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Two-electron and one-photon transitions in highly charged nickel-like ions*

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This paper calculates the transition wavelengths and probabilities of the two-electron and one-photon (TEOP) transition from the $(3s^{-1}_{1/2}4d_j)_{J=1,2}$ to $(3p^{-1}_{3/2}4s_{1/2})_{J=1}$ and the $(3p^{-1}_{1/2}4s_{1/2})_{J=1}$ to $(3d^{-1}_{j}4d_{j'})_{J=1,2}$ for highly charged Ni-like ions with atomic number Z in the range $47 \leq Z \leq 92$. In the calculations, the multi-configuration Dirac–Fock method and corresponding program packages GRASP92 and REOS99 were used, and the relativistic effects, correlation effects and relaxation effects were considered systematically. It is found that the TEOP transitions are very sensitive to the correlation of electrons, and the probabilities will be enhanced sharply in some special Z regions along the isoelectronic sequence. The present TEOP transition wavelengths are compared with the available data from some previous publications, good agreement is obtained.

Keywords: multiconfiguration Dirac–Fock method, two-electron and one-photon transition, strong configuration mixing

PACC: 3120B, 3130, 3270F

1. Introduction

Two-electron and one-photon (TEOP) transition refers to a transition in which two electrons change their states and only one photon is emitted or absorbed. Such multi-electron transitions were first predicted by Heisenberg[1] 80 years ago. In 1931, Goudsmit and Gropper[2] derived the selection rules of TEOP transitions with $\Delta l_1 = \pm 1$ and $\Delta l_2 = 0, \pm 2$. In 1975, Wölfli *et al*[3] reported the first experimental observation of the TEOP transition for Ni and Fe in a heavy-ion collision experiment. Since then, the TEOP transition has attracted much attentions and been intensively studied both experimentally[4−6] and theoretically,[7−10] because it gives very valuable information on electron–electron correlation, and demonstrates the contribution of configuration mixing and interelectronic-electrostatics.

In the past years, most of the studies focused mainly on TEOP transitions involving double inner-shell K vacancies,[3−9] in which two L shell electrons jump into the K shell and release one photon. There were few studies on outer-shell transitions, because the branching ratios of those transitions are usually small, and which make measurements very difficult. Most recently, our researches on energy-crossings for highly charged Ne-like ions show that the strong configuration mixing affects intensively some outer-shell TEOP transitions, which make the transition probabilities increasing by several orders of magnitude and becoming comparable with electric dipole transitions in particular Z regions.[11] Zhang *et al*[12] studied dielectronic recombination processes related to outer-shell doubly excited states $4l4l'$ and $4l5l'$ in Co-like Pd ions, and found that the contributions from some TEOP transitions to total rate coefficients are also very important, and it is more than 10%. In addition, Rosmej *et al*[10] have observed the higher-order TEOP transitions with the type $1s2l3l' \rightarrow 1s^2 4l'' + h\nu$ in Li-like ions in optically thick laser produced plasmas, and found

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that those transitions can provide sensitive diagnostic means for hot plasmas. It is well known, for highly charged Ni-like ions, the outer-shell $n = 3 \rightarrow 4$ transition spectra has very important applications in plasma diagnostics and x-ray lasers.[13−21] Many researches have shown that the energy-crossing and strong configuration mixing are also existed in highly charged Ni-like ions.[13−16] For example, in 1991, Quinet and Biemont [13] investigated the $n = 3 - 4$ transitions connected with x-ray spectra of AgXX-PbLV ions, and predicted the strong configuration mixings between the $(3d_{5/2}^{-1}4f_{7/2})_{J=1}$ and $(3p_{3/2}^{-1}4s_{1/2})_{J=1}$ states at $Z \sim 55$, and between the $(3p_{1/2}^{-1}4s_{1/2})_{J=1}$ and $(3p_{3/2}^{-1}4d_{3/2})_{J=1}$ states at $Z \sim 78 - 79$. In 2000, Safronova *et al*[14] calculated the excitation energies and oscillator strengths for $3l - 4l'$ particle-hole states of Ni-like ions ($Z = 29 - 100$) by using a relativistic many-body perturbation theory, and pointed out that there are strong configuration mixing between the states of the odd-parity with $J = 1$ in the range of $Z = 43 - 59$. As already pointed out by Nakamura *et al*[22] in an electron-beam ion trap (EBIT) experiment for highly charged Ne-like ions, the strong configuration mixings will result in an anomalous behaviour in the Z-dependence of electric dipole transition probabilities, and a great enhancement of the transition probabilities for correlated multielectron transitions and forbidden transitions.

In this paper, based on the precise calculation of the wavefunctions for all of $3l^{-1}4l'$ single excited states of Ni-like ions in the range $Z = 47 - 92$, by using the multi-configuration Dirac–Fock (MCDF) method,[23−25] two kinds of TEOP transitions $(3s_{1/2}^{-1}4d_j)_{J=1,2} \rightarrow (3p_{3/2}^{-1}4s_{1/2})_{J=1}$ and $(3p_{1/2}^{-1}4s_{1/2})_{J=1} \rightarrow (3d_j^{-1}4d_{j'})_{J=1,2}$ are studied systematically. The wavelengths and probabilities are presented along the sequence to assist future experiments. Some anomalistic behaviours of the TEOP transition probabilities are found and analysed. It is found that those anomalies cannot be neglected in practical applications, such as simulations and identifications of plasma spectra.[10,12]

2. Results and discussions

The Ni-like ions have a stable closed-shell ground configuration $3s^23p^63d^{10}$. Their low-lying excited configurations are $3d^94l'$, $3p^53d^{10}4l'$, and $3s3p^63d^{10}4l'$ ($l' = s, p, d, f$), denoted as $3l^{-1}4l'$. In this study, to generate atomic state wavefunctions and energies, the atomic structure program package GRASP92[24] has been used. In the calculations, the active space method[26] is used to produce all correlation configurations, in which all single excitation from the $3l$ inner-shell of the ground configuration into the virtual unoccupied $4l'(l' = s, p, d, f)$ orbital are taken into account. To decrease computational time and consider relaxation effects,[27,28] which are very important for transition probabilities, we divide all levels belong to the $3s^23p^63d^{10}$ and $3l^{-1}4l'$ configurations into different groups according to their parity and total angular momentum, and make calculations of energy levels and wavefunctions in the (extended) optimal level model.[24] Finally, in order to incorporate the effects caused by orbital relaxation and inorthonormality of the wavefunctions induced by separate calculations for different level groups, another program package REOS99[25] are used in the calculations of the TEOP transition probabilities.

In Tables 1 and 2, the TEOP transition wavelengths are presented along the Ni-like sequence for two kinds of transitions, namely the $(3s_{1/2}^{-1}4d_j)_{J=1,2} \rightarrow (3p_{3/2}^{-1}4s_{1/2})_{J=1}$ and $(3p_{1/2}^{-1}4s_{1/2})_{J=1} \rightarrow (3d_j^{-1}4d_{j'})_{J=1,2}$ transitions. As a comparison, some available theoretical data are also collected in the tables. It is noticed that the present TEOP transition wavelengths are in the far vacuum ultraviolet, and gradually extend to x-ray regions with the increase of atomic number Z. Those values are generally higher than that of decay of the inner-shell K^{-2} states by one order of magnitude for low-Z atoms, such as Cr, Fe and Cu.[8] Comparing the present results with the previous theoretical values predicted by Dong *et al*,[15] Aggarwal *et al*[29] and Hagelstein,[30] we obtain good agreements. For both low-Z and high-Z Ni-like ions, the discrepancy is less than 0.8%.

In Fig.1, the TEOP transition probabilities as function of atomic number Z are plotted for the three transitions, namely from the $(3s_{1/2}^{-1}4d_{3/2})_{J=1}$, $(3s_{1/2}^{-1}4d_{3/2})_{J=2}$ and $(3s_{1/2}^{-1}4d_{5/2})_{J=2}$ states to the $(3p_{3/2}^{-1}4s_{1/2})_{J=1}$ state, respectively. Usually, the above transitions are unallowed by electric dipole transition rule, but due to electron-electron correlation effects, those transitions are no longer forbidden. From the figure, we can see that the Z-dependant features of the transition probabilities are very obvious. At certain Z regions, such as $Z \sim 49$, 55 and 59, the transition probabilities are greatly en-

hanced with sharp features. And there is maximum transition probability of $9.494 \times 10^8 s^{-1}$ for the $(3s^{-1}_{1/2}4d_{3/2})_{J=2} \rightarrow (3p^{-1}_{3/2}4s_{1/2})_{J=1}$ transition around $Z \sim 55$. In order to explain the above trends in transition probabilities, we studied the energy structures and atomic state wavefunctions connected with those transitions. Figure 2(a) shows the trends of excited energies (relative to the ground state) as function of Z for the four levels $(3d^{-1}_{5/2}4f_{5/2})_{J=1}$, $(3d^{-1}_{5/2}4f_{7/2})_{J=1}$, $(3d^{-1}_{3/2}4f_{5/2})_{J=1}$ and $(3p^{-1}_{3/2}4s_{1/2})_{J=1}$. It can be seen clearly that the $(3p^{-1}_{3/2}4s_{1/2})_{J=1}$ level firstly crosses with $(3d^{-1}_{3/2}4f_{5/2})_{J=1}$ at $Z = 49 - 50$, and then with $(3d^{-1}_{5/2}4f_{7/2})_{J=1}$ and $(3d^{-1}_{5/2}4f_{5/2})_{J=1}$ again at $Z = 55-56$ and $58-59$ respectively. However, such energy

Table 1. Wavelengths (nm) of the $(3s^{-1}_{1/2}4d_j)_{J=1,2} \rightarrow (3p^{-1}_{3/2}4s_{1/2})_{J=1}$ TEOP transitions along the Ni-like sequence. The upper levels of the transition are indicated at the top of each column.

Z	$(3s^{-1}_{1/2}4d_{3/2})_{J=1}$		$(3s^{-1}_{1/2}4d_{3/2})_{J=2}$		$(3s^{-1}_{1/2}4d_{5/2})_{J=2}$	
	this work	others	this work	others	this work	others
47	4.8089		4.8027		4.7679	
48	4.5644		4.5582		4.5230	
49	4.3419		4.3358		4.3001	
50	4.1087		4.1028		4.0671	
51	3.9131		3.9073		3.8711	
52	3.7268		3.7211		3.6845	
53	3.5510		3.5455		3.5086	
54	3.3854		3.3800		3.3428	
55	3.2306		3.2254		3.1879	
56	3.0809		3.0759		3.0382	
57	2.9412		2.9364		2.8985	
58	2.8092		2.8045		2.7665	
59	2.6809		2.6763		2.6383	
60	2.5628	2.5710[a]	2.5585	2.5670[a]	2.5204	2.5295[a]
61	2.4496		2.4455		2.4074	
62	2.3419	2.3497[a]	2.3379	2.3460[a]	2.2999	2.3086[a]
63	2.2393	2.2469[a]	2.2354	2.2434[a]	2.1976	2.2060[a]
64	2.1415	2.1602[b]	2.1379	21563[b]	2.1002	2.1181[b]
65	2.0484		2.0449		2.0074	
66	1.9596		1.9562		1.9190	
67	1.8748		1.8716		1.8347	
68	1.7939		1.7909		1.7544	
69	1.7167		1.7138		1.6777	
70	1.6429		1.6402		1.6045	
71	1.5724		1.5699		1.5346	
72	1.5051		1.5026		1.4679	
73	1.4407	1.4462[a]	1.4384	1.4441[a]	1.4042	1.4.102[a]
74	1.3791	1.3844[a]	1.3769	1.3824[a]	1.3433	1.3.491[a]
75	1.3202		1.3182		1.2851	
76	1.2639	1.2630[c]	1.2620	1.2613[c]	1.2296	1.2294[c]
77	1.2101		1.2082		1.1764	
78	1.1585	1.1576[c]	1.1568	1.1561[c]	1.1256	1.1255[c]
79	1.1092		1.1075		1.0771	
80	1.0620	1.0611[c]	1.0604	1.0598[c]	1.0307	1.0306[c]
81	1.0168		1.0153		0.9863	
82	0.9735	0.9728[c]	0.9722	0.9716[c]	0.9438	0.9437[c]
83	0.9321		0.9308		0.9032	
84	0.8925	0.8918[c]	0.8913	0.8908[c]	0.8644	0.8643[c]
85	0.8546		0.8534		0.8272	
86	0.8183		0.8172		0.7917	
87	0.7835		0.7825		0.7578	
88	0.7502		0.7492		0.7252	
89	0.7183		0.7174		0.6941	
90	0.6878		0.6869		0.6644	
91	0.6585		0.6577		0.6359	
92	0.6306		0.6298		0.6087	

[a] Aggarwal *et al.*[29]
[b] Hagelstein.[30]
[c] Dong *et al.*[15]

Table 2. Wavelengths (nm) of $(3p_{1/2}^{-1}4s_{1/2})_{J=1} - (3d_j^{-1}4d_{j'})_{J=1,2}$ TEOP transitions along the Ni-like sequence. The lower levels of the transition are indicated at the top of each column.

Z	$(3d_{5/2}^{-1}4d_{3/2})_{J=1}$		$(3d_{5/2}^{-1}4d_{5/2})_{J=1}$		$(3d_{5/2}^{-1}4d_{3/2})_{J=2}$		$(3d_{5/2}^{-1}4d_{5/2})_{J=2}$	
	this work	others	this work	others	this work	others	this work	others
47	9.5772		9.8880		9.8443		10.0732	
48	9.2030		9.5085		9.4588		9.6912	
49	8.8400		9.1401		9.0841		9.3196	
50	8.4880		8.7826		8.7202		8.9584	
51	8.1470		8.4360		8.3672		8.6075	
52	7.8166		8.1002		8.0250		8.2670	
53	7.4968		7.7751		7.6936		7.9368	
54	7.1874		7.4606		7.3728		7.6169	
55	6.8883		7.1566		7.0627		7.3072	
56	6.5993		6.8628		6.7631		7.0075	
57	6.3203		6.5792		6.4740		6.7179	
58	6.0512		6.3055		6.1951		6.4382	
59	5.7918		6.0415		5.9264		6.1682	
60	5.5418	5.5970[a]	5.7872	5.8395[a]	5.6676	5.7238[a]	5.9078	5.9642[a]
61	5.3012		5.5422		5.4187		5.6568	
62	5.0697	5.1220[a]	5.3063	5.3557[a]	5.1793	5.2325[a]	5.4150	5.4686[a]
63	4.8472	4.8982[a]	5.0794	5.1276[a]	4.9494	5.0012[a]	5.1824	5.2347[a]
64	4.6333	4.6051[b]	4.8612	4.8297[b]	4.7285	4.6985[b]	4.9585	4.9253[b]
65	4.4281		4.6516		4.5167		4.7434	
66	4.2311		4.4501		4.3135		4.5367	
67	4.0422		4.2567		4.1189		4.3382	
68	3.8612		4.0711		3.9324		4.1477	
69	3.6878		3.8931		3.7540		3.9651	
70	3.5217		3.7225		3.5833		3.7899	
71	3.3629		3.5589		3.4200		3.6222	
72	3.2110		3.4023		3.2640		3.4615	
73	3.0658	3.1033[a]	3.2524	3.2877[a]	3.1150	3.1525[a]	3.3077	3.3464[a]
74	2.9271	2.9634[a]	3.1090	3.1431[a]	2.9728	3.0090[a]	3.1607	3.1981[a]
75	2.7949		2.9720		2.8373		3.0204	
76	2.6692	2.7081[c]	2.8417	2.8795[c]	2.7086	2.7477[c]	2.8869	2.9280[c]
77	2.5512		2.7194		2.5878		2.7616	
78	2.4484	2.4766[c]	2.6135	2.6398[c]	2.4827	2.5108[c]	2.6533	2.6824[c]
79	2.3118		2.4686		2.3430		2.5048	
80	2.2110	2.2430[c]	2.3637	2.3949[c]	2.2401	2.2721[c]	2.3976	2.4314[c]
81	2.1188		2.2680		2.1459		2.2997	
82	2.0080	2.0360[c]	2.1504	2.1775[c]	2.0328	2.0607[c]	2.1795	2.2090[c]
83	1.9188		2.0570		1.9419		2.0841	
84	1.8324	1.8604[c]	1.9661	1.9938[c]	1.8538	1.8818[c]	1.9913	2.0212[c]
85	1.7494		1.8788		1.7693		1.9022	
86	1.6701		1.7951		1.6886		1.8168	
87	1.5944		1.7151		1.6116		1.7353	
88	1.5222		1.6386		1.5381		1.6573	
89	1.4532		1.5655		1.4680		1.5829	
90	1.3874		1.4956		1.4011		1.5117	
91	1.3246		1.4288		1.3374		1.4438	
92	1.2646		1.3650		1.2765		1.3789	

[a] Aggarwal *et al.*[29]
[b] Hagelstein.[30]
[c] Dong *et al.*[15]

level crossings never occurred for the TEOP transition upper levels $(3s_{1/2}^{-1}4d_j)_{J=1,2}$ in the whole Z regions from 47 to 92. Also, we compared the present results of energy level crossings with previous predictions by Quinet and Biemont[13] and Safronova *et al*,[14] good consistencies are obtained both for the levels and Z regions of crossing. In Fig.2(b), the four main wave function components of the $(3p_{3/2}^{-1}4s_{1/2})_{J=1}$ level are plotted as function of Z to study the mixing of configurations. It can be seen from the figure that for

the main wavefunction components, the contributions from all of $(3d_j^{-1}\,4f_{j'})_{J=1}$ levels are 23.5%, 44.5% and 21.4% at $Z = 49$, 55 and 59, respectively. This indicates that there are strong configuration mixings existed among those crossing levels. Such strong configuration mixings are responsible for the great enhancement of the TEOP transition probabilities at $Z \sim 49$, 55 nd 59, respectively.

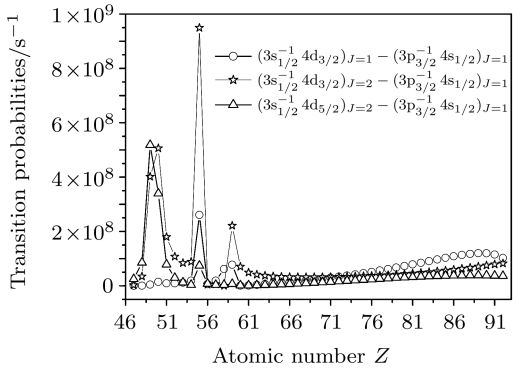


Fig.1. TEOP transition probabilities (s^{-1}) from the upper levels $(3s_{1/2}^{-1}\,4d_j)_{J=1,2}$ to the $(3p_{3/2}^{-1}4s_{1/2})_{J=1}$ level as functions of Z.

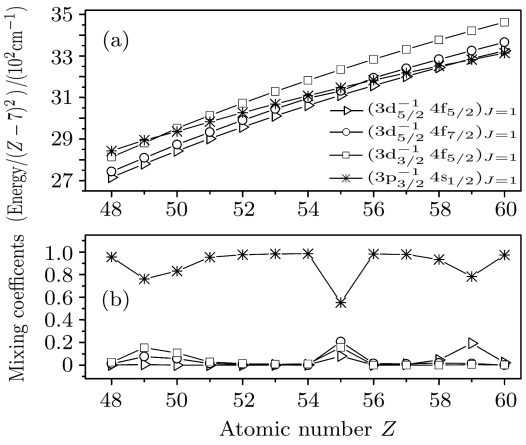


Fig.2. (a) The excited energy (relative to the ground state) as function of Z for the $(3d_{3/2}^{-1}\,4f_{5/2})_{J=1}$, $(3d_{5/2}^{-1}\,4f_{7/2})_{J=1}$, $(3d_{5/2}^{-1}\,4f_{5/2})_{J=1}$ and $(3p_{3/2}^{-1}\,4s_{1/2})_{J=1}$ levels. (b) Main wavefunction components of the $(3p_{3/2}^{-1}\,4s_{1/2})_{J=1}$ level as function of Z.

In Fig.3, the TEOP transition probabilities from the higher excited state $(3p_{1/2}^{-1}\,4s_{1/2})_{J=1}$ to the lower states $(3d_{5/2}^{-1}\,4d_{5/2})_{J=1,2}$ and $(3d_{5/2}^{-1}\,4d_{3/2})_{J=1,2}$ are illustrated as function of Z. The figure shows that the trends of transition probabilities increase with Z before $Z = 79$ and then decrease after $Z = 81$ for all of the transitions. And there are some complicated changes with Z in the region of $Z = 79-81$. Comparing with the transition probabilities plotted in Fig.1, we find that this kind of transitions are stronger than that of $(3s_{1/2}^{-1}4d_j)_{J=1,2} \rightarrow (3p_{3/2}^{-1}4s_{1/2})_{J=1}$ transitions. The TEOP transition probabilities generally exceed $10^8\,s^{-1}$, especially approach $10^{12}\,s^{-1}$ at $Z = 78$ and 81. So strong transitions should be observed in many experiments such as EBIT, electron-beam ion source (EBIS), or heavy-ion storage ring. As mentioned by Quinet and Biemont[13] and Dong *et al*,[15] there are several energy level crossings at $Z \sim 74-84$ regions for highly charged Ni-like ions. In this study, we also studied the energy level crossings and configuration mixings both for the upper and lower levels related to $(3p_{1/2}^{-1}4s_{1/2})_{J=1} \rightarrow (3d_j^{-1}\,4d_{j'})_{J=1,2}$ transitions. In Fig.4(a), the results of energy level crossing are plotted for the upper level $(3p_{1/2}^{-1}\,4s_{1/2})_{J=1}$, and in Fig.4(b), the corresponding main wavefunction components of

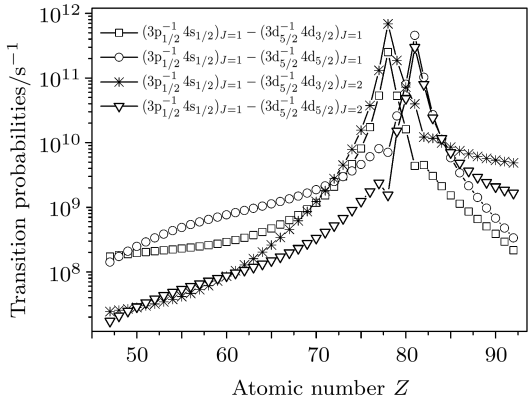


Fig.3. TEOP transition probabilities (s^{-1}) from the level $(3p_{1/2}^{-1}4s_{1/2})_{J=1}$ to the lower levels $(3d_j^{-1}\,4d_{j'})_{J=1,2}$ as function of Z.

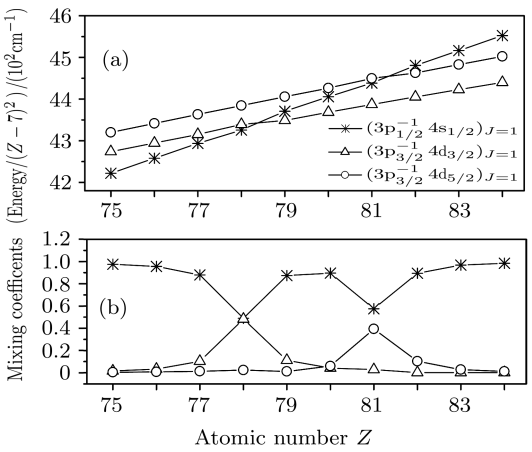


Fig.4. (a) The excited energy (relative to the ground state) as function of Z for the $(3p_{1/2}^{-1}\,4s_{1/2})_{J=1}$ and $(3p_{3/2}^{-1}\,4d_{3/2})_{J=1}$ as well as $(3p_{3/2}^{-1}\,4d_{5/2})_{J=1}$ levels. (b) Main wave function components of the $(3p_{1/2}^{-1}\,4s_{1/2})_{J=1}$ level as function of Z.

it are presented. From the figure, we can see that two crossings occur between the $(3p_{1/2}^{-1}\,4s_{1/2})_{J=1}$ level and the $3p_{3/2}^{-1}\,4d_{3/2}(1)$ and $3p_{3/2}^{-1}\,4d_{5/2}(1)$ levels at $Z \sim 78$ and 81, respectively, which result in strong mixing of wavefunctions among those crossing levels. It is clearly that just those crossings of the transition upper levels, which caused the sharp enhancement of the TEOP transition probabilities in Fig.3 at $Z \sim 78$ and 81.

3. Conclusion

In summary, we studied the TEOP transitions of $(3s_{1/2}^{-1}4d_j)_{J=1,2} \rightarrow (3p_{3/2}^{-1}4s_{1/2})_{J=1}$ and $(3p_{1/2}^{-1}4s_{1/2})_{J=1} \rightarrow (3d_j^{-1}4d_{j'})_{J=1,2}$ for highly charged Ni-like ions, by using the MCDF method. The transition wavelengths and probabilities are presented for all ions with atomic numbers Z from 47 to 92, which will conduce to observation of experiments. It is found that the TEOP transition probabilities are strongly dependant on configuration mixing. Due to energy level crossings of the lower level $(3p_{3/2}^{-1}4s_{1/2})_{J=1}$ or the upper level $(3p_{1/2}^{-1}4s_{1/2})_{J=1}$ related with the transitions, their wavefunctions are strongly mixed with $(3d_j^{-1}\,4f_{j'})_{J=1}$ or $(3p_j^{-1}\,4d_{j'})_{J=1}$ levels at particular Z regions, respectively, which results in a great enhancement of TEOP transition probabilities around the crossing regions. Such transition processes are very important and can not be neglected in practical applications. Also, in the present study, comparisons are made for the transition wavelengths and energy level crossings with previous available data and theoretical predictions, good agreements are obtained. We hope this study of outer-shell TEOP transition in highly charged Ni-like ions will contribute to further understanding of TEOP processes based on strong configuration mixing, and can be tested in the future.

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