

The Calculations of Oscillator Strengths and Transition Probabilities for Atomic Fluorine

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Abstract

Oscillator strengths for transitions between individual lines belonging to some doublet and quartet terms, and multiplet transition probabilities of atomic fluorine have been calculated using weakest bound electron potential model theory (WBEPMT). In the determination of relevant parameters, we employed numerical non-relativistic Hartree-Fock (NRHF) wave functions for expectation values of radii and the necessary energy values have been taken from experimental energy data in the literature. Oscillator strengths and transition probabilities obtained in this work have been compared to experimental and theoretical values given in the literature.

Key Words: Transition probabilities, oscillator strengths, the weakest bound electron potential model theory, atomic fluorine.

1. Introduction

Determination of physical parameters such as oscillator strengths, transition probabilities and atomic lifetimes are very important in research areas where atomic data is widely used. Hence, the reliability of the values of these parameters is mainly based in the performance of calculation methods used. Especially, the lifetimes belonging to neutral fluorine is very important for physical applications. The determination of lifetimes depends on accuracy of transition probabilities obtained. Moreover, transition probabilities, oscillator strengths and lifetimes are basic physical parameters that are often used to present data in evaluating the properties of plasma.

Fluorine is the most reactive of all elements of periodic table and no chemical substance is capable of freeing fluorine from any of its compounds. For this reason, fluorine does not exist free in nature and is extremely difficult for scientists to isolate [1]. Therefore, data for this atom is scarce in the literature. However, several methods have been used to study the transition probabilities, oscillator strengths and lifetimes for atomic fluorine. Absolute transition probabilities in the visible and near-infrared region of the spectrum for FI, CII, CIII and BrI have been measured by Bengston et al. [2] using a gas-driven shock tube technique. Extensive sets of oscillator strengths have been calculated by Kurucz and Peytremann [3] using a semi-empirical approach. Relative transition probabilities and lifetimes relevant to level $2p^43p$ have been measured by Vujnovic et al. for F-I [4] using wall-stabilized arc technique. The oscillator strengths of multiplets for F-I have been calculated by Baliyan and Bhatia [5] using configuration interaction wave

functions. The oscillator strengths for multiplets of atomic fluorine have been calculated by the Opacity Project team [6] using the R-matrix method. Relativistic quantum defect orbital (RQDO) calculations with and without polarization results have been carried out by Velasco et al. [7]. Musielok have been studied regularities of line strengths in spectra of N-I, F-I and Ne-II [8]. Relative transition probabilities between lines of 3s-3p and 3p-3d have been measured by Musielok et al. [9] for neutral fluorine in the visible and near-infrared region of spectrum applying a wall-stabilized high-current arc technique. Lifetimes for metastable state ($3s\ 4P_{5/2}$) in fluorine atom were determined by Shimizu et al. [10], measuring the decay curve of the fluorescence intensity as a function of distance from the plasma source. Transition probabilities and oscillator strengths have been calculated by Tachiev and Fischer [11] using Multiconfiguration Hartree-Fock Method. Recently, Zheng and Wang have calculated theoretical transition probabilities and oscillator strengths for some individual and multiplet transitions of 3s-3p transition array in neutral fluorine using the NCA method for expectation values of radii in the WBEPMT framework [12].

2. Theoretical approximation

The determination of oscillator strengths and transition probabilities theoretically for multi-electron systems is an important, but also difficult, problem in atomic physics, to be overcome. The difficulties arise from the issues in distinguishing, or indistinguishing, equivalent electrons and the necessity of taking into account many configurations or orbital basis set functions in calculations. Therefore, new methods need to be developed for the calculations of transition probabilities and oscillator strengths, especially those associated with high-lying levels. Towards alleviating these difficulties, Zheng [13] has proposed the weakest bound electron potential model theory (WBEPMT). He has suggested a new model potential to describe the electronic motion in a multi-electron atom or ion in his papers [13–16]. The WBEPMT theory is based on the idea that a system of electrons can be divided into two groups: one being the weakest bound electron; the other being the non-weakest bound electrons. The weakest bound electron in a given many-electron system is that electron that is most weakly bound to the system compared to the other electrons. Therefore, the weakest bound electron in a given atomic or ionic system is also the electron which can most easily be excited or ionized. By the separation of the electrons in a given system, complex many-electron problem can be simplified as the single electron problem and so can be solve more easily [17–21].

Electric dipole transition probability from one level, labeled by γJM , to another level, labeled by $\gamma' J' M'$, can be expressed as [22]

$$A(\gamma JM \rightarrow \gamma' J' M') = \frac{64\pi^4 e^2 a_0^2 (E_{J'} - E_J)^3}{3h} S \sum_{Mq} \begin{pmatrix} J & 1 & J' \\ -M & q & M' \end{pmatrix}^2 \quad (1)$$

The total transition probability from γJM to all M' levels of $\gamma' J'$ can be determined via the relation

$$A = \frac{64\pi^4 e^2 a_0^2 (E_{J'} - E_J)^3}{3h(2J' + 1)} S. \quad (2)$$

Oscillator strength from one level, labeled by γJ , to another level, labeled by $\gamma' J'$, has been given [22] as

$$f_{ij} = \frac{8\pi^2 m c a_0^2 \sigma}{3h(2J + 1)} S = \frac{(E_j - E_i)}{3h(2J + 1)} S = 3,0376 \cdot 10^{-6} (E_j - E_i) S. \quad (3)$$

Here, $(E_j - E_i)$ is the energy difference between relevant levels and S is the electric dipole line strength. $(E_j - E_i)$ has units of kaysers (cm^{-1}) and S in atomic units of $e^2 a_0^2$. Line strength is determined according

to the coupling schemes and the transition types in atomic or ionic systems. As well known, LS coupling in light atoms is the dominant coupling scheme. In this coupling, electric dipole line strength for $l_1^n l_2 \rightarrow l_1^n l_3$ type transitions scheme can be given as [22]

$$\begin{aligned} \sqrt{S_{LS}} &\equiv \langle [(\dots\alpha_1 L_1, l_2) L (\dots S_1 s_2) S] J | \mathbf{r}_N^{(1)} | [(\dots\alpha'_1 L'_1, l'_2) L' (\dots S'_1 s'_2) S'] J' \rangle \\ &= \delta_{\alpha_1 L_1 S_1, \alpha'_1 L'_1 S'_1} \delta_{s s'} (-1)^{S+J'+L_1+l'_2} [J, J', L, L']^{1/2} \left\{ \begin{matrix} L & S & J \\ J' & 1 & L' \end{matrix} \right\} \left\{ \begin{matrix} L_1 & l_2 & L \\ 1 & L' & l'_2 \end{matrix} \right\} \end{aligned} \quad (4)$$

If there were n equivalent electrons in a shell, the expression for line strength should be multiplied by the factor of $n(l_1^n \alpha_1 L_1 S_1 \left\{ \begin{matrix} l_1^{n-1} \alpha'_1 L'_1 S'_1 \end{matrix} \right\})$ in $l_1^n \rightarrow l_1^{n-1} l_2$ type transitions,

$$\begin{aligned} \sqrt{S_{LS}} &\equiv \langle \alpha_1 L_1, S_1, J | \mathbf{r}^{(1)} | (\alpha'_1 L'_1, S'_1, l_2) L' S' J' \rangle \\ &= \delta_{S_1 S'} (-1)^{L'_1+l_2+S_1+J'} (n. [L_1, L', J, J'])^{1/2} x \\ &\quad \left\{ \begin{matrix} L_1 & S & J \\ J' & 1 & L' \end{matrix} \right\} \left\{ \begin{matrix} l_2 & L'_1 & L_1 \\ L' & 1 & l'_2 \end{matrix} \right\} \end{aligned} \quad (5)$$

$$P_{l_2 l'_2}^{(1)} = l_> \langle n_i, l_i | r^k | n_f, l_f \rangle = l_> \int_0^\infty r^{k+2} R_{n_i l_i}(r) R_{n_f l_f}(r) dr$$

$$\left\{ \begin{matrix} L & S & J \\ J' & 1 & L' \end{matrix} \right\} = W(\text{abcd};\text{ef}).$$

Here, n is number of equivalent electrons in a shell and the bracketed term is the coefficient of fractional parentage. Tables of numerical values of the coefficients of fractional parentage for p shells are given in literature [22, 23]. $W(\text{abcd};\text{ef})$ is known as the Racah coefficient or Wigner's 6-j symbol, and it is used to describe the coupling between two or more angular momentums. $P_{l_2 l'_2}^{(1)}$ is known to be radial transition integral. In this work, equation (5) has been employed for transitions processed by equivalent electrons, and equation (4) has been employed for the case of non-equivalent electrons in a shell or for the transitions between two excited levels on the determination of line strengths.

According to WBEPM theory, in the Schrödinger equation of the weakest bound electron, in solving the radial equation by employing some transformations, the radial wave function of the weakest bound electron [20, 24] can be obtained as

$$R = C \exp\left(-\frac{Z^* r}{n^*}\right) r^{l^*} L_{n^*-l^*-1}^{2l^*+1}\left(\frac{2Z^* r}{n^*}\right), \quad (6)$$

where, $L_{n^*-l^*-1}^{2l^*+1}\left(\frac{2Z^* r}{n^*}\right)$ is the general Laguerre polynomial and C is normalization constant given to be

$$C = \left(\frac{2Z^*}{n^*}\right)^{l^*+3/2} \left[\frac{2n^*}{(n^*-l^*-1)!} \Gamma(n^*-l^*+1) \right]^{-1/2}. \quad (7)$$

Here, parameters n^* and l^* have been given to be

$$n^* = n + d \quad l^* = l + d. \quad (8)$$

Quantities Z^* , n^* , l^* are defined to be the effective nuclear charge, effective principal quantum number, effective azimuthal quantum number, respectively, and d is an adjustable parameter. In WBEPM theory, the determination of parameters Z^* , n^* and l^* is sufficient for the calculation of oscillator strengths and transition probabilities. These parameters were obtained by solving together equations (9) and (10):

$$I = -\varepsilon = \frac{Z^{*2}}{2n^{*2}} \quad (9)$$

$$\langle r \rangle = \frac{3n^{*2} - l^*(l^* + 1)}{2Z^*} \quad (10)$$

Here, I is the ionization energy and $\langle r \rangle$ is the expectation value for radius of the weakest bound electron. It is well known that some difficulties in obtaining the parameters directly from theory are still present. Therefore, Zheng suggest that ionization energies for the weakest bound electron is taken from experimental energy values in literature and expectation value of radius of the weakest bound electron is obtained from many different methods such as NCA, HF, MCHF, RHF, HKS, etc. [25].

In this study, for determination of relevant parameters, ionization energies used in the equation (7) are taken from experimental values [26]; and to determine the expectation values of radii for all levels, we used the computer program HF96, based on the numerical non-relativistic Hartree-Fock wave functions [27, 28].

3. Results and Conclusion

In this study, oscillator strengths for transitions between the individual lines belonging to doublet and quartet terms in some 2p-3s, 3s-3p transitions and multiplet atomic transition probabilities of some 3p-3d and 3s-3p transitions for atomic fluorine have been calculated using weakest bound electron potential model theory. The parameters required for the calculations of the oscillator strengths and transition probabilities have been determined using the procedure mentioned above. Using these parameters, the values of oscillator strengths obtained are presented in Table 1 and transition probabilities are presented in Table 2, in comparison with the experimental and theoretical data given in the literature. It can be seen from Table 1 that our oscillator strength results are in well agreement with the values in literature. Since no data has been presented in accepted values from NIST [29] for the transitions of 3p-3d, our data for transition probabilities are compared to the most theoretical or experimental results currently available in the literature. Because lack of sufficient data on atomic fluorine in the literature for the purpose of comparison, we have used transition probabilities derived from calculations of relativistic quantum defect orbital (RQDO) oscillator strengths. Oscillator strengths derived from atomic transition probabilities have been measured by Bengtson et al. [2]. In Table 2 one can see the transition probabilities results obtained in this paper are in agreement with the experimental and theoretical data in the literature.

Atomic fluorine is a multi-electron system having seven valance electrons, except the $1s^2$ core electrons. There are important interactions among the configurations, particularly in the excited states. It is not easy to deal with these multi-electron systems using known ab-initio methods, since too many configurations may be required for a sufficient representation. In order to obtain accurate physical data in an ab initio method, many configurations and orbital basis set functions should be considered to include these interactions. Experimentally, the measurement of transition probabilities and oscillator strengths are still very difficult for several reasons. The results obtained using the experimental methods have usually been measured with uncertainties between $\pm 10 - 50$ %. For example, Bengston et al. [2] have estimated the uncertainty in the range of $\pm 20 - 50$ % and Musielok et al. [8] is $\pm 18 - 40$ %. Moreover, it can be seen from the literature that the measured values obtained using different experimental methods may have been different for the same transitions. Considering the estimated uncertainties on the experimental data, our results are in

agreement with the experimental results in the literature. The WBEPM theory is a method to calculate the oscillator strengths and transition probabilities for atoms with a simple calculation procedure. Accuracy and reliability of the results calculated using WBEPMT strongly depends on the accuracy of the expectation values of radii used in determination of relevant parameters. The values of the transition probability and oscillator strength will be better if the expectation values have enough accuracy. The method used in this work requires quite shorter time than other methods need for the computation procedure. The calculations for transition probabilities and oscillator strengths belonging to either low lying or highly excited levels can, and thus easily and in a shorter time, be performed. We suppose that this method can be considered as a useful method for especially highly excited states.

Table 1. Oscillator strengths and comparison with theoretical and experimental data for atomic fluorine.

Lower State (L)	Upper State (U)	TERMS		Statical Weight		This Work	NIST DATA Ref. [29]	Velasco et al. Ref.[7]	Tachiev and Fischer Ref. [11]	Bengtson et al. Ref.[2]
		L	U	L	U					
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	4P	4S	6	4	0,124	0,110	0,0936	0,101	0,0942
				4	4	0,122	0,110	0,0941	0,126	0,0991
				2	4	0,121	0,110	0,0944	0,148	-
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	4P	4P	6	6	0,229	0,210	0,1915	0,256	0,249
				6	4	0,099	0,091	0,0824	0,118	0,220
				4	6	0,144	0,130	0,1229	0,0963	0,100
				4	4	0,043	0,039	0,0366	0,048	-
				4	2	0,136	0,120	0,1146	0,139	0,145
2	2	0,053	0,0490	0,0458	0,0405	-				
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	4P	4D	6	8	0,465	0,420	0,374	0,449	0,376
				6	6	0,106	0,096	0,0844	0,0657	0,0610
				6	4	0,011	0,011	0,0094	0,00485	0,0072
				4	6	0,364	0,330	0,2958	0,377	0,313
				4	4	0,187	0,170	0,1505	0,163	0,120
				4	2	0,0294	0,027	0,0235	0,0216	0,013
				2	4	0,289	0,260	0,2355	0,320	0,305
2	2	0,291	0,270	0,2357	0,293	0,260				
$2s^2 2p^5$	$2s^2 2p^4(^3P)3s$	2P	2P	4	4	0,0655	-	0,1285	0,0817	-
				4	2	0,0121	-	0,0246	0,0165	-
				2	4	0,0237	-	0,0510	0,0318	-
				2	2	0,0486	-	0,0981	0,0648	-
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	2P	2S	4	2	0,122	0,110	0,0967	0,141	0,164
				2	2	0,119	0,110	0,0970	0,0491	0,135
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	2P	2D	4	6	0,523	0,470	0,4289	0,449	0,423
				4	4	0,059	0,053	0,0479	0,0772	0,048
				2	4	0,0578	0,530	0,0479	0,469	0,383

Table 2. Transition probabilities and comparison with other values from literature for atomic fluorine ($\times 10^8 sn^{-1}$).

Lower (L)	Upper (U)	L	U	Wavelength Å	This Work	Kurucz and Peytremann Ref. [3]	Velasco et al. Ref.[7]	Tachiev and Fischer Ref. [11]	Musielok et al. Ref.[9]
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	4D	4F	8862,6	0,486	0,332	0,601	0,524	0,320
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	4P	4D	8263,2	0,412	0,338	0,506	0,577	0,334
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	4S	4P	9892,3	0,219	0,161	0,271	0,539	0,127
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	4D	4D	9130,0	0,112	0,109	0,139	0,144	-
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	4P	4P	7973,9	0,247	0,135	0,264	0,176	0,118
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	4D	4P	8778,1	0,0137	0,0487	0,0171	0,0359	-
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	2D	2D	9567,4	0,103	0,102	0,127	0,114	-
$2s^2 2p^4(^3P)3p$	$2s^2 2p^4(^3P)3d$	2S	2P	9760,1	0,228	0,0959	0,280	0,370	0,0656
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	4P	4S	6304,2	0,702	0,577	0,464	0,611	0,658
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	4P	4P	7445,8	0,391	0,368	0,321	0,406	0,444
$2s^2 2p^4(^3P)3s$	$2s^2 2p^4(^3P)3p$	4P	4D	6859,0	0,503	0,463	0,389	0,483	0,462

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