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Abstract

Oscillator strengths between various doublet states of OII ions are calculated in which extensive multi-configuration wave functions are used. The lower levels for the transitions are of the $2p^3\ {}^2D^o$ and $2p^3\ {}^2P^o$ states, and the upper levels are $2p^4$, 3s, and 3d states. The results, which are estimated to have errors of less than 10% for individual transitions, agree quite well with the beam foil experiments, as well as with the calculations by use of the non-closed shell many electron theory (NCMET). The agreement with the rocket measurements is also good except for the 538/581 Å pair, in which the 538 Å line is believed to be blend with the other stronger quartet line. However, a comparison with the recent branching ratio measurement indicates that discrepances between the present calculation and the experiment do exist for certain transistions.

(I) Introduction

We report a calculation for the oscillator strengths of the OII ions between various doublet states by the use of extensive configuration interaction wave functions. Studies of various oxygen ions have practical, experimental, and theoretical interests. From the practical side, accurate atomic data are essential for the interpretations of the physical conditions of astrophysical plasmas. For example, the recent Voyager flyby of the Jupiter has revealed bright extreme-ultraviolet (EUV) lines of oxygen and sulfur ions in the vicinity of the satellite Io[1]. In addition, some EUV transistions between various doublet states of OII ions have been identified in the day airgrow spectrum. The spectrum was observed in a rocket measurement [2,3]. From the experimental side the use of beam foil techniques to determine the lifetimes of various ionic states has been quite popular[4,5]. Other recent experimental investigations on the OII ions include the branching ratio measurements[6,7]. On the theoretical side, accurate calculations of the oscillator strengths for OII ions are of recent interest. Since OII ions are singly ionized species, strong configuration interactions exist in the calculations of oscillator strengths. Furthermore, since OII are also open shell ions, various correlation effects must be included for accurate calculations. Previous theoretical investigations include the calculations by use of the non-closed shell many electron theory (NCMET)[8] and the first order theory of oscillator strengths (FOTOS)[9], which is itself a subset of the full NCMET theory. The oscillator strengths for these open shell and singly ionized ions are sensitive to the wave functions used, as well as to the procedures by which the parameters in the wave functions are determined (optimized). Such sensitivities have been documented in the literature[10,11,12]. The results for some of the transitions obtained by these two calculations differ from each other considerably. It is felt, because of these experimental and theoretical interests, that an independent extensive calculation for the oscillator strengths of OII ions is worthwhile.

This work presents such a calculation. The wave functions used are of extensive configuration-interaction type. The program CIV3 of Hibbert[13] is used in the present calculation. In section (II) we will describe the wave functions as well as the procedures to determine the parameters for the wave functions. In section (III) we will present our results. Comparisons with other calculations and with experiments will also be given.

(II) Theory and Calculations

In the program CIV3 of Hibbert[13], the wave functions are expressed as linear combinations of configuration-interaction-type wave functions.

$$\Psi = \Sigma\, a_i\, \Phi_i \;, \qquad (1)$$

with Φ_i constructed from one-electron orbitals

$$u_{nlm} = r^{-1} P_{nl}(r) Y_{lm}(\theta,\phi) \chi(m_s), \tag{2}$$

In Eq.(2), u is a product of a radial function, a spherical harmonic and a spin function. The radial functions are linear combinations of Slater orbitals

$$P_{nl}(r) = \sum_{j=1}^{k} C_{jnl} r^{I_j} e^{-\xi_j r} \tag{3}$$

Wave functions are obtained by solving the eigenvalue problem

$$< \Psi_i | H | \Psi_j > = \delta_{ij} E_j \tag{4}$$

We will discuss later in this article how various parameters for the orbital wave functions are determined. Once the wave functions for both the upper and lower states are obtained, the absorption oscillator strengths can be calculated. The oscillator strengths (expressed in atomic units) in the length and velocity forms are;

$$f_L = 2/3 \frac{\Delta E}{g_i} | <\Psi_i |\Sigma_k \bar{r}_k |\Psi_f >|^2 \qquad \text{(length)} \tag{5}$$

$$f_V = 2/3 \frac{(\Delta E)^{-1}}{g_i} | <\Psi_i |\Sigma_k \bar{p}_k |\Psi_f >|^2 \qquad \text{(velocity)} \tag{6}$$

where r and p are the coordinate and momentum operators respectively, and ΔE the energy difference between the initial (Ψ_i) and and final (Ψ_f) states. The summations in equations (5) and (6) are summed over the number of electrons. A necessary (but not sufficient) condition for an accurate calculation for the oscillator strengths is the consistence between the length and velocity values.

The procedure to choose the configurations to represent various ionic states is the following; Since OII is an open shell ion, we include the three major correlation effects in the present calculation. These effects are;

(1) internal effects that include the configurations for which the electrons occupy the Hartree-Fock (H-F) sea, (For example, for the $2p^3$ $^2P^o$ state the H-F sea includes the 1s, 2s and 2p orbitals. Therefore, the $2p^5$ $^2P^o$ configuration represents the internal correlation effect.)

(2) semi-internal effects include the configurations in which only one electron is outside the H-F sea, and

(3) all-external effects include the configurations in which two or more electrons are outside the H-F sea.

In this work, however, we limit the all-external effects to the configurations in which no more than two electrons are outside the H-F sea. Such an limitation is called the quasi-external effect by Sinanoglu[8].

For illustrative purposes, we show in table 1 the configurations that are used to represent the $2s2p^4$ ^2D state together with their classifications. For the semi-internal correlation effects we include contributions from both the N=3 shell and the N=4 shell. However, for the quasi-external effects only the contributions from the N=3 shell (except for 4f) are included. Also implicitly, we do have some contributions from higher shells. Since some of the orbitals do not necessarily have spectroscopic meanings, the '3l' orbital therefore represents the average contributions from the higher shells.

The parameters for different orbitals are optimized individually according to different transitions. For example, for the transition between the $2p^3\ {}^2D^o$ - ${}^2D$ states, we use the 1s, 2s and 2p orbitals that are optimized on the $2p^3\ {}^2D^o$ state in the single configuration H-F approximation. The parameters for these orbitals have been published by Clementi and Roetti[14]. The 3s orbital is then optimized on the 3s ${}^2D$ excited state, and the 3p and 3d orbitals, etc., are optimized on the $2p^4\ {}^2D$ excited state. Therefore, in this case, only the 3s orbital has spectroscopic meaning, while others are simply correlation orbitals.

In order to avoid the variational collapse[8], care must be taken for a state that is not the lowest state in a given symmetry (the total angular momentum, total spin, and parity). For example, in the optimization of the 3s orbital for the $2p^2\ 3s\ {}^2D$ state (which has the second lowest energy in its symmetry), the configuration of the $2s2p^4$ is also included. We then optimize the 3s on the second lowest energy eigenstate. The Hylleraas-Undheim-MacDonald theorem would guarantee that the calculated energy be an upper bound to the true energy for the 3s ${}^2D$ state.

For the calculations of the 3d states, we optimized various orbitals by the following procedure. Since 3d also contributes to the ground doublet states, we optimize the 3d orbitals on the average energy of the ground state and the 3d excited state. The 4d orbital was then optimized on the 3d excited state. As a result, the 3d excited state is represented by the combination of 3d and 4d. Here again the individual nd orbital does not have spectroscopic meanings. Furthermore, in the optimization procedure we also include the 3s and the $2p^4$ states in the expansion. Since the 3d state has the third lowest energy for a given set of (π, L, S), we have to include the two lower states to avoid the possibilities of variational collapse.

Most of the transitions reported in this work are done by the procedures described above. In other words we first construct a good representation for the lower state. The upper state is represented by the extensive configuration-interaction type wave functions that include the internal, semi-internal and quasi-external effects. In such a procedure we have found the theoretical energy difference agrees quite well with the experimental observed wave length for most of the transitions reported in this work. However, for the transition between the $^2P^o$ - ^2S states we have found that the theoretical energy differences between the upper and lower states are not consistent with the experimental values. An explanation is suggested as the following; Since the ^2S states are located at higher positions, the orbitals which are good for the lower $2p^3$ $^2P^o$ state may not be good for the upper states. Therefore we treat the $2p^2$ 3s ^2S state as a state with an 3s electron attaching to the $2p^2$ ^1S core of the OIII ion. As a result, the orbital parameters for the 1s, 2s and 2p are those of the OIII ^1S state. The 3s orbital is then optimized on the 3s ^2S excited state. By doing this we have found that the energy differences between the lower and upper states are consistent with the experimental wave lengths.

(III) Results and Discussions

We present our results in table 2 as well as those by Sinanoglu and coworkers who used the program "ATOM". Such a program is based on the non-closed shell many electron theory (NCMET)[6]. The general agreements between the present calculations and the f_L values of the NCMET results are quite good, with the present f_L and f_V values being more consistent than those in Ref. (8). It should be mentioned that these two sets of results are obtained by two different programs, although the methods of selecting various configurations are very similar. Also, by judging the differences between the oscillator strengths in the length and velocity forms, we estimate the errors for the present calculations are within 10% for the individual transitions.

The comparisions with the FOTOS[9] calculations are good except for the 673 Å and 538 Å transitions. In these cases substantial disagreements have been found. This may reflect the sensitivity of the optimization procedures (for the various orbital parameters) used in Ref. (9). It should also be mentioned that some of the transitions reported in this work have been calculated by the present authors using less extensive wave functions[15]. Also in

Ref. (15) the parameters used to represent various state wave functions were optimized for the quartet states. The present results hence represent improvements over the previous calculations in Ref. (15).

Comparisions of the present results with different experiments are shown in tables II and III. It is seen that the present results agree quite well with those by the beam foil experiments[16-19] (table II). The comparision with the branching ratio experiment (table III) is less satisfactory for certain transitions. Since the errors for the present calculations are estimated to be within 10% for the individual transitions, the error for a given ratio pair is hence of 20%. It is seen that some of the present results differ from the branching ratio experiment[7], even when the combined experimental and theoretical errors are included. For example, the discrepancy for the 482/515 Å pair shows a factor of two difference, and the 555/601 Å pair shows a difference of about 60%. Of course we also have good agreement for the 538/581 Å pair. Generally the present ratios (with the longer wavelength as the denominator) are smaller than the branching ratio experiments. However, the present results seem to agree better with the EUV airglow rocket measurements, except for the 538/581 Å ratio. The observed 538 Å line ($2p^4\ {}^2P$ - $2p^3\ {}^2D^o$) is believed to be blend with the 538 Å ($3s\ {}^4P$ - $2p^3\ {}^4S^o$) line where the latter has a larger oscillator strength.

This work presents an extensive calculation for the oscillator strengths for OII ions between various doublet states. The discrepancies between the theoretical calculations and the branching ratio experiments indicate that further theoretical and experimental investigations on such systems are worthwhile. From the theoretical point of view, improvements of the wave functions may be made if one also includes (1) the semi-internal correlation effects coming from the higher shells (higher than N=4), (2) the external effects for which more than two electrons are outside the H-F sea, and (3) the quasi-external contributions coming from higher shells (higher than N=3). Of course, such improvements may have small effects on the oscillator strengths. It is hoped, therefore, that the present calculations would stimulate further experimental investigations, which in turn would provide a more stringent criterion for the test of various theoretical calculations.

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TABLE I - Configurations used to represent the $2s2p^4\ {}^2D$ state

Internal

$2s2p^4$

Semi-internal

$2s^2 2p^2 3s$

$2p^4 3s$

$2s^2 2p^2 3d$

$2p^4 3d$

$2s\ 2p^3 3p$

$2s^2 2p^2 4s$

$2p^4 4s$

$2s^2 2p^2 4d$

$2p^4 4d$

$2s2p^3 4f$

Quasi-external

$2s2p^2 3s^2$

$2s2p^2 3p^2$

$2s2p^2 3d^2$

$2s2p^2 4f^2$

$2p^3 3s3p$

$2p^3 3p3d$

$2p^3 3d4f$

$2s2p^2 3s3d$

$2s2p^2 3p4f$

$2p^3 3s4f$

$2s^2 2p3s3p$

$2s^2 2p3p3d$

$2s^2 2p3d4f$

$2s^2 2p3s4f$

TABLE II Oscillator strengths for O II ions between various doublet states

Transition	λ(nm)	Present f_L	Present f_V	NCMET[a] f_L	NCMET[a] f_V	FOTOS[b]	Experiments	
$^2D^0$, $2s2p^4$ ^2D	71.8	0.148	0.158	0.141	0.167	-	0.18±0.02[c]	0.17±0.02[d]
$^2D^0$, $2p^23s$ ^2D	55.5	0.052	0.051	-	-	-		
$^2D^0$, $2p^2(^3P)3d$ ^2D	48.2	0.0247	0.0240	-	-	-		
$^2D^0$, $2p^23s$ ^2P	61.7	0.106	0.118	0.092	0.126	0.085	0.13±0.01[e]	0.118±0.006[f]
$^2D^0$, $2s2p^4$ ^2P	53.8	0.164	0.164	0.158	0.184	0.109	0.16±0.002[e] 0.22±0.07[d]	0.19±0.002[f]
$^2D^0$, $2p^2(^3P)3d$ ^2P	48.4	0.055	0.052	-	-	0.056		
$^2P^0$, $2s2p^4$ ^2D	79.7	0.0308	0.0303	0.030	0.043	-		
$^2P^0$, $2p^23s$ ^2D	60.1	0.048	0.048	-	-	-		
$^2P^0$, $2p^2(^3P)3d$ ^2D	51.5	0.109	0.106	-	-	-		
$^2P^0$, $2p^23s$ ^2P	67.3	0.035	0.037	0.036	0.037	0.183	0.036±0.002[f]	
$^2P^0$, $2s2p^4$ ^2P	58.1	0.094	0.103	0.086	0.120	0.086	0.102±0.004[e]	0.085±0.003[f]
$^2P^0$, $2p^2(^3P)3d$ ^2P	51.8	0.129	0.140	-	-	0.121		
$^2P^0$, $2s2p^4$ ^2S	64.4	0.104	0.113	0.097	0.102	-	0.084±0.01[d]	
$^2P^0$, $2p^23s$ ^2S	-	0.011	0.011	-	-	-		

a: Refs. 8 and 10; b: Ref. 11 c: Ref. 16 d: Ref. 17 e: Ref. 4 f: Ref. 5

TABLE III Comparisons with experimental measurements

$\lambda(\text{Å})$	Upper state	Present (f_L)	NCMET (f_L)[a]	Branching[b] ratio exp.	Rocket[c] measurement
482/515	$3d\ ^2D$	$\frac{0.0247}{0.109} = 0.23$	-	0.56 or 0.62±0.12	-
538/581	$2p^4\ ^2P$	$\frac{0.164}{0.094} = 1.74$	$\frac{0.158}{0.086} = 1.84$	1.55 or 1.75±0.35	>5.5
555/601	$3s\ ^2D$	$\frac{0.052}{0.048} = 1.08$	-	1.85 or 1.65±0.33	1.0±0.5
617/673	$3s\ ^2P$	$\frac{0.106}{0.035} = 3.03$	$\frac{0.092}{0.036} = 2.56$	4.1 or 4.3±0.9	3.6±1.1
718/797	$2p^4\ ^2D$	$\frac{0.148}{0.031} = 4.77$	$\frac{0.141}{0.030} = 4.7$	6.6 or 7.3±1.5	5.9±3.0

a : Ref. 8
b : Ref. 7
c : Ref. 3