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Oscillator strengths for spin-changing P–D transitions in He I including the effect of a finite nuclear mass and intermediate coupling

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Abstract. We have calculated the electric dipole (E1) oscillator strengths and spontaneous decay rates for 12 spin-changing P–D transitions of atomic helium. We included the effects of the finite nuclear mass and the anomalous magnetic moment of the electron. The specific transitions for ⁴He are $n\ ^1P_1^o - n'\ ^3D_{1,2}$ and $n\ ^3P_{1,2}^o - n'\ ^1D_2$ with $n = 2, 3, 4$ and $n' = 3, 4$. To include the effects of intermediate coupling between pure LS and jj , we used the Breit formulation for the spin-orbit and spin-other-orbit operators and combined the results of the exact diagonalization of the 2×2 energy matrix with pseudostate expansions to perform the perturbation sums over intermediate states. We calculated both the length and velocity gauges as a check on numerical accuracy and the validity of the transition operators.

1. Introduction

With this paper we wish to extend our previous calculations of spin-changing radiative transitions in neutral helium to P - D transitions and include the effects of the finite nuclear mass and the anomalous magnetic moment of the electron. In Paper I [1] we published oscillator strengths (f -values) and transition rates (A -values) for the lowest S–P and P–D transitions and in Paper II [2] the five lowest S–P transitions. These calculations summed the spin-dependent Breit interaction as a first-order perturbation over all intermediate states, but assumed infinite nuclear mass. In Paper III [3] we applied the same perturbation analysis to 24 S–P transitions and included the electron anomaly and the true nuclear mass, which partially cancel each other so it is important to include both. The present paper extends those results to 12 P–D transitions with corrections to the wave functions and operators for the nuclear mass and electron anomaly and the operators for the electron anomaly. In a recent related paper [4] we applied the same theoretical approach to the helium-like ions of C V, N VI and O VII.

In another earlier paper [5] we tabulated an extensive set of He I f -values for both spin-permitted and spin-forbidden transitions $n^{2S+1}L_J - n'^{2S'+1}L'_J$ with $n, n' \leq 10$; $S, S' = 0, 1$; $L, L' \leq 6$, all for infinite nuclear mass. The relevant physics is different for high L because the electrostatic singlet-triplet splitting becomes small relative to the spin-dependent Breit interaction, and so only $\mathbf{L} + \mathbf{S} = \mathbf{J}$ remains a

good quantum number. As L increases, there is a progressive change from pure LS -coupling to pure jj -coupling for high L [6]. In the intermediate case, the dominant mixing is between the pair of LS -coupled states with the same n , L , and J , but different S , for example the singlet-triplet pair $1s3d\ ^1D_2$ and $1s3d\ ^3D_2$. Consequently Ref. [5] included only this mixing by diagonalizing the corresponding 2×2 matrix in place of a first-order perturbation sum over all intermediate states, which fails where the mixing is strong. This use of exact diagonalization is necessary for transitions such as $3\ ^1D_2 - 4\ ^1F_3$ and is almost adequate for $n\ ^1S_0 - n\ ^3P_1$ and $n\ ^3S_1 - n\ ^1P_1$, where the principal quantum numbers are the same, but inadequate for transitions such as $1\ ^1S_0 - 2\ ^3P_1$ or $2\ ^3S_1 - 3\ ^1P_1$. For the P - D transitions in this paper we use a combination of exact diagonalization and summation over intermediate states to treat the case of intermediate coupling between LS and jj .

In Sections 2 and 3 below we repeat the theoretical discussion in Paper III [3] for the true nuclear mass and the electron anomaly and show how the summation over intermediate states is modified to use the exact diagonalization of the 1D_2 and 3D_2 states. We use reduced atomic units in which we relate lengths r and energies ϵ to laboratory values by $R = a_0(m_e/\mu)r$ and $E = \alpha^2 m_e c^2 (\mu/m_e)\epsilon$. Here a_0 , α , m_e and c are the familiar atomic constants [7], $\mu = m_e M/(m_e + M)$ is the reduced mass of the electron, and M is the mass of the nucleus. The usual atomic units (a.u.) result if $M = \infty$.

2. Theory for sums over intermediate states

Solution of the mass-polarized nonrelativistic Schrödinger equation [8]

$$\begin{aligned} H_M \psi_M^0 &= \left[-\frac{1}{2} (\nabla_1^2 + \nabla_2^2) - \frac{\mu}{M} (\nabla_1 \cdot \nabla_2) \right. \\ &\quad \left. - Z \left(\frac{1}{r_1} + \frac{1}{r_2} \right) + \frac{1}{r_{12}} \right] \psi_M^0 \\ &= \epsilon_M^0 \psi_M^0 \end{aligned} \quad (1)$$

provides the unperturbed energies ϵ_M^0 and wave functions ψ_M^0 [9] for nuclear mass M . This equation is in reduced-mass a.u., so we must multiply these energies by μ/m_e to obtain a.u. and multiply all operators used with these ψ_M^0 by one power of μ/m_e for each power of $1/r$ in the operator. These wave functions contain no spin corrections.

When the electron spin changes, the relevant spin-orbit (SO) and spin-other-orbit (SOO) perturbations are the respective Breit operators

$$B_{3Z} = \frac{\alpha^2 Z}{4} \left[\left(\frac{\mathbf{r}_1}{r_1^3} \times \mathbf{p}_1 \right) \cdot \sigma_1 + \left(\frac{\mathbf{r}_2}{r_2^3} \times \mathbf{p}_2 \right) \cdot \sigma_2 \right] \quad (2)$$

$$\begin{aligned} B_{3e} &= \frac{\alpha^2}{4r_{12}^3} [(\mathbf{r}_{12} \times \mathbf{p}_2 - \mathbf{r}_{12} \times \mathbf{p}_1) \cdot (\sigma_1 + \sigma_2) \\ &\quad + (\mathbf{r}_{12} \times \mathbf{p}_2) \cdot \sigma_1 - (\mathbf{r}_{12} \times \mathbf{p}_1) \cdot \sigma_2]. \end{aligned} \quad (3)$$

In [10] Stone formulated the finite-mass corrections and included the effects of the anomalous magnetic moment of the electron $a_e \simeq \alpha/(2\pi)$. Following Drake and Yan [11], who approximated Stone's m_e/M with $y = \mu/M$, the SO and SOO operators become

$$B_{3Z\text{Ma}_e} = (\mu/m_e)^3 [(1 + 2a_e + 2y + 2a_e y) B_{3Z} \quad (4)$$

$$\begin{aligned}
 & + (1 + a_e)y\Delta_3] \\
 B_{3eMa_e} &= (\mu/m_e)^3 [B_{3e} + \frac{a_e\alpha^2}{4r_{12}^3}(\mathbf{r}_{12} \times \mathbf{p}_2 - \mathbf{r}_{12} \times \mathbf{p}_1) \\
 & \cdot (\sigma_1 + \sigma_2)]
 \end{aligned} \tag{5}$$

$$\Delta_3 = \frac{\alpha^2 Z}{2} \left[\left(\frac{\mathbf{r}_1}{r_1^3} \times \mathbf{p}_2 \right) \cdot \sigma_1 + \left(\frac{\mathbf{r}_2}{r_2^3} \times \mathbf{p}_1 \right) \cdot \sigma_2 \right] = 2B_{3Z}. \tag{6}$$

where the a_e term in (5) contributes only for triplet - triplet transitions. Note that the equations corresponding to (4) and (5) in Ref. [11] are in reduced mass atomic units, so the prefactors there are $(\mu/M)^2 \simeq 1 - 2y$ instead of $(\mu/M)^3 \simeq 1 - 3y$.

The mass-corrected dipole length and velocity interaction operators are

$$H_{I,L} = (\mu/m_e)^{-1} Z_r (z_1 + z_2) \tag{7}$$

$$H_{I,V} = (\mu/m_e)^1 Z_p \left(\frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right), \tag{8}$$

where

$$Z_r = \frac{M + Zm_e}{M + Nm_e}, \quad Z_p = \frac{M + Zm_e}{M} \tag{9}$$

and the number of electrons $N = 2$. As outlined in the appendix of [5], these last factors correct the dipole operators for the motion of the nucleus relative to the center-of-mass. When $N \neq Z$, there are additional small corrections proportional to $N - Z$ in the length and velocity operators due to the motion of the centre of mass relative to the inertial frame defined by the electromagnetic field. In the absence of external fields, the centre of mass R_c is an ignorable coordinate, so these extra terms do not contribute for spontaneous emission.

The commutator relation

$$\begin{aligned}
 & i[H_{I,L}, H_0 + B_{3Z} + B_{3e}] \\
 & = (H_{I,V} + B_{I,3Z} + B_{I,3e})
 \end{aligned} \tag{10}$$

relates the dipole operators H_{IL} and H_{IV} in (7) and (10), the unperturbed Hamiltonian H_0 in (1) for infinite nuclear mass and the Breit operators B_{3Z} and B_{3e} from (2) and (3) to the corresponding interaction operators

$$B_{I,3Z} = \frac{-\alpha^2 Z}{4} \left[\left(\frac{\mathbf{r}_1}{r_1^3} \times \hat{\mathbf{e}} \right) \cdot \sigma_1 + \left(\frac{\mathbf{r}_2}{r_2^3} \times \hat{\mathbf{e}} \right) \cdot \sigma_2 \right] \tag{11}$$

$$B_{I,3e} = \frac{-\alpha^2}{4r_{12}^3} [(\mathbf{r}_{12} \times \hat{\mathbf{e}}) \cdot \sigma_1 - (\mathbf{r}_{12} \times \hat{\mathbf{e}}) \cdot \sigma_2]. \tag{12}$$

Following Drake [12] these terms provide a correction to the velocity element through use of the expanded energies $\epsilon = \epsilon^0 + \epsilon^1$ and wave functions $\psi = \psi^0 + \psi^1$ and retaining only first-order terms so that

$$\begin{aligned}
 & i(\epsilon_a^0 - \epsilon_b^0) [\langle {}^3\psi_b^0 | H_{I,L} | {}^1\psi_a^1 \rangle + \langle {}^3\psi_b^1 | H_{I,L} | {}^1\psi_a^0 \rangle] \\
 & = \langle {}^3\psi_b^0 | H_{I,V} | {}^1\psi_a^1 \rangle + \langle {}^3\psi_b^1 | H_{I,V} | {}^1\psi_a^0 \rangle + C_\infty.
 \end{aligned} \tag{13}$$

Thus the length matrix element multiplied by the nonrelativistic energy difference equals the velocity element plus the correction

$$\begin{aligned}
 C_\infty &= \frac{\alpha^2}{4} \langle {}^3\psi_b^0 | B_{I,3Z} + B_{I,3e} | {}^1\psi_a^0 \rangle \\
 &= \frac{\sqrt{2}\alpha^2}{4} \left\langle {}^3\psi_b^0 \left| \frac{Z}{r_1^3} z_1 - \frac{Z}{r_2^3} z_2 + \frac{2}{r_{12}^3} (z_1 - z_2) \right| {}^1\psi_a^0 \right\rangle,
 \end{aligned} \tag{14}$$

which depends on only the initial and final nonrelativistic states as indicated by the superscript 0.

Enhancing (10) to include the mass and electron corrections then gives an equation connecting (4) and (5) with the corresponding extensions of (11) and (12)

$$B_{1,3ZMa_e} = (\mu/m_e)^3(1 + 2a_e + 2y + 2a_e y)B_{1,3Z}$$

$$\Delta_{I,3ZMa_e} = (\mu/m_e)^3 2(y + a_e y)B_{I,3Z} \quad (15)$$

$$B_{1,3eMa_e} = (\mu/m_e)^3 B_{1,3e}. \quad (16)$$

Then the correction to the sum of matrix elements with the velocity interaction operator is

$$C_{Ma_e} = (\mu/m_e)^2 \frac{\sqrt{2}\alpha^2}{4} \left[(1 + 2a_e + 4y + 4a_e y) \left\langle {}^3D \left| \frac{Z}{r_1^3} z_1 - \frac{Z}{r_2^3} z_2 \right| {}^1P^o \right\rangle + \left\langle {}^3D \left| \frac{2}{r_{12}^3} (z_1 - z_2) \right| {}^1P^o \right\rangle \right]. \quad (17)$$

where we have written the equation explicitly for the $2^1P^o - 3^3D^e$ transition.

In this finite-mass extension of (14), including the electron anomaly, B_{3Z} requires a factor $(\mu/m_e)^3(1 + 2a_e + 2y + 2a_e y)$, Δ_3 requires $(\mu/m_e)^3(1 + a_e)y$ and B_{3e} only $(\mu/m_e)^3$ as shown in (14) and (15), while the interaction operators require the mass factors in (15) and (16). If we label the intermediate states with the quantum numbers m and n , use nonrelativistic wave functions and reduced energies from (13), and multiply all energies by (μ/m_e) to give a.u., the equivalence of the length and velocity formulations in (13) becomes $\Delta\epsilon_M M_{LMa_e} = M_{VMa_e} + C_{Ma_e}$ or

$$\begin{aligned} & Z_r \frac{\epsilon(2^1P^o) - \epsilon(3^3D)}{(\mu/m_e)} \left[\sum_m^N \langle {}^3D_2 | z_1 + z_2 | m^3P_1^o \rangle \frac{\langle m^3P_1^o | B_{3ZMa_e} + B_{3eMa_e} | 2^1P_1^o \rangle}{\epsilon(2^1P^o) - \epsilon(m^3P^o)} \right. \\ & + \sum_m^N \langle {}^3D_1 | z_1 + z_2 | m^3P_1^o \rangle \frac{\langle m^3P_1^o | B_{3ZMa_e} + B_{3eMa_e} | 2^1P_1^o \rangle}{\epsilon(2^1P^o) - \epsilon(m^3P^o)} \\ & + \sum_n^N \frac{\langle {}^3D_2 | B_{3ZMa_e} + B_{3eMa_e} | n^1D_2 \rangle}{\epsilon(3^3D) - \epsilon(n^1D)} \langle n^1D_2 | z_1 + z_2 | 2^1P_1^o \rangle \left. \right] \\ & = Z_p \left[\sum_m^N \left\langle {}^3D_2 \left| \frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right| m^3P_1^o \right\rangle \frac{\langle m^3P_1^o | B_{3ZMa_e} + B_{3eMa_e} | 2^1P_1^o \rangle}{\epsilon(2^1P^o) - \epsilon(m^3P^o)} \right. \\ & + \sum_m^N \left\langle {}^3D_1 \left| \frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right| m^3P_1^o \right\rangle \frac{\langle m^3P_1^o | B_{3ZMa_e} + B_{3eMa_e} | 2^1P_1^o \rangle}{\epsilon(2^1P^o) - \epsilon(m^3P^o)} \\ & + \sum_n^N \frac{\langle {}^3D_2 | B_{3ZMa_e} + B_{3eMa_e} | n^1D_2 \rangle}{\epsilon(3^3D) - \epsilon(n^1D)} \left\langle {}^1D_2 \left| \frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right| 2^1P_1^o \right\rangle \left. \right] \\ & + C_{Ma_e}. \end{aligned} \quad (18)$$

Again for clarity this is the specific example for $2^1P_1^o - 3^3D_2^e$ with the J -values included to emphasize the need for both angular-momentum and parity equality to obtain non-zero Breit terms, but opposite parity and $\Delta J = 0, \pm 1$ for the dipole

operator (unless both J 's are zero). Thus we must include dipole elements between $^3P_1^o$ and both 3D_2 and 3D_1 . Similarly for $^3P_{1,2}^o - ^1D_2$ there are dipole contributions between 3D_2 and both $^3P_1^o$ and $^3P_2^o$.

As described in [13] and [1] we replace each sum over the intermediate states in (18), including the integral over the continuum, by a sum over the asymptotically complete set of N discrete pseudostates obtained by diagonalizing the nonrelativistic Hamiltonian in an orthogonalized basis set of N Hylleraas functions of the appropriate symmetry. Thus we have a set of pseudostates $1sn p \ ^3P_1^o$ interacting with $1s2p \ ^1P_1^o$ and $1snd \ ^1D_2$ interacting with $1s3d \ ^3D_2$ in our example of the $1s2p \ ^1P_1^o - 1s3d \ ^3D_2$ transition.

3. Theory for intermediate coupling

In Eq. (18) the third and fourth summations use first-order perturbation theory to estimate the effect of the mixing of the 1D and 3D states on the dipole length and velocity matrix elements. When the principal quantum numbers are the same, the energy difference is small allowing that term to dominate all others by more than a factor 100. We can obtain a better value for this term by considering the perturbed two-state system $|n^1D\rangle$ and $|n^3D\rangle$ expanded them in terms of the unperturbed $|n^1D_2\rangle^0$ and $|n^3D_2\rangle^0$,

$$\begin{aligned} |n^1D_2\rangle &= |n^1D_2\rangle^0 \cos \theta + |n^3D_2\rangle^0 \sin \theta \\ |n^3D_2\rangle &= -|n^1D_2\rangle^0 \sin \theta + |n^3D_2\rangle^0 \cos \theta \end{aligned} \quad (19)$$

from which we obtain the matrix equation

$$\begin{pmatrix} \langle n^1D_2 | H_0 | n^1D_2 \rangle & \langle n^1D_2 | B_3 | n^3D_2 \rangle \\ \langle n^3D_2 | B_3 | n^1D_2 \rangle & \langle n^3D_2 | H_0 | n^3D_2 \rangle \end{pmatrix} = \begin{pmatrix} E_{11} & B_{12} \\ B_{12} & E_{22} \end{pmatrix} \quad (20)$$

for the Hamiltonian operator $H = H_0 + B$. The total perturbation, exact to all orders, is then the sine of the mixing angle θ required to diagonalize this matrix, where

$$\frac{\tan 2\theta}{2} = \frac{B_{12}}{E_{11} - E_{22}}. \quad (21)$$

The right-hand side is just the first-order factor in Eq. (18), but in an exact diagonalization both E_{11} and E_{22} include also the diagonal matrix elements B_{11} and B_{22} of the Breit interaction. Drake [8] has calculated $\sin \theta = -0.01560952$ for 3D and -0.01139597 for 4D including QED effects as well the nuclear mass and the electron anomaly.

Once we have a corrected length matrix element $\Delta\epsilon_M M_{LMa_e}$ in Eq. (18) we can calculate oscillator strengths f and transition rates A

$$g_l f_{lu} = \frac{2}{3\Delta\epsilon} (\Delta\epsilon_M M_L)^2 \quad (22)$$

$$g_u A_{ul} = \frac{2\alpha^4 c}{a_0} \Delta\epsilon^2 g_l f_{lu} = 3.2130011 \times 10^{10} \Delta\epsilon^2 g_l f_{lu}, \quad (23)$$

where $\Delta\epsilon$ is the nonrelativistic energy difference in a.u. and g_l and g_u are the lower and upper statistical weights respectively. Note that Drake and Morton [5] revised the definition of f in [8] to avoid the use of the Z_r and Z_p factors in the relation (22) between f and A , but Z_p still must be applied in calculating H_{IV} and Z_r for H_{IL} if $Z \neq 2$.

The relativistic calculations described here used $\alpha = 7.297\,352\,537\,6 \times 10^{-3}$ for the fine-structure constant, $a_e = 1.159\,652\,181 \times 10^{-3}$ for the anomalous magnetic moment of the electron and $y = (\mu/M) = 1.370\,745\,62 \times 10^{-4}$ for the ratio of the reduced mass of the electron to the alpha particle. All these are within one part in 10^8 or less of the latest recommended values of the fundamental constants [7].

4. Results and Discussion

Tables 1 to 4 give the results of our calculations for 12 intersystem P – D transitions. The detailed listings give the three components for both length $\Delta\epsilon M_L$ and velocity M_V matrix elements where the number of figures indicates the level of convergence with increasing size of the basis sets. The correction $C_{\alpha a_e}$ always is better determined. The length-velocity ratio $(M_V + C_{\alpha a_e} - \Delta\epsilon M_L)/\Delta\epsilon M_L$ provides a guide to the true accuracy of the calculations. Except for a possibly fortuitous 7×10^{-7} , the ratios range between 2×10^{-5} and 4×10^{-4} . The f - and A -values in the tables are based on $\Delta\epsilon M_L$. Comparison with $f_{2 \times 2}$ indicate that the P – D results from the simple 2×2 diagonalizations are reliable to 2 or 3 significant figures.

As described in Paper III [3], Pachucki [14] identified an additional interaction proportional to a_e due to the magnetic component of the radiation field. The extra contribution to the length matrix element $\Delta\epsilon M_L$ is

$$P_{Ma_e} = -(\mu/m_e)^2 a_e [B_{I,3Z} - B_{I,3e}], \quad (24)$$

where the factor $(\mu/m_e)^2$ allows for the reduced atomic units appropriate for the finite nuclear mass. This was a small correction for some of the S – P transitions in Paper III, but negligible for all the P – D cases listed here because both $B_{I,3Z}$ and $B_{I,3e}$ are smaller. As a fraction of $\Delta\epsilon M_L$, the two largest P_{Ma_e} are 1.84×10^{-7} and 1.46×10^{-7} for $2^1P_1^\circ - 3^3D_2$ and $2^3P_1^\circ - 3^1D_2$.

5. Future Calculations

In our studies of $1S^\circ - 3P^\circ$ and $3S^\circ - 1P^\circ$ transitions, it was important to include the doubly excited $2pnp\ 3P^\circ$ and $2pnp\ 1P^\circ$ respectively in the sums over intermediate states. Similarly with $1P^\circ - 3D^\circ$ and $3P^\circ - 1D^\circ$ we need to investigate the contributions of the doubly excited $2pnd\ 3D^\circ$ and $2pnd\ 1D^\circ$ states. Also we would like to extend the tables to include higher principal quantum numbers.

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Table 1. Matrix Elements M , oscillator strengths f and rates A for $1^1P_1^o - 3^3D_{2,1}$ transitions. M_L is the length form, M_V is the velocity form, and $C_{\alpha\alpha_e}$ is the correction to M_V . In each case the 3^3D levels are above the $1^1P_1^o$ level.

E1 Transition	$2^1P_1^o - 3^3D_{2,1}$	$2^1P_1^o - 4^3D_{2,1}$	$3^1P_1^o - 4^3D_{2,1}$
$\Delta\epsilon$ (a.u.) theory	$6.819\,112\,257 \times 10^{-2}$	$9.253\,524\,812 \times 10^{-2}$	$2.385\,225\,514 \times 10^{-2}$
$1/\lambda$ (cm $^{-1}$) theory	$1.496\,622\,149 \times 10^4$	$2.030\,913\,947 \times 10^4$	$5.234\,964\,903 \times 10^3$
$\Delta\epsilon M_L$ from $n^3P_1^o$	$-0.111\,710 \times 10^{-3}$	$-0.053\,71 \times 10^{-3}$	$-0.058\,671 \times 10^{-3}$
$\Delta\epsilon M_L$ from $n^3P_1^o$	$-0.064\,496 \times 10^{-3}$	$-0.031\,01 \times 10^{-3}$	$-0.033\,874 \times 10^{-3}$
$\Delta\epsilon M_L$ from n^1D_2	$7.286\,850 \times 10^{-3}$	$2.548\,15 \times 10^{-3}$	$3.008\,032 \times 10^{-3}$
$\Delta\epsilon M_L$ sum	$7.110\,644 \times 10^{-3}$	$2.463\,42 \times 10^{-3}$	$2.915\,488 \times 10^{-3}$
M_V from $n^3P_1^o$	$-0.113\,052 \times 10^{-3}$	$-0.054\,598 \times 10^{-3}$	$-0.058\,943 \times 10^{-3}$
M_V from $n^3P_1^o$	$-0.065\,271 \times 10^{-3}$	$-0.031\,523 \times 10^{-3}$	$-0.034\,031 \times 10^{-3}$
M_V from n^1D_2	$7.290\,545 \times 10^{-3}$	$2.550\,566 \times 10^{-3}$	$3.008\,771 \times 10^{-3}$
$C_{\alpha\alpha_e}$	$-0.003\,038\,9 \times 10^{-3}$	$-0.001\,984\,1 \times 10^{-3}$	$-0.000\,610\,5 \times 10^{-3}$
M_V sum + $C_{\alpha\alpha_e}$	$7.109\,183 \times 10^{-3}$	$2.462\,462 \times 10^{-3}$	$2.915\,188 \times 10^{-3}$
$M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L$	-1.461×10^{-6}	-9.6×10^{-7}	-3.00×10^{-7}
$(M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L)/\Delta\epsilon M_L$	-2.1×10^{-4}	-3.9×10^{-4}	-1.03×10^{-4}
$f(1^1P_1^o - 3^3D_2)$	$1.677\,72 \times 10^{-4}$	$1.494\,26 \times 10^{-5}$	$8.104\,27 \times 10^{-5}$
$f(1^1P_1^o - 3^3D_1)$	$1.355\,57 \times 10^{-8}$	$2.309\,43 \times 10^{-6}$	$1.069\,01 \times 10^{-8}$
$A(s^{-1})(3^3D_2 - 1^1P_1^o)$	$1.503\,97 \times 10^4$	$2.466\,61 \times 10^3$	$8.888\,63 \times 10^2$
$A(s^{-1})(3^3D_1 - 1^1P_1^o)$	$2.025\,29 \times 10^0$	$6.353\,75 \times 10^{-1}$	$1.954\,12 \times 10^{-1}$
$f_{2x2}(1^1P_1^o - 3^3D_2)$	$1.684\,5 \times 10^{-4}$	$1.499\,3 \times 10^{-5}$	$8.153\,9 \times 10^{-3}$

Table 2. Matrix Elements M , oscillator strengths f and rates A for $3^3D_{2,1} - 1^1P_1^o$ transitions. M_L is the length form, M_V is the velocity form, and $C_{\alpha\alpha_e}$ is the correction to M_V . In each case the $1^1P_1^o$ level is above the 3^3D levels.

E1 Transition	$3^3D_{2,1} - 3^1P_1^o$	$3^3D_{2,1} - 4^1P_1^o$	$4^3D_{2,1} - 4^1P_1^o$
$\Delta\epsilon$ (a.u.) theory	$4.918\,704\,127 \times 10^{-4}$	$2.456\,414\,571 \times 10^{-2}$	$2.200\,201\,604 \times 10^{-4}$
$1/\lambda$ (cm $^{-1}$) theory	$1.079\,530\,775 \times 10^2$	$5.391\,206\,825 \times 10^3$	$4.828\,884\,361 \times 10^1$
$\Delta\epsilon M_L$ from $n^3P_1^o$	$-0.015\,543\,180 \times 10^{-4}$	$-0.089\,690 \times 10^{-4}$	$-0.140\,594\,2 \times 10^{-5}$
$\Delta\epsilon M_L$ from $n^3P_1^o$	$-0.008\,973\,859 \times 10^{-4}$	$-0.051\,783 \times 10^{-4}$	$-0.081\,172\,1 \times 10^{-5}$
$\Delta\epsilon M_L$ from n^1D_2	$1.086\,645\,859 \times 10^{-4}$	$6.397\,072 \times 10^{-4}$	$7.338\,665\,5 \times 10^{-5}$
$\Delta\epsilon M_L$ sum	$1.062\,128\,820 \times 10^{-4}$	$6.255\,599 \times 10^{-4}$	$7.116\,899\,1 \times 10^{-5}$
M_V from $n^3P_1^o$	$-0.015\,727\,8 \times 10^{-4}$	$-0.089\,158 \times 10^{-4}$	$-0.141\,54 \times 10^{-5}$
M_V from $n^3P_1^o$	$-0.009\,080\,4 \times 10^{-4}$	$-0.051\,475 \times 10^{-4}$	$-0.081\,72 \times 10^{-5}$
M_V from n^1D_2	$1.086\,991\,0 \times 10^{-4}$	$6.395\,753 \times 10^{-4}$	$7.340\,57 \times 10^{-5}$
$C_{\alpha\alpha_e}$	$-0.000\,205\,542 \times 10^{-4}$	$0.001\,089\,9 \times 10^{-4}$	$-0.001\,097\,7 \times 10^{-4}$
M_V sum + $C_{\alpha\alpha_e}$	$1.061\,977\,2 \times 10^{-4}$	$6.256\,210 \times 10^{-4}$	$7.116\,22 \times 10^{-4}$
$M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L$	-1.516×10^{-8}	6.11×10^{-8}	6.80×10^{-9}
$(M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L)/\Delta\epsilon M_L$	-1.4×10^{-4}	9.8×10^{-5}	-9.6×10^{-5}
$f(3^3D_2 - 1^1P_1^o)$	$3.109\,93 \times 10^{-6}$	$2.159\,41 \times 10^{-6}$	$3.139\,85 \times 10^{-6}$
$f(3^3D_1 - 1^1P_1^o)$	$3.638\,27 \times 10^{-10}$	$2.425\,80 \times 10^{-10}$	$6.654\,86 \times 10^{-10}$
$A(s^{-1})(1^1P_1^o - 3^3D_2)$	$4.029\,13 \times 10^{-2}$	$6.977\,47 \times 10^1$	$8.139\,41 \times 10^{-3}$
$A(s^{-1})(1^1P_1^o - 3^3D_1)$	$2.828\,18 \times 10^{-6}$	$4.702\,94 \times 10^{-3}$	$1.035\,08 \times 10^{-6}$
$f_{2x2}(3^3D_2 - 1^1P_1^o)$	$3.100\,8 \times 10^{-6}$	$2.140\,8 \times 10^{-6}$	$3.131\,8 \times 10^{-6}$
$f_{2x2}(3^3D_1 - 1^1P_1^o)$	$3.673\,5 \times 10^{-10}$	.	$6.633\,8 \times 10^{-10}$

Table 3. Matrix Elements M , oscillator strengths f and rates A for ${}^3P_{1,2}^o - {}^1D_2$ transitions. M_L is the length form, M_V is the velocity form, and $C_{\alpha\alpha_e}$ is the correction to M_V . In each case the 3D_2 level is above the ${}^1P^o$ levels.

E1 Transition	$2\ {}^3P_{1,2}^o - 3\ {}^1D_2$	$2\ {}^3P_{1,2}^o - 4\ {}^1D_2$	$3\ {}^3P_{1,2}^o - 3\ {}^1D_2$
$\Delta\epsilon$ (a.u.) theory	$7.754\,164\,731\times 10^{-2}$	$1.018\,792\,144\times 10^{-1}$	$2.462\,497\,812\times 10^{-3}$
$1/\lambda$ (cm $^{-1}$) theory	$1.701\,842\,446\times 10^4$	$2.235\,990\,303\times 10^4$	$5.404\,557\,996\times 10^2$
$\Delta\epsilon M_L$ from $n\ {}^1P_1^o$	$-0.130\,571\ \times 10^{-3}$	$-0.066\,99\ \times 10^{-3}$	$-0.091\,269\,1\times 10^{-4}$
$\Delta\epsilon M_L$ from $n\ {}^3D_2$	$6.234\,804\ \times 10^{-3}$	$2.342\,57\ \times 10^{-3}$	$4.782\,896\,2\times 10^{-4}$
$\Delta\epsilon M_L$ from $n\ {}^3D_2$	$3.599\,666\ \times 10^{-3}$	$1.352\,49\ \times 10^{-3}$	$2.761\,406\,4\times 10^{-4}$
$\Delta\epsilon M_L$ sum	$9.703\,899\ \times 10^{-3}$	$3.628\,07\ \times 10^{-3}$	$7.453\,033\,4\times 10^{-4}$
M_V from $n\ {}^1P_1^o$	$-0.129\,053\,8\times 10^{-3}$	$-0.065\,966\ \times 10^{-3}$	$-0.090\,265\ \times 10^{-4}$
M_V from $n\ {}^3D_2$	$6.231\,614\,3\times 10^{-3}$	$2.340\,443\ \times 10^{-3}$	$4.780\,977\ \times 10^{-4}$
M_V from $n\ {}^3D_2$	$3.599\,666\,0\times 10^{-3}$	$1.351\,256\ \times 10^{-3}$	$2.760\,299\ \times 10^{-4}$
$C_{\alpha\alpha_e}$	$0.003\,046\,2\times 10^{-3}$	$0.002\,032\,1\times 10^{-3}$	$0.001\,807\,1\times 10^{-4}$
M_V sum + $C_{\alpha\alpha_e}$	$9.703\,430\,8\times 10^{-3}$	$3.627\,765\ \times 10^{-3}$	$7.452\,818\ \times 10^{-4}$
$M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L$	-4.684×10^{-7}	-3.069×10^{-7}	-2.153×10^{-8}
$(M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L)/\Delta\epsilon M_L$	-4.8×10^{-5}	-8.5×10^{-5}	-2.9×10^{-5}
$f\ ({}^3P_1^o - {}^1D_2)$	$1.067\,86\times 10^{-4}$	$1.129\,51\times 10^{-5}$	$1.986\,36\times 10^{-5}$
$f\ ({}^3P_2^o - {}^1D_2)$	$2.228\,07\times 10^{-5}$	$2.393\,97\times 10^{-6}$	$4.128\,80\times 10^{-6}$
$A(s^{-1})\ ({}^1D_2 - {}^3P_1^o)$	$1.237\,79\times 10^4$	$2.260\,07\times 10^3$	$2.322\,05\times 10^0$
$A(s^{-1})\ ({}^1D_2 - {}^3P_2^o)$	$4.304\,36\times 10^3$	$7.983\,63\times 10^2$	$8.044\,26\times 10^{-1}$
$f_{2x2}({}^3P_1^o - {}^1D_2)$	$1.063\,2\times 10^{-4}$	$1.127\,6\times 10^{-5}$	$1.985\ 9\times 10^{-5}$
$f_{2x2}({}^3P_2^o - {}^1D_2)$	$2.230\,7\times 10^{-5}$	$2.393\,3\times 10^{-6}$	$4.123\ 2\times 10^{-6}$

Table 4. Matrix Elements M , oscillator strengths f and rates A for $3^3P_{1,2}^o - 1^1D_2$ transitions. M_L is the length form, M_V is the velocity form, and $C_{\alpha\alpha_e}$ is the correction to M_V . The 4^1D_2 level is above the 3 and $4^3P_{1,2}^o$ levels, but $4^3P_1^o$ is above 3^1D_2 .

E1 Transition	$3^3P_{1,2}^o - 4^1D_2$	$3^1D_2 - 4^3P_{1,2}^o$	$4^3P_{1,2}^o - 4^1D_2$
$\Delta\epsilon$ (a.u.) theory	$2.680\,006\,492 \times 10^{-2}$	$2.329\,218\,431 \times 10^{-2}$	$1.045\,382\,794 \times 10^{-3}$
$1/\lambda$ (cm $^{-1}$) theory	$5.881\,934\,369 \times 10^3$	$5.112\,043\,566 \times 10^3$	$2.294\,350\,033 \times 10^2$
$\Delta\epsilon M_L$ from $n^1P_1^o$	$-0.062\,137 \times 10^{-3}$	$-0.015\,694\,2 \times 10^{-3}$	$-0.077\,924\,7 \times 10^{-4}$
$\Delta\epsilon M_L$ from n^3D_2	$2.365\,030 \times 10^{-3}$	$0.843\,170\,1 \times 10^{-3}$	$3.049\,424\,5 \times 10^{-4}$
$\Delta\epsilon M_L$ from n^3D_2	$1.365\,451 \times 10^{-3}$	$0.486\,804\,5 \times 10^{-3}$	$1.760\,586\,0 \times 10^{-4}$
$\Delta\epsilon M_L$ sum	$3.668\,344 \times 10^{-3}$	$1.314\,280\,4 \times 10^{-3}$	$4.732\,085\,8 \times 10^{-4}$
M_V from $n^1P_1^o$	$-0.061\,908 \times 10^{-3}$	$-0.015\,700\,9 \times 10^{-3}$	$-0.077\,432 \times 10^{-4}$
M_V from n^3D_2	$2.364\,543 \times 10^{-3}$	$0.843\,190\,8 \times 10^{-3}$	$3.048\,499 \times 10^{-4}$
M_V from n^3D_2	$1.365\,169 \times 10^{-3}$	$0.486\,816\,4 \times 10^{-3}$	$1.760\,052 \times 10^{-4}$
$C_{\alpha\alpha_e}$	$0.000\,472\,65 \times 10^{-3}$	$-0.000\,026\,9 \times 10^{-3}$	$0.000\,879\,9 \times 10^{-4}$
M_V sum + $C_{\alpha\alpha_e}$	$3.668\,276 \times 10^{-3}$	$1.314\,279\,5 \times 10^{-3}$	$4.731\,998 \times 10^{-4}$
$M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L$	-6.8×10^{-8}	-1.0×10^{-9}	-8.8×10^{-9}
$(M_V + C_{\alpha\alpha_e} - \Delta\epsilon M_L)/\Delta\epsilon M_L$	-1.9×10^{-5}	$-7. \times 10^{-7}$	-1.8×10^{-5}
$f(3^3P_1^o - 1^1D_2)$	$4.397\,43 \times 10^{-5}$		$1.877\,00 \times 10^{-5}$
$f(1^1D_2 - 3^3P_1^o)$	.	$3.919\,58 \times 10^{-6}$	
$f(3^3P_2^o - 1^1D_2)$	$9.275\,88 \times 10^{-6}$		$3.953\,47 \times 10^{-6}$
$f(1^1D_2 - 3^3P_2^o)$	.	$1.356\,56 \times 10^{-6}$	
$A(s^{-1})(1^1D_2 - 3^3P_1^o)$	$6.088\,82 \times 10^2$		$3.954\,36 \times 10^{-1}$
$A(s^{-1})(3^3P_1^o - 1^1D_2)$	.	$1.138\,73 \times 10^2$	
$A(s^{-1})(1^1D_2 - 3^3P_2^o)$	$2.140\,61 \times 10^2$		$1.388\,16 \times 10^{-1}$
$A(s^{-1})(3^3P_2^o - 1^1D_2)$	.	$2.364\,66 \times 10^2$	
$f_{2x2}(3^3P_1^o - 1^1D_2)$	$4.360\,5 \times 10^{-5}$		$1.876\,5 \times 10^{-5}$
$f_{2x2}(1^1D_2 - 3^3P_1^o)$	.	$3.958\,0 \times 10^{-6}$	
$f_{2x2}(3^3P_2^o - 1^1D_2)$	$9.306\,7 \times 10^{-6}$		$3.948\,5 \times 10^{-6}$
$f_{2x2}(1^1D_2 - 3^3P_2^o)$	.	$1.350\,4 \times 10^{-6}$	