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Free-free transitions in collisions between slow electrons and neutral oxygen atoms

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The absorption coefficients for the free-free transitions in collisions between slow electrons and neutral oxygen atoms have been calculated for wavelengths in the range of 1 to 30 μm and temperatures between 5000 and 50 000 K. The wave functions of the unbound electron are the solutions of a one-electron Schrödinger-like continuum equation that includes the Coulomb, exchange, and polarization interactions with the oxygen atom. The polarization potential is determined by a first-principles calculation based on the method of polarized orbitals. Our absorption coefficients are in good agreement with those of John and Williams [J. Quant. Spectrosc. Radiat. Transfer **17**, 169 (1977)], but are much smaller than the experimental data of Taylor and Caledonia [J. Quant. Spectrosc. Radiat. Transfer **9**, 681 (1969)] and of Kung and Chang [J. Quant. Spectrosc. Radiat. Transfer **16**, 579 (1976)].

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I. INTRODUCTION

During an encounter with an atom, an electron may emit (bremsstrahlung) or absorb (inverse bremsstrahlung) a photon in a manner in which the atom is not affected energetically. Such free-free transitions of electrons are an important source of emission and absorption processes in the stellar atmospheres and the low-temperature plasmas [1–3].

The free-free transitions with the neutral atomic oxygen as a host have been studied theoretically by several groups [4–7]. Since the free-free transitions assume a particular importance at low incident electron energies, usually below the first excitation threshold, the target polarization is an important factor to consider in the theoretical calculation. Thus, in the work of Mjolsness and Ruppel [4] and of Geltman [5], an empirical polarization potential is included in the calculation of the continuum wave functions. John [6] obtained the absorption coefficients from the momentum-change cross sections by means of a formula suggested by Dalgarno and Lane [8]. Later, John and Williams [7] adopted the multichannel theory of Morgan and John [9] to calculate the absorption coefficients, utilizing the results of a close-coupling calculation of the electron-atom scattering [10]. The polarization effect was not included in the latter calculation [10], although target correlation was taken into account by the use of multiconfiguration (MC) target wave functions.

In this work, we account for the target polarization by means of the method of polarized orbitals, which Temkin [11] devised to study the *e*-O scattering and later extended to the *e*-H problem [12]. Henry has also applied this method to study the elastic scattering of the *e*-O system and photodetachment from O$^-$ [13]. In the polarized-orbitals method, the target polarization is made a part of the atomic wave functions, which depend parametrically on the incident-electron coordinates. The polarization potential is obtained from the polarized orbitals and is included in the scattering equation.

In Sec. II, we briefly discuss the basic formulation of free-free absorption and emission coefficients, and describe the method by which the free-electron functions are obtained. The polarized-orbitals method of Temkin, from which the polarization potentials are derived, is described in Sec. III. A short description of the numerical procedure is contained in Sec. IV. In Sec. V, we compare our results with the work of Geltman [5], with that of John and Williams [7], and with experiments [14,15]. Section VI concludes this paper.

II. THEORY

A. Absorption and emission coefficients

We study the free-free transition process,

$$e^-(\mathbf{k}_i)+\mathrm{O}(2p^4\,{}^3P)\rightarrow e^-(\mathbf{k}_f)+\mathrm{O}(2p^4\,{}^3P)\pm\hbar\omega\ , \qquad (1)$$

in which a photon is emitted ($+\hbar\omega$) or absorbed ($-\hbar\omega$). The conservation of energy gives the relationship

$$\frac{(k_i\hbar)^2}{2m}=\frac{(k_f\hbar)^2}{2m}\pm\hbar\omega\ . \qquad (2)$$

It is appropriate to construct the wave functions of the $(e^-+\mathrm{O})$ system that are eigenfunctions of the total orbital (L) and spin (S) angular momenta if we neglect the spin-orbit interaction. Then the transitions of interest are of the type,

$$[2p^4(S_1L_1)k_ilSL]\rightarrow[2p^4(S_1L_1)k_fl'SL']\ , \qquad (3)$$

where $S_1=L_1=1$ for the ${}^3P$ state, and (l,l') are the partial waves of the incident and scattered electrons. The dipole matrix elements for the above transition have been worked out [16]. Using these results, the formula for the absorption cross sections σ_{abs} [1,2] can be generalized, viz.,

$$\sigma_{\text{abs}}(k_i,\Delta k^2)=\frac{256\pi^2\alpha a_0^5}{3k_i^2k_f(\Delta k^2)^3}M^2\ , \qquad (4)$$

where α is the fine-structure constant,

$$\Delta k^2=|k_i^2-k_f^2|\ , \qquad (5)$$

$$M^2=\sum_{ll'} l_> \left\{ \sum_{SLL'} \frac{(2S+1)}{2(2S_1+1)} \frac{(2L+1)(2L'+1)}{(2L_1+1)} W^2(lLl'L';L_1 1)|M_{l,l'}^{LL'S}|^2 \right\} . \quad (6)$$

In the above, $l_>$ is the greater of l and l', W is the Racah coefficient, and

$$M_{l,l'}^{LL'S}=\int_0^\infty P_{k_i l}^{LS}(r)\frac{dV(r)}{dr}P_{k_f l'}^{L'S}(r)dr \ , \quad (7)$$

where $r^{-1}P_{k_i l}^{LS}(r)$ is the radial part of the continuum function of the free electron, and $V(r)$ is the potential that affects the free electron. If the dependency of $M_{l,l'}^{LL'S}$ on (L,L',S) is suppressed, the quantity inside the curly brackets in Eq. (6) reduces to $M_{l,l'}^2$ so that Eq. (4) reverts back to Eq. (6) of Ref. [2].

The (mean) absorption coefficient is obtained by averaging the cross sections over the Maxwellian distribution function $f(v,T)$ corresponding to the electron temperature T, viz.,

$$\kappa(\lambda,T)=\int_0^\infty \sigma_{\text{abs}}(k_i,\Delta k^2)f(v_i,T)dv_i \ , \quad (8)$$

where

$$f(v,T)dv=\frac{4}{\sqrt{\pi}}\left[\frac{m}{2kT}\right]^{3/2}\exp\left[-\frac{mv^2}{2kT}\right]v^2dv \ , \quad (9)$$

$$=198.0\Theta^{3/2}\exp(-31.3296\Theta k_i^2)k_i d(k_i^2) \ , \quad (10)$$

with

$$\Theta=5040/[T\ (\text{K})] \ , \quad (11)$$

so that

$$\kappa(\lambda,T)=\frac{5.05\times10^{-39}\Theta^{3/2}}{(\Delta k^2)^3}\int_0^\infty \frac{\exp(-31.3296\Theta k_i^2)}{k_i k_f} \times M^2 d(k_i^2) \ . \quad (12)$$

The wavelength λ and Δk^2 are related as

$$[\lambda\ (\text{Å})]=911.8/[\Delta k^2\ (\text{a.u.})] \ . \quad (13)$$

The cross sections in Eq. (4) are expressible in units of cm^5 [1] after a substitution of $a_0=0.529\times10^{-8}$ cm, so that the absorption coefficients in Eq. (12) are also in units of cm^5. The absorption cross sections and coefficients are frequently multiplied by the electron density n that would give rise to a pressure of 1 dyn/cm^2 at temperature T,

$$[n\ (\text{cm}^{-3})]=0.724\times10^{16}/[T\ (\text{K})] \quad (14)$$

per dyn/cm^2 [1], so that the cross sections and coefficients are now expressible in cm^4/dyn. The photons involved in the absorption also induce emission so that the absorption coefficients are sometimes multiplied by a factor $[1-\exp(-h\nu/kT)]$ [1]. In this paper, we do not include this factor unless specifically stated otherwise.

The expression of the emission cross sections has been given in Refs. [4,5]. However, a more pertinent quantity in applications is the emissivity in units of W cm^3/(μm sr) [5], which we found to be

$$J(\lambda,T)=\frac{0.794\,814\times10^{-31}}{[\lambda(\mu\text{m})]^2}\Theta^{3/2}\int_{v_0}^\infty \frac{\exp(-31.3296\Theta k_i^2)}{k_i k_f} \times M^2 d(k_i^2) \ , \quad (15)$$

where v_0 is the threshold velocity of the free electron for emission, i.e.,

$$\tfrac{1}{2}mv_0^2=\hbar\omega \ , \quad (16)$$

and the symbol $[\lambda\ (\mu\text{m})]$ indicates that λ is to be expressed in μm. The emissivity in this work was computed by Eq. (15). Geltman [5] also gave the relationship

$$J(\lambda,T)=\frac{1.19\times10^4}{[\lambda(\mu\text{m})]^5}\exp\left[-\frac{1.439\times10^4}{[\lambda(\mu\text{m})][T\ (\text{K})]}\right]\kappa(\lambda,T) \ , \quad (17)$$

which can be used to check the consistency between Eqs. (12) and (15).

B. Free-electron function $P_{kl}^{LS}(r)$

The reduced radial function $P_{kl}^{LS}(r)$ is obtained as the solution of the integro-differential equation

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-V_{\text{Coul}}^L(r)-V_{\text{pol}}^L(r)+k^2\right]P_{kl}^{LS}(r)$$

$$=\sum_{n'l'\lambda} W_{n'l'\lambda,kl}^{LS}\mathcal{P}_{n'l'}(r)+\sum_{n'l'}\delta_{l'l}C_{n'l'}\mathcal{P}_{n'l'}(r) \ , \quad (18)$$

where V_{Coul}^L and V_{pol}^L are the Coulomb potential due to the unperturbed atomic orbitals and the polarization correction (to be discussed in Sec. III), respectively. The first term on the right-hand side is the exchange interaction term, and the second term is to ensure the orthogonality with the bound atomic orbitals $\mathcal{P}_{nl}$. The dependency on the angular momenta L and S is indicated as superscripts. Because the $2p$ shell in O($1s^22s^22p^4$) is not completely filled, the composite nine-electron wave function of the e-O system may contain a term corresponding to the $1s^22s^22p^5$ configuration of the O$^-$ ion, which is not considered in the present work. Inclusion of the $1s^22s^22p^5$ configuration would introduce additional terms to Eq. (18), as discussed in Ref. [17], and would greatly increase the complexity of the computational procedure.

With regard to the present problem of O$^-[1s^22s^22p^4(^3P)kl\,^{2,4}L]$, the unperturbed orbitals of the oxygen atom are

$$\phi_{nlm}^0(\mathbf{r})=Y_{lm}(\hat{\mathbf{r}})r\mathcal{P}_{nl}(r) \ , \quad (19)$$

and the Coulomb potential is

$$V^L_{\text{Coul}}(r)=2\left\{-\frac{Z}{r}+2y_0(1s,1s|r)+2y_0(2s,2s|r)\right.$$
$$\left.+4y_0(2p,2p|r)+\tfrac{1}{5}v^L_2 y_2(2p,2p|r)\right\}, \tag{20}$$

where Z is the nuclear charge,

$$y_\lambda(nl,n'l'|r)=r^{-\lambda-1}\int_0^r \mathcal{P}_{nl}(t)\mathcal{P}_{n'l'}(t)t^\lambda dt$$
$$+r^\lambda\int_r^\infty \mathcal{P}_{nl}(t)\mathcal{P}_{n'l'}(t)t^{-\lambda-1}dt\ , \tag{21}$$

and v^L_2 is equal to $l/(2l+3)$, -1, and $(l+1)/(2l-1)$ for $L=l+1,l,l-1$, respectively. The exchange terms are

$$\sum_{n'l'\lambda} W^{LS}_{n'l'\lambda,kl}(r)\mathcal{P}_{n'l'}(r)=2\left\{-\frac{1}{2l+1}y_l(1s,kl|r)\mathcal{P}_{1s}(r)-\frac{1}{2l+1}y_l(2s,kl|r)\mathcal{P}_{2s}(r)\right.$$
$$\left.+w^{LS}_{l+1}y_{l+1}(2p,kl|r)\mathcal{P}_{2p}(r)+w^{LS}_{l-1}y_{l-1}(2p,kl|r)\mathcal{P}_{2p}(r)\right\}, \tag{22}$$

where $y_l(nl,kl|r)$ can be obtained from Eq. (21) by substituting $P^{LS}_{kl}(t)$ for $\mathcal{P}_{n'l'}(t)$. The coefficients w^{LS}_λ are shown in Table I. Throughout the work, we have used the wave functions of Clementi and Roetti [18] for the unperturbed orbitals. Finally, Eq. (18) is to be solved subject to the boundary condition,

$$\lim_{r\to\infty} P^{LS}_{kl}(r)=\sin(kr-\tfrac{1}{2}l\pi+\eta^{LS}_{kl})\ , \tag{23}$$

where η^{LS}_{kl} is the phase shift due to interaction with the atom. Determination of the polarization potential $V^L_{\text{pol}}(r)$ in Eq. (18) will be taken up in Sec. III.

TABLE I. Values of ω^{LS}_λ in Eq. (22).

		w^{LS}_λ	
S	L	$\lambda=l+1$	$\lambda=l-1$
$\frac{3}{2}$	$\begin{Bmatrix} l+1 \\ l \\ l-1 \end{Bmatrix}$	$-\frac{3(l+1)}{(2l+1)(2l+3)}$	$-\frac{3l}{(2l-1)(2l+1)}$
$\frac{1}{2}$	$l+1$	$\frac{3l(2l+5)}{2(2l+1)(2l+3)^2}$	$-\frac{3l}{(2l-1)(2l+1)}$
$\frac{1}{2}$	l	$\frac{3(l-2)}{2(2l+1)(2l+3)}$	$\frac{3(l+3)}{2(2l-1)(2l+1)}$
$\frac{1}{2}$	$l-1$	$-\frac{3(l+1)}{(2l+1)(2l+3)}$	$\frac{3(2l-3)(l+1)}{2(2l-1)^2(2l+1)}$

III. METHOD OF POLARIZED ORBITALS

In this section, we briefly recall the essential steps in Temkin's method of polarized orbitals [11], ultimately leading to the polarization potential $V^L_{\text{pol}}(r)$ in Eq. (18). The details are found in the works of Temkin and coworkers [11–13]. Here the distortion of the target atom caused by the perturbation of the free electron at $\mathbf{r}_{N+1}$ is treated in an adiabatic, dipole approximation with the proviso that the perturbing electron is outside the atomic electrons. Thus the perturbation is taken as

$$H'=\left[\frac{4\pi}{3}\right]\frac{1}{r^2_{N+1}}\sum_{i=1}^{N} r_i\varepsilon(r_i,r_{N+1})$$
$$\times\sum_{\mu=-1}^{1} Y^*_{1\mu}(\hat{\mathbf{r}}_i)Y_{1\mu}(\hat{\mathbf{r}}_{N+1})\ , \tag{24}$$

$$\varepsilon(r_i,r_{N+1})=\begin{cases}1 & \text{for } r_{N+1}\geq r_i\\ 0 & \text{for } r_{N+1}<r_i\ .\end{cases} \tag{25}$$

To construct the wave function of O(^3P), we start with the unperturbed one-electron functions of the oxygen atom [18] as shown in Eq. (19). Following Temkin, we add a polarization correction to each ϕ^0_{nlm} to form a polarized orbital, which depends parametrically on $\mathbf{r}_{N+1}$ as

$$\phi_{nlm}(\mathbf{r},\mathbf{r}_{N+1})=\phi^0_{nlm}(\mathbf{r})+\lambda\phi^{\text{cor}}_{nlm}(\mathbf{r},\mathbf{r}_{N+1})\ , \tag{26}$$

$$\lambda\phi^{\text{cor}}_{nlm}(\mathbf{r},\mathbf{r}_{N+1})=\varepsilon(r,r_{N+1})\sum_{l'm'}Y_{1,m-m'}(\hat{\mathbf{r}}_{N+1})$$
$$\times\phi'_{nlm\to l'm'}(\mathbf{r})\ . \tag{27}$$

It is convenient to define

$$\phi'_{nlm\to l'm'}(\mathbf{r})=c(lm\to l'm')Y_{l'm'}(\hat{\mathbf{r}})rP_{nlm\to l'm'}(r)\ , \tag{28}$$

where

$$c(lm\to l'm')=2(-1)^{m'-m}\left[\frac{4\pi(2l+1)}{(2l'+1)}\right]^{1/2}c(1m'-mlm;l'm')c(10l0;l'0)\ . \tag{29}$$

In the above, $c(j_1m_1j_2m_2;jm)$ is the Clebsch-Gordan coefficient; thus we see that $|l'-l|=1$ and $|m'-m|=0,1$.

The radial function $P_{nlm\to l'm'}(r)$ is obtained as the solution of the differential equation,

$$\left[\frac{d^2}{dr^2}-\frac{l'(l'+1)}{r^2}-V'_{\mathrm{Coul}}(r)+E_{nl}\right]P_{nlm\to l'm'}(r)=\sum_{n''l''\lambda}W'_{n''l''\lambda,l'm'}(r)P_{nlm\to l'm'}(r)+\sum_{n''l''}\delta_{l'',l'}C_{n''l''}\mathcal{P}_{n''l''}(r)+r\mathcal{P}_{nl}(r)\ . \tag{30}$$

Here the Coulomb (V'_{Coul}) and exchange (W') potentials are obtainable by subjecting to the Hartree-Fock procedure the determinantal wave functions in which the parent orbitals $\phi^0_{nlm}(\mathbf{r})$ are replaced by the polarized version of Eq. (26). The function $P_{nlm\to l'm'}(r)$ approaches zero as $r\to\infty$, and for small r,

$$\lim_{r\to 0} P_{nlm\to l'm'}(r)=ar^{l'+1}\ . \tag{31}$$

In this work, we have obtained the $P_{nlm\to l'm}$ functions associated with the unperturbed orbitals $nl=2s$ and $2p$. For later reference, they are listed in Table II and are referred to simply as P_i therein. From these polarized orbitals, we obtained the dipole polarizability of $5.084a_0^3$ compared with the experimental value of 5.2 ± 0.4 [19]. Other theoretical values range from 4.63 to 5.41 [20]. In general the polarized orbitals $P_{nlm\to l'm'}$ depend on m and m' as well as on l and l' due to the difference in exchange term in Eq. (30), so that only two pairs are identical among the fifteen functions in Table II; that is, P_5 and P_6, and P_{10} and P_{12}. This dependency on m and m' manifests itself, for example, in the calculation of dipole polarizability in which a difference up to 20% is found in the matrix elements.

When the target wave functions are described by the unperturbed orbitals ϕ^0, the Coulomb potential $V^L_{\mathrm{Coul}}(r)$ seen by the free electron (coordinate $\mathbf{r}$) consists of constituent terms due to all occupied $n'l'$ orbitals, such as

$$v_{n'l'}(r)=\int Y^*_{lm}(\hat{\mathbf{r}})Y_{lm}(\hat{\mathbf{r}})|\mathbf{r}-\mathbf{r}'|^{-1}\times\phi^{0*}_{n'l'}(\mathbf{r}')\phi^0_{n'l'}(\mathbf{r}')d\mathbf{r}'d\hat{\mathbf{r}}\ . \tag{32}$$

As a consequence of the polarization of the $n'l'$ orbital, augmentation of the target orbitals by the polarization correction $\lambda\phi^{\mathrm{cor}}_{nlm}$ in accordance with Eqs. (26) and (27) produces additional (polarization) terms, to the first order in λ, of the form

$$v_{n'l'm'\to l''m''}(r)=\int Y^*_{lm}(\hat{\mathbf{r}})Y_{lm}(\hat{\mathbf{r}})|\mathbf{r}-\mathbf{r}'|^{-1}\times\phi^{0*}_{n'l'}(\mathbf{r}')\phi'_{n'l'm'\to l''m''}(\mathbf{r}')d\mathbf{r}'d\hat{\mathbf{r}}\ . \tag{33}$$

The polarization potentials associated with the Coulomb interaction, which can be derived variationally [11], are composed of a series of such integrals, and can be cast into the general form

$$V^L_{\mathrm{pol}}(r)=-\frac{2}{r^4}\sum_j C_jF_{u(j)}(l)\int_0^r\mathcal{P}_j(t)P_{B(j)}(t)t\,dt\ . \tag{34}$$

The notation used here requires some explanation. We have a summation over j, which ranges from 1 to 15 for $L=l+1$, 1 to 21 for $L=l$, and 1 to 31 for $L=l-1$, as shown in Table III. For each value of j, we also list C_j, $u(j)$, $\mathcal{P}_j$, and $B(j)$ in Table III for the three possible choices of $L=l+1$, l, and $l-1$. To identify $P_{B(j)}$, let us take an example of, say, $j=5$ with $L=l+1$. The associated $B(j)$ is 7 according to Table III. We then go to the entry of $i=7$ in Table II and find that $P_{B(j=5)}$ is $P_{2p,1\to2,2}$. From Table IV we find $F_{u(j)}$ for each j in a similar way. $\mathcal{P}_j$ is the reduced radial function of the unperturbed target orbitals as defined in Eq. (19), with $\mathcal{P}_j=\mathcal{P}_{2s}$ for $j\le3$ and $\mathcal{P}_j=\mathcal{P}_{2p}$ for $j>3$.

The exchange potential is also modified by the inclusion of polarization. The effects of the polarization on the exchange term have been examined by Henry [13] in his work on the elastic scattering of electrons from the oxygen atom. The inclusion of this exchange term was found to change the s-wave ($l=0$) cross sections by only 10%. For the higher partial waves ($l>0$), the difference is even smaller (4%), so that the influence of the polarization of the orbitals via exchange is seen to be rather marginal. For this reason, we do not consider in this paper the polarization correction on the electron exchange. Also omitted from Eq. (18) for simplicity is a term due to the Laplacian acting on the step function $\varepsilon(r_i,r_{N+1})$ [13].

TABLE II. Polarized corrections $P_{nlm\to l'm'}$ that are equivalently referred to simply as P_i.

i	$nl,m\to l',m'$	
1	$2s,0$	$1,1$
2	$2s,0$	$1,0$
3	$2s,0$	$1,-1$
4	$2p,1$	$0,0$
5	$2p,0$	$0,0$
6	$2p,-1$	$0,0$
7	$2p,1$	$2,2$
8	$2p,1$	$2,1$
9	$2p,1$	$2,0$
10	$2p,0$	$2,1$
11	$2p,0$	$2,0$
12	$2p,0$	$2,-1$
13	$2p,-1$	$2,0$
14	$2p,-1$	$2,-1$
15	$2p,-1$	$2,-2$

IV. NUMERICAL PROCEDURES

The integro-differential equations of Eqs. (18) and (30) are solved noniteratively by using the Lagrange-multiplier technique, as we have done previously [21]. The inhomogeneity terms, which arise due to the electron exchange, orthogonality, and perturbation, are set to zero after $r=13.5a_0$. This corresponds to the r value at which the $2p$ function has decreased to 10^{-5} of its peak value. At this point, the Lagrange multipliers are determined, and the complete solution is constructed as a linear combination of the particular integrals and homogeneous solution. Beyond $r=13.5a_0$, Eqs. (18) and (30) are considered to be homogeneous differential equations.

For the free-electron functions, the phase shift η is determined at various points 50 to $250a_0$ apart starting at $450a_0$, until two successive values agree within 0.01%. To solve for the polarization correction functions of Eq. (30), the numerical solution is first initiated with a certain arbitrary value of a in Eq. (31). The resulting solution obtained by numerical integration in general would diverge at large r, say, tending to $+\infty$ as $r \rightarrow \infty$. The value of a used here is denoted by a_+. We then change the value of a until the resulting solution tends to $-\infty$ at large r, and this new choice of a is denoted by a_-. By successive interpolation between a_+ and a_-, we develop a numerical solution for $P_{nlm \rightarrow l'm'}(r)$ that monotonically

TABLE III. List of constituent parts that describe the polarization potential $V^L_{\mathrm{pol}}(r)$ in Eq. (34).

j	C_j	$u(j)$	$\mathcal{P}_j$	$B(j)$
		$L=l+1$		
1	$\frac{4}{3}$	1	2s	1
2	$\frac{4}{3}$	2	2s	2
3	$\frac{4}{3}$	1	2s	3
4	$\frac{4}{3}$	1	2p	4
5	$\frac{8}{5}$	1	2p	7
6	$\frac{4}{5}$	2	2p	8
7	$\frac{4}{15}$	1	2p	9
8	$\frac{2}{3}$	2	2p	5
9	$\frac{2}{5}$	1	2p	10
10	$\frac{8}{15}$	2	2p	11
11	$\frac{2}{5}$	1	2p	12
12	$\frac{2}{3}$	1	2p	6
13	$\frac{2}{15}$	1	2p	13
14	$\frac{2}{5}$	2	2p	14
15	$\frac{4}{5}$	1	2p	15
		$L=l$		
1	$\frac{4}{3}$	3	2s	1
2	$\frac{4}{3}$	4	2s	2
3	$\frac{4}{3}$	3	2s	3
4	$\frac{2}{3}$	5	2p	4
5	$\frac{4}{5}$	5	2p	7
6	$\frac{2}{5}$	6	2p	8
7	$\frac{2}{15}$	5	2p	9
8	$\frac{2}{3}$	7	2p	5
9	$\frac{2}{5}$	8	2p	10
10	$\frac{8}{15}$	7	2p	11
11	$\frac{2}{5}$	8	2p	12
12	$\frac{2}{3}$	3	2p	6
13	$\frac{2}{15}$	3	2p	13
14	$\frac{2}{5}$	4	2p	14
15	$\frac{4}{5}$	3	2p	15
16	$-\frac{2}{3}$	9	2p	5
17	$-\frac{2}{5}$	9	2p	10
18	$\frac{4}{15}$	9	2p	11
19	$-\frac{2}{3}$	9	2p	4
20	$-\frac{2}{5}$	9	2p	8
21	$\frac{4}{15}$	9	2p	9
		$L=l-1$		
1	$\frac{4}{3}$	10	2s	1
2	$\frac{4}{3}$	11	2s	2
3	$\frac{4}{3}$	10	2s	3
4	$\frac{2}{3}$	12	2p	4
5	$\frac{4}{5}$	12	2p	7
6	$\frac{2}{5}$	13	2p	8
7	$\frac{2}{15}$	12	2p	9
8	$\frac{2}{3}$	14	2p	5
9	$\frac{2}{5}$	15	2p	10
10	$\frac{8}{15}$	14	2p	11
11	$\frac{2}{5}$	15	2p	12
12	$\frac{2}{3}$	16	2p	6
13	$\frac{2}{15}$	16	2p	13
14	$\frac{2}{5}$	17	2p	14
15	$\frac{4}{5}$	16	2p	15
16	$-\frac{2}{3}$	18	2p	5
17	$-\frac{2}{5}$	18	2p	10
18	$\frac{4}{15}$	18	2p	11
19	$-\frac{2}{3}$	18	2p	4
20	$-\frac{2}{5}$	18	2p	8
21	$\frac{4}{15}$	18	2p	9
22	$\frac{4}{3}$	19	2p	6
23	$\frac{4}{15}$	19	2p	13
24	$\frac{4}{3}$	19	2p	4
25	$\frac{4}{15}$	19	2p	9
26	$\frac{2}{3}$	20	2p	6
27	$-\frac{4}{15}$	20	2p	13
28	$\frac{2}{5}$	20	2p	14
29	$\frac{2}{3}$	20	2p	5
30	$-\frac{4}{15}$	20	2p	11
31	$\frac{2}{5}$	20	2p	12

decreases up to $r=20a_0$.

The dipole matrix elements are computed by the velocity form instead of the acceleration form shown in Eq. (7). The length and acceleration forms may be derived from and are equivalent to the velocity form if the wave functions are exact eigenfunctions of the atomic Hamiltonian. Using a short-hand notation of $\gamma=(LSkl)$, we have

$$M_{l,l'}^{LL'S}=\frac{(\Delta k^2)a_0}{2}\int_0^\infty P_\gamma(r)\left[\frac{d}{dr}+\frac{l_>(l'-l)}{r}\right]P_{\gamma'}(r)dr\ , \tag{35}$$

where $l_>$ is the greater of l and l'. The limits of integral $(0,\infty)$ are divided into two regions $(0,R)$ and (R,∞), where R is the value of r at which the asymptotic form of Eq. (23) sets in. The integration in the interval $(0,R)$ is carried out numerically. For the interval (R,∞), the integrals are expressed in closed forms analogous to those given in Ref. [22].

TABLE IV. The l-dependent function $F_i(l)$ in the polarization potential $V_{\text{pol}}^L(r)$ in Eq. (34).

i	$F_i(l)$
1	$\frac{(l+1)}{(2l+3)}$
2	$\frac{1}{(2l+3)}$
3	$\frac{l(l+2)}{(l+1)(2l+3)}$
4	$\frac{(l+3)}{(l+1)(2l+3)}$
5	$\frac{l(l+3)}{(l+1)(2l+3)}$
6	$\frac{(l+6)}{(l+1)(2l+3)}$
7	$\frac{1}{(l+1)}$
8	$\frac{l}{(l+1)}$
9	$\frac{l}{(l+1)(2l+3)}$
10	$\frac{(2l^3-l^2-l+1)}{l(2l-1)(2l+1)}$
11	$\frac{(2l^2+l-2)}{l(2l-1)(2l+1)}$
12	$\frac{(4l^4+4l^3-3l^2-4l+6)}{l(2l-1)(2l+1)(2l+3)}$
13	$\frac{(4l^3+8l^2+9l-15)}{l(2l-1)(2l+1)(2l+3)}$
14	$\frac{(4l^3+20l^2-13l-3)}{l(2l-1)(2l+1)(2l+3)}$
15	$\frac{(4l^4+8l^3-9l^2+3)}{l(2l-1)(2l+1)(2l+3)}$
16	$\frac{(8l^4+4l^3-8l^2+3)}{l(2l-1)(2l+1)(2l+3)}$
17	$\frac{(8l^3+4l^2-6)}{l(2l-1)(2l+1)(2l+3)}$
18	$\frac{(2l-3)}{l(2l+1)(2l+3)}$
19	$\frac{1}{(2l+1)(2l+3)}$
20	$\frac{(2l-1)}{(2l+1)(2l+3)}$

Using our computational procedures, we obtain virtually identical results for various entries in Tables 3 and 5 of Ref. [2]. In these calculations of free-free transitions in a H atom, the difference between the velocity and acceleration forms was typically 1.5% or less.

V. RESULTS

In Eq. (6), we have $L_1=S_1=1$ for the present problem (^3P ground state of the O atom), and S takes on $\frac{1}{2}$ and $\frac{3}{2}$. We have also set the limit of $(l,l')\leq 4$, and (L,L') to all values consistent with (l,l'). For a given value of the wavelength λ (equivalently, of Δk^2), we have computed the cross sections at 200 different values of incident-electron energy from 0 to 1.2 a.u. as shown in Table V. The process of averaging over the Maxwell-Boltzmann distribution in Eqs. (12) and (15) was carried out by interpolating between these 200 points. The resulting continuous absorption coefficients in Eq. (12) are shown in Table VI and the emissivity of Eq. (15) in Table VII.

Geltman [5] made an extensive calculation of the free-free absorption coefficients for a number of neutral-atom systems, including the oxygen atom. A Hartree-Fock-Slater-type potential was used to describe the Coulomb and exchange interaction of the free electron with the neutral atom, and an empirical polarization potential was added. The matrix elements are then evaluated in the acceleration form. At 10 000 K, Geltman's values are 25 to 30% smaller than our values as shown in Table VIII. A more detailed comparison of Table 4 of Ref. [5] and Table VI of the present paper shows that the coefficients of Ref. [5] are smaller than the present values at the lower electron temperatures and longer wavelengths of

TABLE V. Quadrature of the incident-electron energy k^2 in a.u. For each region, k^2 runs from k_A^2 to k_B^2 in increments of δk^2.

Region	k_A^2	δk^2	k_B^2
1	0.0	6.25×10^{-4}	0.025
2	0.025	1.25×10^{-3}	0.050
3	0.050	2.50×10^{-3}	0.100
4	0.100	5.0×10^{-3}	0.200
5	0.200	1.0×10^{-2}	1.200

TABLE VI. Absorption coefficients $\kappa(\lambda, T)$ of Eq. (12) in units of cm^5. The wavelengths λ are in μm, and the temperature T in kelvins. Numbers inside the brackets indicate the power of 10.

T (K) $\lambda(\mu$m)	5000	10 000	15 000	20 000	30 000	50 000
1.0	9.31[−40]	1.53[−39]	2.18[−39]	2.87[−39]	4.28[−39]	6.19[−39]
2.0	5.25[−39]	9.72[−39]	1.46[−38]	1.99[−38]	3.07[−38]	4.58[−38]
3.5	2.30[−38]	4.63[−38]	7.20[−38]	9.98[−38]	1.56[−37]	2.37[−37]
5.0	6.12[−38]	1.28[−37]	2.02[−37]	2.83[−37]	4.48[−37]	6.83[−37]
7.5	1.91[−37]	4.15[−37]	6.65[−37]	9.37[−37]	1.49[−36]	2.28[−36]
10.0	4.35[−37]	9.66[−37]	1.56[−36]	2.20[−36]	3.50[−36]	5.36[−36]
15.0	1.41[−36]	3.19[−36]	5.15[−36]	7.28[−36]	1.16[−35]	1.79[−35]
20.0	3.29[−36]	7.41[−36]	1.20[−35]	1.70[−35]	2.74[−35]	4.22[−35]
25.0	6.30[−36]	1.43[−35]	2.32[−35]	3.30[−35]	5.32[−35]	8.21[−35]
30.0	1.07[−35]	2.44[−35]	3.98[−35]	5.68[−35]	9.16[−35]	1.42[−34]

TABLE VII. Emissivity $J(\lambda, T)$ of Eq. (15) in units of W cm^3/(μm sr). The wavelengths λ are in units of μm, and the temperature T in K. Numbers inside the brackets indicate the power of 10.

T (K) $\lambda(\mu$m)	5000	10 000	15 000	20 000	30 000	50 000
1.0	6.22[−37]	4.32[−36]	9.94[−36]	1.66[−35]	3.10[−35]	5.24[−35]
2.0	4.63[−37]	1.76[−36]	3.37[−36]	5.17[−36]	8.92[−36]	1.44[−35]
3.5	2.30[−37]	6.96[−37]	1.24[−36]	1.84[−36]	3.09[−36]	4.88[−36]
5.0	1.31[−37]	3.66[−37]	6.37[−37]	9.35[−37]	1.55[−36]	2.43[−36]
7.5	6.53[−38]	1.72[−37]	2.94[−37]	4.28[−37]	7.02[−37]	1.10[−36]
10.0	3.89[−38]	9.97[−38]	1.69[−37]	2.44[−37]	3.98[−37]	6.18[−37]
15.0	1.88[−38]	4.57[−38]	7.60[−38]	1.09[−37]	1.77[−37]	2.75[−37]
20.0	1.06[−38]	2.57[−38]	4.27[−38]	6.13[−38]	9.95[−38]	1.55[−37]
25.0	6.99[−39]	1.65[−38]	2.73[−38]	3.92[−38]	6.37[−38]	9.90[−38]
30.0	4.77[−39]	1.14[−38]	1.89[−38]	2.72[−38]	4.42[−38]	6.88[−38]

TABLE VIII. Comparisons of the absorption coefficients $\kappa(\lambda, T)$ of Eq. (12) in cm^5 with other theoretical works [5,7] and with the experimental values of Ref. [14]. Numbers inside the brackets indicate the power of 10.

λ (μm) Method	2.0	3.5	5.0	10
Present ($T=10\,000$ K)	9.72[−39]	4.63[−38]	1.28[−37]	9.66[−37]
Ref. [5] ($T=10\,000$ K)	7.13[−39]		8.97[−38]	6.68[−37]
Ref. [7] ($T=9\,700$ K)	9.6[−39]	4.67[−38]	1.31[−37]	
Expt. [14] ($T=9\,700$ K)	29[−39]	10[−38]	2.6[−37]	
λ (μm) Method	1.14	1.52	2.28	4.56
Present ($T=5\,000$ K)	1.2[−39]	2.5[−39]	7.3[−39]	4.9[−38]
Ref. [7] ($T=5\,040$ K)	1.09[−39]	2.28[−39]	6.60[−39]	4.38[−38]

the absorbed photon. At higher temperatures the difference becomes smaller, and at 20 000 K the two sets are nearly identical. John [6] derived the free-free absorption coefficients involving various atoms and molecules by means of the formula suggested by Dalgarno and Lane [8]. The data of John for oxygen [6] are reported to be in good agreement with those of Geltman [5], particularly for $\lambda > 1.0\ \mu$m.

A new theoretical treatment was subsequently offered by John and Williams [7] in which they applied the multichannel theory [9] to obtain the free-free absorption coefficients for the *e*-O scattering system. For the continuum orbitals, they used the scattering data from the three-state ($^3P, ^1D, ^1S$ of the ground configuration) close-coupling calculation of Saraph [10]. The bound states were described by the three-configuration wave functions. In Table VIII, we compare their absorption coefficients at 9700 K, computed by the velocity form, with ours at 10 000 K. In making this comparison, two points should be mentioned. First, we estimate our absorption coefficients at 9700 K to be about 3% smaller than the ones at 10 000 K shown in Table VIII. Secondly, the coefficients of John and Williams contain the contributions from cases other than the oxygen atom being in the ground ^3P state before and after the collision. However, the ^3P-^3P contribution is expected to occupy greater than 90% of the total at 9700 K, since its percentage is 90% at 12 600 K and 99% at 5040 K (see Table 3 of Ref. [7]). Thus, after accounting for the other contributions, the absorption coefficients of this work and of Ref. [7] differ by about 10% or less at 10 000 K. In Table 5 of Ref. [7], John and Williams also give the absorption coefficients that include the factor for the stimulated emission. In Table VIII of this paper, we include their values at 5040 K, adjusted so as to exclude the stimulated-emission factor and to be expressible in units of cm^5. These values are seen to be about 10% smaller than our interpolated counterparts at 5000 K. Thus the agreement is quite good.

From the solutions of Eq. (18), we have also calculated the elastic cross sections at several energies so as to compare with the cross-section calculations of Henry [13] based on a similar polarized-orbitals approach. Our elastic cross sections for electron impact on oxygen atoms are somewhat ($\sim$25%) larger than those of Henry. For instance, at 0.5, 1.0, and 4.0 eV, our elastic cross sections are 3.7×10^{-16}, 5.2×10^{-16}, and 7.6×10^{-16} cm^2 respectively, compared to the corresponding values of 3.0×10^{-16}, 3.8×10^{-16}, and 5.8×10^{-16} cm^2 as read from Fig. 2 of Ref. [13]. The difference may be attributed to the differing approximations made in the present work, within the method of polarized orbitals, and that of Henry [13]. Henry included the term arising from the Laplacian acting on the step function [Eq. (25)] as well as the exchange-polarization terms that were omitted in our calculations. On the other hand, the differential equation for the polarization correction to the orbitals in Henry's paper involves an approximation that is not used in our work. Comparison with the experimental elastic cross sections has been addressed in the earlier theoretical papers [10,13], but the scatter of the different sets of experimental data are such that definitive conclusions are difficult to draw.

From a shock-heated plasma experiment, Taylor and Caledonia [14] obtained the absorption coefficients, which are shown in Table VIII as "Expt." In a similar experiment Kung and Chang [15] found the absorption coefficients of 7.8×10^{-38} and 3×10^{-36} cm^5 for $\lambda=3.1$ and 9.85 μm, respectively, both at the electron temperature of 9700 K. Those experimental values are about two to three times larger than the present values and those of Ref. [7]. Beyond the obvious difficulties associated with the experiments that are discussed in Refs. [14] and [15], we can offer no clear explanation for the discrepancy between the experiment and theory. In view of the generally good agreement among different theoretical calculations, further experimental works would be valuable.

VI. CONCLUSION

In an electron-atom collision, the polarization of the target atom is an important and yet difficult feature to incorporate into the theoretical formalism. In this paper, we approached the problem of the target polarization with the method of polarized orbitals. We found that this method gives the dipole polarizability of $5.084a_0^3$, which is quite comparable to the range of values 4.63 to 5.41 by other calculations [20].

With respect to the free-free absorption coefficients, our values show very good agreement with the previous theoretical calculations, particularly with the results of John and Williams [7]. However, the theoretical absorption coefficients are smaller by a factor of about two or three compared to the experimental values. Further experimental works are needed to clarify this discrepancy.

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