,  $Q(x)$ , (explained in the text) is multiplied to get the cross section for the processes of Eq. (A2). The BK formulas are now given for both the direct processes of Eq. (A2) and their inverses. By inverse process is meant the process obtained by reversing the direction of the arrow. The formulas for the inverse processes are only approximate in that small changes in velocities and reduced masses are ignored. The argument,  $x$ , of  $Q(x)$  [see Eq. (8b)] denotes the  $x$  value appropriate to the process. The cross sections in Tables III and IV are labeled by the terms of the atom and ion of Eq. (A2); e.g.,  $Q(^2S+1L \rightarrow ^2S'+1L')$ . Any other process between the ground-state terms of the ion and the atom violates the conservation of multiplicity, and therefore is forbidden in the absence of spin-dependent forces. Since the value of  $Q(x)$  differs only slightly among these possible processes for a given target atom, the ratios of the cross sections are nearly equal to the ratios of the numerical factors. Although the values of the cross sections are not representative of the actual cross section, except for very large impact energies, these ratios are perhaps good approximations to the ratios of the exact cross sections.

TABLE IV. Oxygen cross sections,  $n=4$ .

Direct	Inverse
$Q(^3P \rightarrow ^3S) = (4/9)Q(x)$	$Q(^4S \rightarrow ^3P) \approx \frac{4}{3}Q(x)$
$Q(^3P \rightarrow ^2D) = (5/9)Q(x)$	$Q(^2D \rightarrow ^3P) \approx \frac{5}{3}Q(x)$
$Q(^3P \rightarrow ^2P) = \frac{1}{3}Q(x)$	$Q(^2P \rightarrow ^3P) \approx \frac{1}{3}Q(x)$
$Q(^1D \rightarrow ^2D) = Q(x)$	$Q(^2D \rightarrow ^1D) \approx \frac{1}{2}Q(x)$
$Q(^1D \rightarrow ^2P) = \frac{1}{3}Q(x)$	$Q(^2P \rightarrow ^1D) \approx (5/36)Q(x)$
$Q(^1S \rightarrow ^2P) = \frac{1}{3}Q(x)$	$Q(^2P \rightarrow ^1S) \approx \frac{1}{3}Q(x)$



## APPENDIX II

In this Appendix some of the wave functions used are written as linear combinations of determinants. For economy of space the  $s$  orbitals are not written, but are understood. Only the first row of the determinant is written, and the notation used in Eq. (6) is used for the  $p$  orbitals; the customary symbols,  $\alpha$  and  $\beta$ , are used to denote the spin functions. The wave functions are labeled by their  $M_L$  and  $M_S$  values as  $\psi(M_L, M_S)$ .

Ground-State Configuration Terms for  $(2p)^3$ 

$$\begin{aligned}
 {}^4S: \quad \psi\left(\frac{3}{2}\right) &= \frac{1}{(7!)^{1/2}} |P_{-1}\alpha P_1\alpha P_0\alpha|, \\
 \psi\left(\frac{1}{2}\right) &= \frac{1}{(3 \times 7!)^{1/2}} (|P_{-1}\beta P_1\alpha P_0\alpha| + |P_{-1}\alpha P_1\alpha P_0\beta| + |P_{-1}\alpha P_1\beta P_0\alpha|) \cdots, \\
 {}^2D: \quad \psi\left(2, \frac{1}{2}\right) &= \frac{1}{(7!)^{1/2}} |P_1\beta P_1\alpha P_0\alpha|, \\
 \psi\left(1, \frac{1}{2}\right) &= \frac{1}{(2 \times 7!)^{1/2}} (|P_0\beta P_1\alpha P_0\alpha| - |P_{-1}\alpha P_1\alpha P_1\beta|), \\
 \psi\left(0, \frac{1}{2}\right) &= \frac{1}{(6 \times 7!)^{1/2}} (-2|P_{-1}\alpha P_1\alpha P_0\beta| + |P_{-1}\beta P_1\alpha P_0\alpha| + |P_{-1}\alpha P_1\beta P_0\alpha|), \\
 \psi\left(-1, \frac{1}{2}\right) &= \frac{1}{(2 \times 7!)^{1/2}} (|P_{-1}\beta P_1\alpha P_{-1}\alpha| - |P_{-1}\alpha P_0\alpha P_0\beta|), \\
 \psi\left(-2, \frac{1}{2}\right) &= \frac{1}{(7!)^{1/2}} |P_0\alpha P_{-1}\alpha P_{-1}\beta| \cdots, \\
 {}^2P: \quad \psi\left(1, \frac{1}{2}\right) &= \frac{1}{(2 \times 7!)^{1/2}} (|P_{-1}\alpha P_1\beta P_1\alpha| + |P_1\alpha P_0\beta P_0\alpha|), \\
 \psi\left(0, \frac{1}{2}\right) &= \frac{1}{(2 \times 7!)^{1/2}} (|P_0\alpha P_1\alpha P_{-1}\beta| - |P_0\alpha P_1\beta P_{-1}\alpha|), \\
 \psi\left(-1, \frac{1}{2}\right) &= \frac{1}{(2 \times 7!)^{1/2}} (|P_{-1}\alpha P_0\beta P_0\alpha| + |P_1\alpha P_{-1}\beta P_{-1}\alpha|) \cdots.
 \end{aligned}$$

Ground-State Configuration Terms for  $(2p)^4$ 

$$\begin{aligned}
 {}^3P: \quad \psi(1, 1) &= \frac{1}{(8!)^{1/2}} |P_1\alpha P_1\beta P_{-1}\alpha P_0\alpha|, \\
 \psi(1, 0) &= \frac{1}{(2 \times 8!)^{1/2}} (|P_1\alpha P_1\beta P_{-1}\beta P_0\alpha| + |P_1\alpha P_1\beta P_{-1}\alpha P_0\beta|), \\
 \psi(0, 1) &= \frac{1}{(8!)^{1/2}} |P_1\alpha P_{-1}\alpha P_0\alpha P_0\beta|, \\
 \psi(0, 0) &= \frac{1}{(2 \times 8!)^{1/2}} (|P_1\alpha P_{-1}\beta P_0\alpha P_0\beta| + |P_1\beta P_{-1}\alpha P_0\alpha P_0\beta|), \\
 \psi(-1, 1) &= \frac{1}{(8!)^{1/2}} |P_{-1}\alpha P_{-1}\beta P_0\alpha P_1\alpha| \cdots, \\
 \psi({}^1S) &= \frac{1}{(3 \times 8!)^{1/2}} (|P_1\alpha P_1\beta P_{-1}\alpha P_{-1}\beta| - |P_1\beta P_{-1}\alpha P_0\alpha P_0\beta| + |P_1\alpha P_{-1}\beta P_0\alpha P_0\beta|);
 \end{aligned}$$

$$\begin{aligned}
{}^1D: \quad \psi(2) &= \frac{1}{(8!)^{1/2}} |P_{1\alpha}P_{1\beta}P_{0\alpha}P_{0\beta}|, \\
\psi(1) &= \frac{1}{(2 \times 8!)^{1/2}} (|P_{1\alpha}P_{1\beta}P_{0\alpha}P_{-1\beta}| - |P_{1\alpha}P_{1\beta}P_{0\beta}P_{-1\alpha}|), \\
\psi(0) &= \frac{1}{(6 \times 8!)^{1/2}} (2|P_{1\alpha}P_{1\beta}P_{-1\alpha}P_{-1\beta}| + |P_{1\beta}P_{-1\alpha}P_{0\alpha}P_{0\beta}| - |P_{1\alpha}P_{-1\beta}P_{0\alpha}P_{0\beta}|), \\
\psi(-1) &= \frac{1}{(2 \times 8!)^{1/2}} (|P_{1\alpha}P_{0\beta}P_{-1\alpha}P_{-1\beta}| - |P_{1\beta}P_{0\alpha}P_{-1\alpha}P_{-1\beta}|), \\
\psi(-2) &= \frac{1}{(8!)^{1/2}} |P_{-1\alpha}P_{-1\beta}P_{0\alpha}P_{0\beta}|.
\end{aligned}$$

Although some of the wave functions for  $p^n({}^{2S+1}L)$  have been omitted from this list, enough are given to illustrate the structure when they are expressed as combinations of determinants. The wave functions for  $p^4({}^1D)$  and  $p^4({}^1S)$  require the following cfp's for their construction:

$$(p^3({}^2P) \parallel p^4({}^1S)) = 1; \quad (p^3({}^2P) \parallel p^4({}^1D)) = -\frac{1}{2}; \quad (p^3({}^2D) \parallel p^4({}^1D)) = -\sqrt{3}/2.$$

#### ACKNOWLEDGMENTS

The author is particularly grateful to Dr. F. R. Innes, a co-worker, for his introducing the author to the important literature of G. Racah, and for many instructive conversations. Gratitude is also expressed to Professor A. Dalgarno for many instructive conversations, and particularly for his suggesting the approximations that were used in estimating the cross sections for capture of *s*-subshell electrons. The author also expresses his gratitude to Professor D. R. Bates for many stimulating communications.