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Theoretical Calculations of Transition Probabilities and Oscillator Strengths for Sc(III) and Y(III)

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The Weakest Bound Electron Potential Model theory is used to calculate transition probability-values and oscillator strength-values for individual lines of Sc(III) and Y(III). In this method, by solving the Schrödinger equation of the weakest bound electron, the expressions of energy eigenvalue and the radial function can be obtained. And a coupled equation is used to determine the parameters which are needed in the calculations. The obtained results of Sc(III) from this work agree very well with the accepted values taken from the National Institute of Standards and Technoligy (NIST) data base, most deviations are within the accepted level. For Y(III) there are no accepted values reported by the NIST data base. So we compared our results of Y(III) with other theoretical results, good agreement is also obtained.

Key words: Weakest bound election potential model theory, Transition probability, Oscillator strength, Sc(III), Y(III)

I. INTRODUCTION

There has been growing interest in the calculations of transition probabilities for atoms and ions because these values are used in many applications of astrophysics, plasma physics, thermonuclear fusion research, and laser isotope separations. The values of transition probabilities can give some important information about the physical properties of an atom or an ion. The ground configurations of Sc(III) and Y(III) are [Ar]3d and [Kr]4d respectively, and theoretical studies of these two systems are of special interest.

Many theoretical methods have been used to investigate transition probabilities and oscillator strengths of Sc(III). Theoretical research on oscillator strengths for the inner-shell excitation of Sc(III) reported by Hibbert *et al.* gave both the Hartree-Fock (HF) and configuration interaction (CI) calculations of oscillator strengths of the $3p^6 3d$-$3p^5 3d^2$ transitions [1,2]. The quantum defect orbital (QDO) method was employed to calculate oscillator strengths for potassium and some of its isoelectronic ions including Sc(III) on the isoelectronic sequence of potassium by Martin *et al.* [3,4]. A core-polarization correction to the dipole transition moment was included in the study by using a core polarization-corrected dipole. All these studies did not consider fine structure effects and only provided multiplet results. The forbidden transitions of Sc(III) have also raised interest for many theorists; electric quadrupole (E_2) and magnetic dipole (M_1) transitions of Sc(III) were reported in Refs.[5,6]. Schippers *et al.* carried out both experimental and theoretical studies of Sc(III) [7]. In their work, the authors first employed the ion-photon beams method to measure the cross sections for the photoionization of Sc(III) and then performed theoretical calculations using the code of Cowan. The theoretical calculations in their study was restricted to the transition between ground state and the inner-shell excitation of Sc(III). The study of transition between high excited states was not included in this work.

There are also many theoretical studies for Y(III). Reffors *et al.* used the computer code of Cowan to calculate gf values for the lines of Y(III) [8]. The uncertainty of the reported gf values was estimated to be within 10%. Brage *et al.* gave oscillator strengths for several transitions of Y(III) using multiconfiguration Hartree-Fock (MCHF) method and made an application of the obtained values to determine the solar abundance of yttrium [9]. All the methods mentioned above must take into account configuration interaction effects in order to get accurate results. For complicated systems such as Sc(III) and Y(III), the possible configurations are so numerous that only some of them can be selected in practice, which is expected to influence the results significantly.

In this work, we calculate the transition probabilities and oscillator strengths of Sc(III) and Y(III) ions with the weakest bound electron potential model (WBEPM) theory and compare our results with the accepted values and other theoretical results. Since the WBEPM theory was presented [22-26], many studies have been carried

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out using it to investigate the atomic properties of many systems [10-21]. In this work, we also introduce the WBEPM theory briefly. The Schrödinger equation is solved to obtain the radial wave function, and we use a couple of equations to obtain the parameters.

II. THEORY AND METHOD

The WBEPM theory is based on the followings: (i) the consideration of successive ionization of free particles (atom and molecule); (ii) the choice of zero of energy in quantum mechanics; (iii) the separation of the weakest bound electron (WBE) and non-weakest bound electrons (NWBE). The WBEPM theory classifies the electrons in an atom system or an ion system into two types: WBE and NWBE. The WBE is the electron which is most weakly bonded to the system and can be excited or ionized most easily, and the rest of electrons are called NWBE. We consider the nucleus and non-weakest bound electrons as an ion core, and the WBE is supposed to move in the central potential of this ion core. An N-electron atom system can be subdivided into N subsystems which correspond with the N species ionized. Also, these N electrons in the N-electron atom system each play a role as WBE in one of the N subsystems. There is only one WBE in each subsystem, and other electrons in the subsystem are NWBE.

According to the WBEPM theory, the Schrödinger equation of WBEi is

$$\left[-\frac{1}{2}\nabla_i^2 + V(r_i)\right]\varphi_i = \varepsilon_i\varphi_i \tag{1}$$

In the WBEPM theory the potential function $V(r_i)$ in Eq.(1) may be written as (in atomic unit):

$$V(r_i) = \frac{-Z_i'}{r_i} + \frac{d_i(d_i+1)+2d_il_i}{2{r_i}^2} \tag{2}$$

in which the first term represents the Coulomb potential and the second term represents the dipole potential produced by the polarization effect, Z_i' is the effective number charge, l_i is the angular quantum number of WBEi, r_i is the distance between the WBEi and the nucleus, and d_i is a parameter which modifies the integral quantum number n_i and angular quantum number l_i into non-integral n_i' and l_i'.

Substituting Eq.(2) into Eq.(1) and solving the Schrödinger equation of the WBEi, the following expressions of energy eigenvalue and the radial function R can be obtained:

$$\varepsilon_i = -\frac{{Z_i'}^2}{2{n_i'}^2} \tag{3}$$

$$R = C\exp\left(-\frac{Z_i'r_i}{n_i'}\right) r^{l_i'} L_{n_i-l_i-1}^{2l_i'+1}\left(\frac{2Z_i'r_i}{n_i'}\right) \tag{4}$$

where n_i' is the effective principal quantum number with n_i'=n_i+d_i, and l_i' is the effective angular quantum number with l_i'=l_i+d_i, C is the normalization factor and $L_{n_i-l_i-1}^{2l_i'+1}\left(\frac{2Z_i'r_i}{n_i'}\right)$ is the generalized Laguerre polynomial.

It is clear that the negative value of ε_i in Eq.(3) should be approximately equal to the ionization energy of that WBEi,

$$I_i = -\varepsilon_i = \frac{{Z_i'}^2}{2{n_i'}^2} \tag{5}$$

Further, the expression of the radial expectation value of the WBEi $\langle r_i\rangle$ can be obtained as [27]:

$$\langle r_i\rangle = \frac{3{n_i'}^2 - l_i'(l_i'+1)}{2Z_i'} \tag{6}$$

The transition probability of (n_f, l_f) to (n_i, l_i) for spontaneous emission (E_f>E_i) is [28,29] (in atomic units)

$$\begin{aligned} A_{fi} = {} & \frac{4}{3}\alpha^3(E_f-E_i)^3\left|\langle n_fl_f|r|n_il_i\rangle\right|^2 \cdot \\ & (2L_f+1)(2L_i+1)(2J_i+1)l_> \times \\ & W^2(l_iL_il_fL_f;L_c1)\times W^2(L_iJ_iL_fJ_f;S1) \end{aligned} \tag{7}$$

where $l_\rangle$=max(l_f, l_i), α is the fine structure constant, E_f and E_i (in Hartree unit) are the energies of (n_f, l_f) and (n_i, l_i) respectively, L_c is the total orbital angular momentum of atomic core and $W(abcd;ef)$ is the Racah coefficient [30,31].

In order to obtain the value of $\langle n_fl_f|r|n_il_i\rangle$, the parameters Z' and d are required. Coupled equations by associating Eq.(5) with Eq.(6) will be employed for the determination of parameters:

$$\varepsilon = -\frac{{Z'}^2}{2{n'}^2} \tag{8}$$

$$\langle r\rangle = \frac{3{n'}^2 - l'(l'+1)}{2Z'} \tag{9}$$

ε or I can be obtained from the experimental atomic energy data. In this work, for Sc(III) they are taken from the NIST website [32]; for Y(III) they are taken from Ref.[33]. The $\langle r\rangle$ value can be calculated from many theoretical methods such as Roothanna Hartree-Fock (RHF), Hartree-Kohn-Sham (HKS), multiconfiguration Hartree-Fock (MCHF), self-interaction-corrected local spin density (SIC-LSD), time-dependent Hartree-Fock (TDHF), Hartree-Slater, and numerical coulomb approximation (NCA) [34-40]. In this work NCA is employed to evaluate $\langle r\rangle$. NCA is a good approximation for excited states, since its calculation is simple and its results agree well with the results obtained from other theoretical methods.

After obtaining the values of Z', n', and l', the matrix element in Eq.(7) can be calculated, and the transition probability between two levels (n_f, l_f) and (n_i, l_i) can also be calculated.

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TABLE I Transition probabilities A and oscillator strengths f for Y(III) compared with others' results.

Transition	$A/10^8$ s^{-1}		f	
	This work	Others' results [9]	This work	Others' results
5s $^2S_{1/2}$-5p $^2P^0_{1/2}$	2.766	3.27	0.3601	0.320 [9][a]
		2.55		0.313 [41][b]
		2.42		0.317 [42][c]
		2.45		0.426 [8][d]
5s $^2S_{1/2}$-5p $^2P^0_{3/2}$	3.153	3.43	0.7506	0.673 [9][a]
		2.92		0.656 [41][b]
		2.79		0.666 [42][c]
		2.82		0.889 [8][d]
6s $^2S_{1/2}$-5p $^2P^0_{1/2}$	2.105	2.75	0.1537	0.207 [9][a]
		2.23		0.196 [41][b]
		2.76		0.213 [8][d]
		2.83		
6s $^2S_{1/2}$-5p $^2P^0_{3/2}$	4.239	4.96	0.1659	0.208 [9][a]
		4.02		0.208 [41][b]
		5.27		0.203 [8][d]
		5.32		
5p $^2P^0_{1/2}$-5d $^2D_{3/2}$	6.694	9.35	0.9093	1.071 [9][a]
		8.12		1.040 [41][a]
		7.77		1.227 [8][d]
		7.89		
5p $^2P^0_{3/2}$-5d $^2D_{3/2}$	1.289	1.69	0.09363	0.106 [9][a]
		1.47		0.106 [41][b]
		1.46		0.117 [8][d]
		1.46		
5p $^2P^0_{3/2}$-5d $^2D_{5/2}$	7.753		0.8376	0.959 [9][a]
				0.950 [41][b]
				1.07 [8][d]
5d $^2D_{3/2}$-4f $^2F^0_{5/2}$	0.4561		0.6347	
5d $^2D_{5/2}$-4f $^2F^0_{5/2}$	0.03113		0.02980	
5d $^2D_{5/2}$-4f $^2F^0_{7/2}$	0.5176		0.6607	

[a] These values are translated from the values of lg(gf) reported in the Ref.[9].
[b] Coulomb approximation calculations from Ref.[41], these values are translated from the values of lg(gf).
[c] Hartree-Fock calculations with core-polarization corrections in both potential and transition matrix from Ref.[42].
[d] These values are translated from the values of lg(gf) reported in the Ref.[8].

III. RESULTS AND DISCUSSION

Employing the method mentioned above, we calculated the transition probabilities and oscillator strengths of transitions between some excited states for Sc(III) and Y(III).

The results for Y(III) transitions are listed in Table I. There are no values on NIST data base for Y(III), so we list some other results in Table I for comparison. As the experimental energy level data for Y(III) is quite limited, we only give results for several transitions in this work. In the future, if more experimental energy level data can be obtained, anyone who wants a specific the value of transition probability A or the value of oscillator strength f can obtain it using the WBEPM theory easily. It can be seen that most of our results agree well with other results.

The results for Sc(III) transitions are listed in Table II. There are many theoretical studies of transitions for Sc(III), but current computations are generally restricted to the study of the values of gf and f. g is statistical weight of a level. Studies of the values of transition rates are quite limited and many works just focus on the transitions between multiplets and the transitions between ground state and low excited states. Because the results for transitions between excited states

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TABLE II Transition probabilities A and oscillator strengths f for Sc(III) compared with the accepted values.

Transition	$A/10^8$ s^{-1}		f	
	This work	NIST [32]	This work	NIST [32]
4s $^2S_{1/2}$-4p $^2P^0_{1/2}$	2.887	3.3	3.236×10^{-1}	0.37
4s $^2S_{1/2}$-4p $^2P^0_{3/2}$	3.001	3.43	6.559×10^{-1}	0.750
4s $^2S_{1/2}$-5p $^2P^0_{1/2}$	2.138×10^{-1}	0.16	3.047×10^{-3}	0.0023
4s $^2S_{1/2}$-5p $^2P^0_{3/2}$	1.831×10^{-1}	0.17	5.199×10^{-3}	0.0048
5s $^2S_{1/2}$-4p $^2P^0_{1/2}$	2.314	3.0	1.246×10^{-1}	0.16
5s $^2S_{1/2}$-4p $^2P^0_{3/2}$	4.651	5.8	1.275×10^{-1}	0.16
5s $^2S_{1/2}$-5p $^2P^0_{1/2}$	5.487×10^{-1}	0.54	4.689×10^{-1}	0.46
5s $^2S_{1/2}$-5p $^2P^0_{3/2}$	5.699×10^{-1}	0.58	9.485×10^{-1}	0.97
5s $^2S_{1/2}$-7p $^2P^0_{1/2}$	1.928×10^{-2}		9.630×10^{-4}	
5s $^2S_{1/2}$-7p $^2P^0_{3/2}$	1.640×10^{-2}		1.636×10^{-3}	
6s $^2S_{1/2}$-4p $^2P^0_{1/2}$	1.195	1.1	2.361×10^{-2}	0.022
6s $^2S_{1/2}$-4p $^2P^0_{3/2}$	2.398	2.3	2.396×10^{-2}	0.023
6s $^2S_{1/2}$-5p $^2P^0_{1/2}$	6.951×10^{-1}	0.80	2.343×10^{-1}	0.27
6s $^2S_{1/2}$-5p $^2P^0_{3/2}$	1.392	1.55	2.386×10^{-1}	0.266
6s $^2S_{1/2}$-6p $^2P^0_{1/2}$	1.596×10^{-1}		6.036×10^{-1}	
6s $^2S_{1/2}$-6p $^2P^0_{3/2}$	1.657×10^{-1}		1.220	
6s $^2S_{1/2}$-7p $^2P^0_{1/2}$	5.140×10^{-3}		1.843×10^{-3}	
6s $^2S_{1/2}$-7p $^2P^0_{3/2}$	3.960×10^{-3}		2.827×10^{-3}	
7s $^2S_{1/2}$-4p $^2P^0_{1/2}$	6.788×10^{-1}	0.60	9.398×10^{-3}	0.0083
7s $^2S_{1/2}$-4p $^2P^0_{3/2}$	1.362	1.2	9.514×10^{-3}	0.0084
7s $^2S_{1/2}$-5p $^2P^0_{1/2}$	3.871×10^{-1}	0.35	4.008×10^{-2}	0.036
7s $^2S_{1/2}$-5p $^2P^0_{3/2}$	7.735×10^{-1}	0.69	4.042×10^{-2}	0.036
7s $^2S_{1/2}$-6p $^2P^0_{1/2}$	2.580×10^{-1}	0.28	3.398×10^{-1}	0.37
7s $^2S_{1/2}$-6p $^2P^0_{3/2}$	5.161×10^{-1}	0.55	3.454×10^{-1}	0.37
7s $^2S_{1/2}$-7p $^2P^0_{1/2}$	5.933×10^{-2}		7.340×10^{-1}	
7s $^2S_{1/2}$-7p $^2P^0_{3/2}$	6.159×10^{-2}		1.483	
8s $^2S_{1/2}$-4p $^2P^0_{1/2}$	4.197×10^{-1}		4.867×10^{-3}	
8s $^2S_{1/2}$-4p $^2P^0_{3/2}$	8.416×10^{-1}		4.921×10^{-3}	
8s $^2S_{1/2}$-5p $^2P^0_{1/2}$	2.361×10^{-1}	0.2	1.557×10^{-2}	0.013
8s $^2S_{1/2}$-5p $^2P^0_{3/2}$	4.715×10^{-1}	0.38	1.565×10^{-2}	0.013
8s $^2S_{1/2}$-6p $^2P^0_{1/2}$	1.500×10^{-1}	0.14	5.454×10^{-2}	0.051
8s $^2S_{1/2}$-6p $^2P^0_{3/2}$	2.992×10^{-1}	0.27	5.485×10^{-2}	0.050
8s $^2S_{1/2}$-7p $^2P^0_{1/2}$	1.122×10^{-1}		4.437×10^{-1}	
8s $^2S_{1/2}$-7p $^2P^0_{3/2}$	2.244×10^{-1}		4.505×10^{-1}	
4p $^2P^0_{1/2}$-4d $^2D_{3/2}$	7.794	9.4	9.290×10^{-1}	1.1
4p $^2P^0_{1/2}$-5d $^2D_{3/2}$	1.490	1.6	6.037×10^{-2}	0.065
4p $^2P^0_{1/2}$-6d $^2D_{3/2}$	6.914×10^{-1}	0.56	1.935×10^{-2}	0.016
4p $^2P^0_{1/2}$-7d $^2D_{3/2}$	4.082×10^{-1}		9.524×10^{-3}	
4p $^2P^0_{3/2}$-4d $^2D_{3/2}$	1.537	1.8	9.333×10^{-2}	0.11
4p $^2P^0_{3/2}$-4d $^2D_{5/2}$	9.232	11	8.396×10^{-1}	1.0
4p $^2P^0_{3/2}$-5d $^2D_{3/2}$	2.887×10^{-1}	0.32	5.913×10^{-3}	0.0066
4p $^2P^0_{3/2}$-5d $^2D_{5/2}$	1.741	1.9	5.347×10^{-2}	0.058
4p $^2P^0_{3/2}$-6d $^2D_{3/2}$	1.336×10^{-1}	0.11	1.888×10^{-3}	0.0016
4p $^2P^0_{3/2}$-6d $^2D_{5/2}$	8.064×10^{-1}	0.67	1.708×10^{-2}	0.014
4p $^2P^0_{3/2}$-7d $^2D_{3/2}$	7.892×10^{-2}		9.280×10^{-4}	
4p $^2P^0_{3/2}$-7d $^2D_{5/2}$	4.762×10^{-1}		8.403×10^{-3}	

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Table II continued.

Transition	$A/10^8$ s^{-1}		f	
	This work	NIST [32]	This work	NIST [32]
5p $^2P^0_{1/2}$-4d $^2D_{3/2}$	7.516×10^{-1}	0.73	2.242×10^{-1}	0.22
5p $^2P^0_{1/2}$-5d $^2D_{3/2}$	1.699	1.83	1.271	1.37
5p $^2P^0_{1/2}$-6d $^2D_{3/2}$	4.204×10^{-1}	0.48	8.969×10^{-2}	0.10
5p $^2P^0_{1/2}$-7d $^2D_{3/2}$	2.044×10^{-1}	0.21	2.733×10^{-2}	0.028
5p $^2P^0_{3/2}$-4d $^2D_{3/2}$	7.689×10^{-2}	0.075	4.488×10^{-2}	0.044
5p $^2P^0_{3/2}$-4d $^2D_{5/2}$	6.884×10^{-1}	0.66	2.694×10^{-1}	0.26
5p $^2P^0_{3/2}$-5d $^2D_{3/2}$	3.356×10^{-1}	0.36	1.277×10^{-1}	0.14
5p $^2P^0_{3/2}$-5d $^2D_{5/2}$	2.016	2.1	1.149	1.2
5p $^2P^0_{3/2}$-6d $^2D_{3/2}$	8.167×10^{-2}	0.095	8.795×10^{-3}	0.010
5p $^2P^0_{3/2}$-6d $^2D_{5/2}$	4.924×10^{-1}	0.56	7.950×10^{-2}	0.090
5p $^2P^0_{3/2}$-7d $^2D_{3/2}$	3.955×10^{-2}	0.041	2.664×10^{-3}	0.0028
5p $^2P^0_{3/2}$-7d $^2D_{5/2}$	2.386×10^{-1}	0.24	2.411×10^{-2}	0.024
6p $^2P^0_{1/2}$-4d $^2D_{3/2}$	2.615×10^{-1}	0.17	1.049×10^{-2}	0.0068
6p $^2P^0_{1/2}$-5d $^2D_{3/2}$	2.639×10^{-1}		3.652×10^{-1}	
6p $^2P^0_{1/2}$-6d $^2D_{3/2}$	5.293×10^{-1}		1.555	
6p $^2P^0_{1/2}$-7d $^2D_{3/2}$	1.587×10^{-1}	0.18	1.193×10^{-1}	0.14
6p $^2P^0_{3/2}$-4d $^2D_{3/2}$	2.697×10^{-2}	0.017	2.155×10^{-3}	0.0014
6p $^2P^0_{3/2}$-4d $^2D_{5/2}$	2.410×10^{-1}	0.16	1.286×10^{-2}	0.0085
6p $^2P^0_{3/2}$-5d $^2D_{3/2}$	2.706×10^{-2}		7.316×10^{-2}	
6p $^2P^0_{3/2}$-5d $^2D_{5/2}$	2.422×10^{-1}		4.390×10^{-1}	
6p $^2P^0_{3/2}$-6d $^2D_{3/2}$	1.047×10^{-1}		1.564×10^{-1}	
6p $^2P^0_{3/2}$-6d $^2D_{5/2}$	6.288×10^{-1}		1.406	
6p $^2P^0_{3/2}$-7d $^2D_{3/2}$	3.091×10^{-2}	0.035	1.172×10^{-2}	0.013
6p $^2P^0_{3/2}$-7d $^2D_{5/2}$	1.863×10^{-1}	0.21	1.059×10^{-1}	0.12
7p $^2P^0_{1/2}$-4d $^2D_{3/2}$	1.542×10^{-1}		3.510×10^{-3}	
7p $^2P^0_{1/2}$-5d $^2D_{3/2}$	8.287×10^{-2}	0.057	1.343×10^{-2}	0.0092
7p $^2P^0_{1/2}$-6d $^2D_{3/2}$	1.103×10^{-1}		5.051×10^{-1}	
7p $^2P^0_{1/2}$-7d $^2D_{3/2}$	2.049×10^{-1}		1.814	
7p $^2P^0_{3/2}$-4d $^2D_{3/2}$	1.584×10^{-2}		7.200×10^{-4}	
7p $^2P^0_{3/2}$-4d $^2D_{5/2}$	1.417×10^{-1}		4.299×10^{-3}	
7p $^2P^0_{3/2}$-5d $^2D_{3/2}$	8.631×10^{-3}	0.0056	2.784×10^{-3}	0.0018
7p $^2P^0_{3/2}$-5d $^2D_{5/2}$	7.699×10^{-2}	0.052	1.659×10^{-2}	0.011
7p $^2P^0_{3/2}$-6d $^2D_{3/2}$	1.132×10^{-2}		1.013×10^{-1}	
7p $^2P^0_{3/2}$-6d $^2D_{5/2}$	1.013×10^{-1}		6.074×10^{-1}	
7p $^2P^0_{3/2}$-7d $^2D_{3/2}$	4.056×10^{-2}		1.825×10^{-1}	
7p $^2P^0_{3/2}$-7d $^2D_{5/2}$	2.437×10^{-1}		1.641	
4d $^2D_{3/2}$-4f $^2F^0_{5/2}$	2.864	2.9	1.063	1.1
4d $^2D_{3/2}$-5f $^2F^0_{5/2}$	7.530×10^{-3}		7.600×10^{-4}	
4d $^2D_{3/2}$-6f $^2F^0_{5/2}$	5.027×10^{-2}	0.063	3.189×10^{-3}	0.0040
4d $^2D_{3/2}$-7f $^2F^0_{5/2}$	8.336×10^{-2}	0.093	4.181×10^{-3}	0.0047
4d $^2D_{5/2}$-4f $^2F^0_{5/2}$	2.037×10^{-1}	0.21	5.057×10^{-2}	0.052
4d $^2D_{5/2}$-4f $^2F^0_{7/2}$	3.055	3.1	1.011	1.0
4d $^2D_{5/2}$-5f $^2F^0_{7/2}$	7.331×10^{-3}		6.590×10^{-4}	
4d $^2D_{5/2}$-5f $^2F^0_{5/2}$	4.890×10^{-4}		3.293×10^{-5}	
4d $^2D_{5/2}$-6f $^2F^0_{7/2}$	5.534×10^{-2}	0.069	3.126×10^{-3}	0.0039
4d $^2D_{5/2}$-6f $^2F^0_{5/2}$	3.689×10^{-3}	0.0045	1.560×10^{-4}	0.00019

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Table II continued.

Transition	$A/10^8$ s^{-1}		f	
	This work	NIST [32]	This work	NIST [32]
4d ^{2}D$_{5/2}$-7f ^{2}F$^0_{7/2}$	9.078×10^{-2}	0.099	4.053×10^{-3}	0.0044
4d ^{2}D$_{5/2}$-7f ^{2}F$^0_{5/2}$	6.052×10^{-3}	0.0067	2.030×10^{-4}	0.00022
5d ^{2}D$_{3/2}$-4f ^{2}F$^0_{5/2}$	2.143×10^{-1}	0.20	1.691×10^{-1}	0.18
5d ^{2}D$_{3/2}$-5f ^{2}F$^0_{5/2}$	8.293×10^{-1}	0.84	1.449	1.5
5d ^{2}D$_{3/2}$-6f ^{2}F$^0_{5/2}$	6.242×10^{-2}	0.043	2.508×10^{-2}	0.017
5d ^{2}D$_{3/2}$-7f ^{2}F$^0_{5/2}$	3.646×10^{-3}		8.480×10^{-4}	
5d ^{2}D$_{5/2}$-4f ^{2}F$^0_{5/2}$	1.024×10^{-2}	0.0098	1.207×10^{-2}	0.012
5d ^{2}D$_{5/2}$-4f ^{2}F$^0_{7/2}$	2.047×10^{-1}	0.20	1.810×10^{-1}	0.18
5d ^{2}D$_{5/2}$-5f ^{2}F$^0_{7/2}$	8.852×10^{-1}	0.89	1.380	1.4
5d ^{2}D$_{5/2}$-5f ^{2}F$^0_{5/2}$	5.901×10^{-2}	0.059	6.901×10^{-2}	0.069
5d ^{2}D$_{5/2}$-6f ^{2}F$^0_{7/2}$	6.573×10^{-2}	0.047	2.351×10^{-2}	0.017
5d ^{2}D$_{5/2}$-6f ^{2}F$^0_{5/2}$	4.382×10^{-3}	0.0031	1.176×10^{-3}	0.00083
5d ^{2}D$_{5/2}$-7f ^{2}F$^0_{7/2}$	3.679×10^{-3}		7.620×10^{-4}	
5d ^{2}D$_{5/2}$-7f ^{2}F$^0_{5/2}$	2.450×10^{-4}		3.810×10^{-5}	
6d ^{2}D$_{3/2}$-4f ^{2}F$^0_{5/2}$	4.342×10^{-2}	0.053	5.261×10^{-3}	0.0064
6d ^{2}D$_{3/2}$-5f ^{2}F$^0_{5/2}$	1.304×10^{-1}		3.480×10^{-1}	
6d ^{2}D$_{3/2}$-6f ^{2}F$^0_{5/2}$	3.001×10^{-1}		1.758	
6d ^{2}D$_{3/2}$-7f ^{2}F$^0_{5/2}$	4.411×10^{-2}	0.034	5.345×10^{-2}	0.041
6d ^{2}D$_{5/2}$-4f ^{2}F$^0_{5/2}$	2.080×10^{-3}	0.0025	3.780×10^{-4}	0.00045
6d ^{2}D$_{5/2}$-4f ^{2}F$^0_{7/2}$	4.159×10^{-2}	0.050	5.665×10^{-3}	0.0068
6d ^{2}D$_{5/2}$-5f ^{2}F$^0_{7/2}$	1.246×10^{-1}		3.726×10^{-1}	
6d ^{2}D$_{5/2}$-5f ^{2}F$^0_{5/2}$	6.229×10^{-3}		2.484×10^{-2}	
6d ^{2}D$_{5/2}$-6f ^{2}F$^0_{7/2}$	3.205×10^{-1}		1.675	
6d ^{2}D$_{5/2}$-6f ^{2}F$^0_{5/2}$	2.137×10^{-2}		8.374×10^{-2}	
6d ^{2}D$_{5/2}$-7f ^{2}F$^0_{7/2}$	4.669×10^{-2}	0.036	5.037×10^{-2}	0.039
6d ^{2}D$_{5/2}$-7f ^{2}F$^0_{5/2}$	3.113×10^{-3}	0.0024	2.519×10^{-3}	0.0019
7d ^{2}D$_{3/2}$-4f ^{2}F$^0_{5/2}$	2.227×10^{-2}		1.495×10^{-3}	
7d ^{2}D$_{3/2}$-5f ^{2}F$^0_{5/2}$	3.262×10^{-2}	0.043	1.276×10^{-2}	
7d ^{2}D$_{3/2}$-6f ^{2}F$^0_{5/2}$	7.088×10^{-2}		5.261×10^{-1}	
7d ^{2}D$_{3/2}$-7f ^{2}F$^0_{5/2}$	1.281×10^{-1}		2.040	
7d ^{2}D$_{5/2}$-4f ^{2}F$^0_{5/2}$	1.066×10^{-3}		1.070×10^{-4}	
7d ^{2}D$_{5/2}$-4f ^{2}F$^0_{7/2}$	2.132×10^{-2}		1.610×10^{-3}	
7d ^{2}D$_{5/2}$-5f ^{2}F$^0_{7/2}$	3.124×10^{-2}	0.041	1.374×10^{-2}	0.017
7d ^{2}D$_{5/2}$-5f ^{2}F$^0_{5/2}$	1.562×10^{-3}	0.0021	9.160×10^{-4}	0.0012
7d ^{2}D$_{5/2}$-6f ^{2}F$^0_{7/2}$	6.771×10^{-2}		5.633×10^{-1}	
7d ^{2}D$_{5/2}$-6f ^{2}F$^0_{5/2}$	3.385×10^{-3}		3.756×10^{-2}	
7d ^{2}D$_{5/2}$-7f ^{2}F$^0_{7/2}$	1.368×10^{-1}		1.943	
7d ^{2}D$_{5/2}$-7f ^{2}F$^0_{5/2}$	9.119×10^{-3}		9.714×10^{-2}	
4f ^{2}F$^0_{5/2}$-5g ^{2}G$_{7/2}$	3.544		1.316	
4f ^{2}F$^0_{5/2}$-6g ^{2}G$_{7/2}$	1.224		1.964×10^{-1}	
4f ^{2}F$^0_{5/2}$-7g ^{2}G$_{7/2}$	5.934×10^{-1}		6.535×10^{-2}	
4f ^{2}F$^0_{5/2}$-8g ^{2}G$_{7/2}$	3.405×10^{-1}		3.036×10^{-2}	
4f ^{2}F$^0_{7/2}$-5g ^{2}G$_{9/2}$	3.675		1.280	
4f ^{2}F$^0_{7/2}$-5g ^{2}G$_{7/2}$	1.313×10^{-1}		3.656×10^{-2}	
4f ^{2}F$^0_{7/2}$-6g ^{2}G$_{7/2}$	4.535×10^{-2}		5.454×10^{-3}	
4f ^{2}F$^0_{7/2}$-6g ^{2}G$_{9/2}$	1.270		1.909×10^{-1}	

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Table II continued.

Transition	$A/10^8$ s^{-1}		f	
	This work	NIST [32]	This work	NIST [32]
4f $^2F^0_{7/2}$-7g $^2G_{7/2}$	2.198×10^{-2}		1.815×10^{-3}	
4f $^2F^0_{7/2}$-7g $^2G_{9/2}$	6.154×10^{-1}		6.353×10^{-2}	
4f $^2F^0_{7/2}$-8g $^2G_{7/2}$	1.261×10^{-2}		8.430×10^{-4}	
4f $^2F^0_{7/2}$-8g $^2G_{9/2}$	3.531×10^{-1}		2.952×10^{-2}	
5f $^2F^0_{7/2}$-5g $^2G_{9/2}$	1.130×10^{-4}		5.881×10^{-2}	
5f $^2F^0_{7/2}$-5g $^2G_{7/2}$	4.035×10^{-6}		1.680×10^{-3}	
5f $^2F^0_{7/2}$-6g $^2G_{7/2}$	3.244×10^{-2}		3.013×10^{-2}	
5f $^2F^0_{7/2}$-6g $^2G_{9/2}$	9.084×10^{-1}		1.054	
5f $^2F^0_{7/2}$-7g $^2G_{7/2}$	1.745×10^{-2}		6.535×10^{-3}	
5f $^2F^0_{7/2}$-7g $^2G_{9/2}$	4.886×10^{-1}		2.287×10^{-1}	
5f $^2F^0_{7/2}$-8g $^2G_{7/2}$	1.035×10^{-2}		2.535×10^{-3}	
5f $^2F^0_{7/2}$-8g $^2G_{9/2}$	2.898×10^{-1}		8.871×10^{-2}	
5f $^2F^0_{5/2}$-5g $^2G_{7/2}$	1.090×10^{-4}		6.049×10^{-2}	
5f $^2F^0_{5/2}$-6g $^2G_{7/2}$	8.760×10^{-1}		1.085	
5f $^2F^0_{5/2}$-7g $^2G_{7/2}$	4.711×10^{-1}		2.353×10^{-1}	
5f $^2F^0_{5/2}$-8g $^2G_{7/2}$	2.795×10^{-1}		9.124×10^{-2}	
6f $^2F^0_{7/2}$-5g $^2G_{9/2}$	1.485×10^{-2}		1.298×10^{-2}	
6f $^2F^0_{7/2}$-5g $^2G_{7/2}$	4.240×10^{-4}		4.630×10^{-4}	
6f $^2F^0_{7/2}$-6g $^2G_{7/2}$	3.525×10^{-6}		3.478×10^{-3}	
6f $^2F^0_{7/2}$-6g $^2G_{9/2}$	9.869×10^{-5}		1.217×10^{-1}	
6f $^2F^0_{7/2}$-7g $^2G_{7/2}$	1.052×10^{-2}		2.667×10^{-2}	
6f $^2F^0_{7/2}$-7g $^2G_{9/2}$	2.946×10^{-1}		9.335×10^{-1}	
6f $^2F^0_{7/2}$-8g $^2G_{7/2}$	6.890×10^{-3}		6.688×10^{-3}	
6f $^2F^0_{7/2}$-8g $^2G_{9/2}$	1.929×10^{-1}		2.341×10^{-1}	
6f $^2F^0_{5/2}$-5g $^2G_{7/2}$	1.528×10^{-2}		1.251×10^{-2}	
6f $^2F^0_{5/2}$-6g $^2G_{7/2}$	9.517×10^{-5}		1.252×10^{-1}	
6f $^2F^0_{5/2}$-7g $^2G_{7/2}$	2.841×10^{-1}		9.602×10^{-1}	
6f $^2F^0_{5/2}$-8g $^2G_{7/2}$	1.860×10^{-1}		2.408×10^{-1}	
7f $^2F^0_{7/2}$-5g $^2G_{9/2}$	6.102×10^{-3}		1.997×10^{-3}	
7f $^2F^0_{7/2}$-5g $^2G_{7/2}$	1.740×10^{-4}		7.131×10^{-5}	
7f $^2F^0_{7/2}$-6g $^2G_{7/2}$	4.050×10^{-4}		1.225×10^{-3}	
7f $^2F^0_{7/2}$-6g $^2G_{9/2}$	1.417×10^{-2}		3.430×10^{-2}	
7f $^2F^0_{7/2}$-7g $^2G_{7/2}$	2.409×10^{-6}		5.240×10^{-3}	
7f $^2F^0_{7/2}$-7g $^2G_{9/2}$	6.746×10^{-5}		1.834×10^{-1}	
7f $^2F^0_{7/2}$-8g $^2G_{7/2}$	4.123×10^{-3}		2.473×10^{-2}	
7f $^2F^0_{7/2}$-8g $^2G_{9/2}$	1.155×10^{-1}		8.654×10^{-1}	
7f $^2F^0_{5/2}$-5g $^2G_{7/2}$	6.276×10^{-3}		1.926×10^{-3}	
7f $^2F^0_{5/2}$-6g $^2G_{7/2}$	1.457×10^{-2}		3.308×10^{-2}	
7f $^2F^0_{5/2}$-7g $^2G_{7/2}$	6.505×10^{-5}		1.886×10^{-1}	
7f $^2F^0_{5/2}$-8g $^2G_{7/2}$	1.113×10^{-1}		8.901×10^{-1}	
5g $^2G_{9/2}$-6h $^2H^0_{11/2}$	1.348		1.642	
5g $^2G_{9/2}$-6h $^2H^0_{9/2}$	2.996×10^{-2}		3.041×10^{-2}	
5g $^2G_{9/2}$-7h $^2H^0_{11/2}$	4.216×10^{-1}		2.007×10^{-1}	
5g $^2G_{9/2}$-7h $^2H^0_{9/2}$	9.369×10^{-3}		3.718×10^{-3}	
5g $^2G_{7/2}$-6h $^2H^0_{9/2}$	1.318		1.672	
5g $^2G_{7/2}$-7h $^2H^0_{9/2}$	4.122×10^{-1}		2.045×10^{-1}	

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Table II continued.

Transition	$A/10^8$ s^{-1}		f	
	This work	NIST [32]	This work	NIST [32]
6g $^2G_{7/2}$-6h $^2H^0_{9/2}$	9.397×10^{-8}		7.917×10^{-3}	
6g $^2G_{7/2}$-7h $^2H^0_{9/2}$	4.240×10^{-1}		1.478	
6g $^2G_{9/2}$-6h $^2H^0_{11/2}$	9.611×10^{-8}		7.773×10^{-3}	
6g $^2G_{9/2}$-6h $^2H^0_{9/2}$	2.136×10^{-9}		1.440×10^{-4}	
6g $^2G_{9/2}$-7h $^2H^0_{11/2}$	4.336×10^{-1}		1.451	
6g $^2G_{9/2}$-7h $^2H^0_{9/2}$	9.635×10^{-3}		2.688×10^{-2}	
7g $^2G_{7/2}$-6h $^2H^0_{9/2}$	2.942×10^{-3}		6.706×10^{-3}	
7g $^2G_{7/2}$-7h $^2H^0_{9/2}$	8.021×10^{-8}		1.551×10^{-2}	
7g $^2G_{9/2}$-6h $^2H^0_{11/2}$	2.888×10^{-3}		6.859×10^{-3}	
7g $^2G_{9/2}$-6h $^2H^0_{9/2}$	5.348×10^{-5}		1.520×10^{-4}	
7g $^2G_{9/2}$-7h $^2H^0_{11/2}$	8.203×10^{-8}		1.523×10^{-2}	
7g $^2G_{9/2}$-7h $^2H^0_{9/2}$	1.823×10^{-9}		2.820×10^{-4}	
8g $^2G_{7/2}$-6h $^2H^0_{9/2}$	1.146×10^{-3}		9.560×10^{-4}	
8g $^2G_{7/2}$-7h $^2H^0_{9/2}$	3.360×10^{-3}		1.819×10^{-2}	
8g $^2G_{9/2}$-6h $^2H^0_{11/2}$	1.126×10^{-3}		9.780×10^{-4}	
8g $^2G_{9/2}$-6h $^2H^0_{9/2}$	2.084×10^{-5}		2.173×10^{-5}	
8g $^2G_{9/2}$-7h $^2H^0_{11/2}$	3.299×10^{-3}		1.861×10^{-2}	
8g $^2G_{9/2}$-7h $^2H^0_{9/2}$	6.109×10^{-5}		4.130×10^{-4}	

are incomplete, the results obtained from our calculation are compared only with data taken from NIST data base [32]. In Table II, column 2 and column 4 list A-values and f-values calculated using WBEPM theory, respectively; and the NIST values of transition probabilities and oscillator strengths are contained in column 3 and column 5 respectively. Table II shows a good agreement between our results and the accepted values.

Sc and Y are rare-earth elements, and the nuclear charge for these two elements are 21 and 39 respectively. As the nuclear charges for these two elements are not very large, the relativistic effects in these two atomic systems are not very effective, so even though the WBEPM theory is a nonrelativistic method, it is still satisfying for these two ions. Another important factor in theoretical calculations for atomic systems is the interaction effects. The ground state configuration of Sc(III) is [Ar]3d which consists of a closed argon core with just one additional 3d electron. The excited states [Ar]nl are formed by excitation of 3d electron from ground state. The configuration of Y(III) is similar to that of Sc(III), the ground state configuration is [Kr]4d and the excited states are [Kr]nl. In this work, we focus on the transitions between the excited states [Ar]nl of Sc(III) and the excited states [Kr]nl of Y(III). For these excitations, there is only one additional electron outside a closed core, so the interaction effects are relativistic ineffective for these transitions. In WBEPM theory, we determine the parameters by fitting experimental energy level data, so the subtle interactions would be partly involved in our calculations.

There are also some other theoretical methods which use model potential to study atomic and ionic transitions. However, our method is quite different from those. The idea of separating the WBE and NWBE means the multi-electron system can be easily treated as a single-electron one. Therefore, the calculation procedure is simplified and the method can be applied to complicated systems. In the *ab initio* method, the problem of interaction effects can be partly resolved through proper mixing of configurations, but for simplicity of calculations in *ab initio* methods, only some selected configurations are included. Sometimes the set of configurations is too small to arrive at accurate transition rates. For complex atomic systems such as Sc(III) and Y(III), in order to get accurate results, a large number of possible configuration functions should be included in the calculation which sometimes makes the calculations impossible to realize.

It should be noted that the parameters Z', n', and l' are obtained with the energy levels and the expectation values $\langle r\rangle$ known. Here values of energy levels are taken from experimental work, so the relativistic effects and the interaction effects are included in the ε, but the values of $\langle r\rangle$ are evaluated using NCA method which is a nonrelativistic method. Also, the interaction effects are not taken into account in NCA method, which is expected to result in some deviations in the determination of parameters. We believe that if more complete relativistic effects and interaction effects can be taken into account, more accurate results would be produced from the WBEPM theory.

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IV. CONCLUSION

Calculations of transition probabilities and oscillator strengths for Sc(III) and Y(III) transitions were carried out using the WBEPM theory. The results are in good agreement with those taken from NIST data base and other results. The present work will be useful for both experimental and theoretical researcher.

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