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Theoretical Study on Energy Structures and Radiative Transition Characteristics of Highly Charged Ni-like Ions

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Abstract

Excitation energies, transition wavelengths and probabilities of the $3s^23p^63d^{10}$, $3s^23p^63d^94l$, $3s^23p^5 3d^{10}4l$, $3s3p^63d^{10}4l\,(l = \mathrm{s,p,d,f})$ states along the Ni-like sequence from $Z = 31$ to 92 are calculated by using the Multi-configuration Dirac-Fock package GRASP92 and a newly developed radiative transition program REOS99. In the calculations, the correlation and relaxation effects are included systematically. Based on the calculations, all possible energy crossings among the level groups with the same parity and total angular momentum have been found. It shows that there are strong configuration interactions between those levels, which cause transition probabilities changes dramatically at many particular Z regions.

Keywords:

energy structure, transition probability, MCDF method, highly charged Ni-like ion

1. Introduction

The Ni-like ions have a stable closed-shell ground configuration $3s^23p^63d^{10}$. Their low-lying excited configurations are $3d^94l$ ($l = \mathrm{s,p,d,f}$), $3p^5\,3d^{10}4l$ and $3s\,3p^6\,3d^{10}4l$ (labled as $3d^{-1}\,4l$, $3p^{-1}\,4l$ and $3s^{-1}\,4l$, respectively), which form 106 fine-structure levels. In general, the emission spectra of the highly charged Ni-like ions can be obviously divided into two different types: one is the $\Delta n \geq 1$ transition with shorter wavelength and stronger intensity, such as the $3d^{10}$–$3d^{-1}\,4p$ transition; the other one is the $\Delta n = 0$ transition with longer wavelength and weaker intensity, for example, the $3d^{-1}\,4s$–$3d^{-1}\,4p$ and $3d^{-1}\,4s$–$3p^{-1}\,4s$ transitions.

For the transitions with $\Delta n \geq 1$, many investigations either in experiment or in theory have been carried out during the last years due to their important applications in X-ray laser study and hot plasmas diagnostic [1-9]. In the X-ray laser study, the $3d^{-1}\,4p$–$3d^{-1}\,4d$ transition of the Ni-like ions on the basis of electron impact excitation is a very important approach to realize X-ray laser. In this scheme, the $3d^{10} - 3d^{-1}\,4p$ transition is directly connected with the fast radiative decay from the laser lower levels $3d^{-1}\,4p$ to the ground state $3d^{10}$. In the hot plasma diagnostic, the allowed electric dipole resonance lines are frequently used because they could be measured easily in hot plasma environment. As a result, many different theoretical methods had been used to calculate the spectra of Ni-like ions up to U^{64+} [1,5-9].

For the $\Delta n = 0$ transitions, ever there existed some investigations for the $3d^{-1}\,4s$–$3d^{-1}\,4p$ and $3d^{-1}\,4p$ –$3d^{-1}\,4d$ transitions in some lowly charged Ni-like ions [10-14]. In order to generate X-ray laser with shorter wavelength for holography of biological living cell specimens within the *water window* (2.3 – 4.4 nm), on the one hand, people continue to search for the $3d^{-1}\,4p$–$3d^{-1}\,4d$ X-ray laser in more high-Z ions; on the other hand, people use the $\Delta n = 0$ transitions among the inner 3s and 3p excited states of highly charged ions [15], such as the transitions $3d^{-1}\,4p$–$3p^{-1}\,4p$ and $3p^{-1}\,4s$–$3p^{-1}\,4p$ etc.. The advantage of using these transitions with an inner-shell excitation is that more shorter wavelengths can be obtained whereas the radiative decay from the lower levels with a $3l$ hole to the ground state $3d^{10}$ is very fast. However, such transition data connected with the inner-shell emission lines are lacking very much up to now.

In the present work, systematic calculations on the 107 energy levels and related E1 transition probabilities are carried out for Ni-like ions in the range of $Z = 31 - 92$. In these calculations, the effects of relativistic, relaxation and correlation have been considered by using the Multi-configuration Dirac-Fock package GRASP92 [16] and a newly developed radiative transition program REOS99 [17]. Based on the calculations, a systematic study on Z-dependence of energies and

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transition probabilities along the whole sequence is carried out. In this paper, main attention is paid to the energy crossings and anomalies of transition probabilities due to strong configuration interactions. It shows that the change of the E1 transition probabilities strongly depend on atomic number Z, the interesting and dramatic changes will take place at particular Z regions existing energy crossings. And two very strong two-electron and one-photon transitions [18-20] (TEOP) were found for Ni-like ions for the first time, we expect it can be tested experimentally in the future.

2. Computational procedures

In this study, wavefunctions and energies have been calculated by the widely used atomic structure package GRASP92 [16]. In order to include correlation and relaxation effects systematically, the 107 levels from the ground state $3s^2 3p^6 3d^{10}$ and the excited states $3l^{-1}4l'$ (l = s, p, d; l' = s, p, d, f) are divided into 13 groups according to their parity and total angular momentum: 6 groups correspond the 51 even-parity levels with $J^P = 0^+, 1^+, 2^+, 3^+, 4^+, 5^+$ respectively, and 7 groups correspond the 56 odd-parity levels with $J^P = 0^-, 1^-, 2^-, 3^-, 4^-, 5^-, 6^-$. For each group of levels, the (extented) optimal level (EOL) calculation of the GRASP92 package [16] is carried out independently to get their wave functions and energies. Also in order to consider the relaxation effects in calculation of probabilities, which are caused by the separate calculations for different level groups, the newly developed program REOS99 [17] is used further.

3. Energy crossings

Based on the calculations of the energies for the low-lying 107 levels of Ni-like ions in the range of $Z = 31 - 92$, the Z-dependence of all energy levels is studied systemically. It is found that there are many energy crossings in many ions, some levels even cross many times with others in some special Z regions along the sequence. As a result, there are very strong configuration interactions among those crossing levels, which result in a series of mixing of the corresponding wave functions, and dramatic changes of transition probabilities. In the past years, there are only a few cases of energy crossings found in previously researches by Safronova *et al.* [1] and Quinet *et al.* [6]. Comparing the present results with the previous predictions, it is found that the crossing levels and the crossing regions presented in this paper are in good agreement with the previous predictions. Also a comparison of transition wavelengths from the 13 excited states with $J^P = 1^-$ to the ground state is made. It shows that our results are very closer to the available experimental results [1,6] and the MBPT calculation by Safronova *et al.* [1]. Especially, a good agreement is found for those wavelengths related with the transitions from the crossing energy levels to the ground state at the crossing regions.

4. Effects of energy crossings on transition probabilities

Here we just show two examples. In Fig. 1, we plot the E1 transition probabilities from the four excited levels $3p_{3/2}^{-1}\ 4s_{1/2}(1)$, $3d_{3/2}^{-1}\ 4f_{5/2}(1)$, $3d_{5/2}^{-1}\ 4f_{7/2}(1)$, and $3d_{5/2}^{-1}\ 4f_{5/2}(1)$ to the ground state $3s^2 3p^6 3d^{10}\ {}^1S_0$. From the Fig. 1, we can see that the transition probabilities change anomaly with Z, which change even more in the region of $Z = 47 - 61$ with sharp features. for the $3p_{3/2}^{-1}\ 4s_{1/2}(1) - {}^1S_0$ transition, there are two minima at $Z = 48$ and $Z = 56$, respectively; for the $3d_{5/2}^{-1}\ 4f_{5/2}$ $(1) - {}^1S_0$ transition, there is one minimum at $Z = 57$. By studying the variety of transition probabilities along the sequence, we find that the energy crossings are responsible for most of irregularly changes of transition probabilities. It shows that the level $3p_{3/2}^{-1}\ 4s_{1/2}(1)$ mixes strongly with the $3d_{3/2}^{-1}\ 4f_{5/2}(1)$ at $Z = 49 - 50$, and then with the $3d_{5/2}^{-1}\ 4f_{7/2}(1)$ at $Z = 55 - 56$, finally it mixes with the $3d_{5/2}^{-1}\ 4f_{5/2}(1)$ level at $Z = 58 - 59$ again. These strong mixtures cause a rapid increase of transition rates of the $3p_{3/2}^{-1}\ 4s_{1/2}(1) - {}^1S_0$ and $3d_{5/2}^{-1}\ 4f_{5/2}(1) - {}^1S_0$ transitions in the regions of $Z = 48 - 50$ and $Z = 57 - 59$, respectively, and finally result in the sharp maximum at $Z = 50$ and 59. Accordingly the transition rates of $3d_{3/2}^{-1}$ $4f_{5/2}(1) - {}^1S_0$ and $3p_{3/2}^{-1}\ 4s_{1/2}(1) - {}^1S_0$ transitions are decreased in those regions due to the strong configuration interactions.

In Fig. 2, the E1 transition probabilities from the

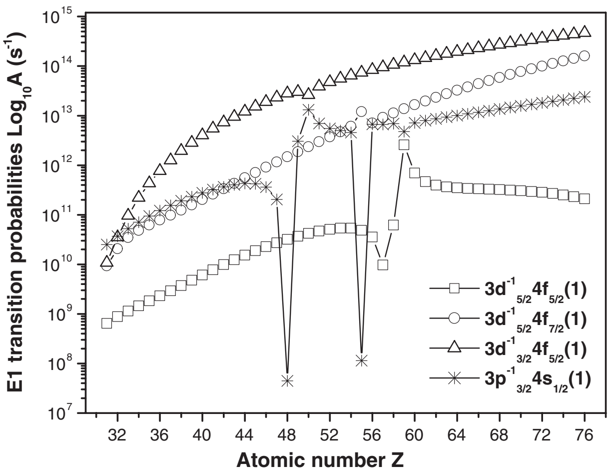

Fig. 1 Z-dependence of the E1 transition probabilities from excited levels with energy crossings to the ground state.

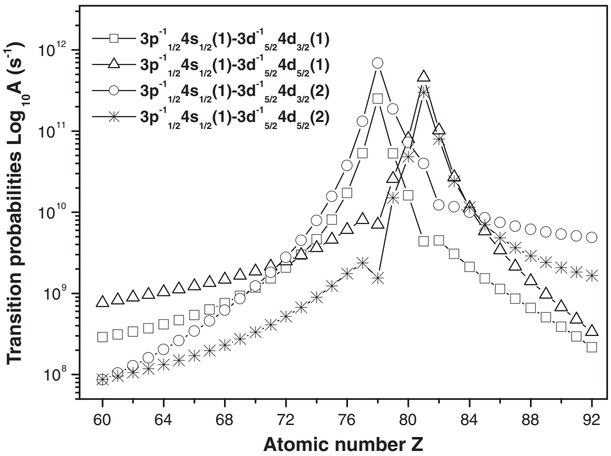

Fig. 2 Z-dependence of the TEOP transition probabilities from the higher level $3p^{-1}_{1/2}\,4s_{1/2}$ (1) with energy crossings to the lower level $3d^{-1}_{j}\,4d_{j'}$ (J) without energy crossings.

higher level $3p^{-1}_{1/2}\,4s_{1/2}(1)$ to the lower level $3d^{-1}_{j}\,4d_{j'}(J)$ are plotted along the sequence. Usually, we know that the above transitions are unallowed by E1 transition rule, but due to the strong configuration mixing among the upper levels $3p^{-1}_{1/2}\,4s_{1/2}(1)$, $3p^{-1}_{3/2}\,4d_{3/2}(1)$ and $3p^{-1}_{3/2}\,4d_{5/2}(1)$ at $Z = 78 - 79$ and $Z = 81 - 82$ respectively, those transitions are enhanced greatly at $Z = 78$ and $Z = 81$. Such transitions were postulated as the two-electron and one-photon transitions (TEOP) by Richtmyer *et al.* [18,19] 80 years ago, and which was firstly detected in heavy-ion collision experiments by Wölfli *et al.* [20]. The selection rules for TEOP transitions are as follows: l_1 can change by ±2 or 0 and l_2 can change by ±1. During the last three decades theoretical and experimental work focused only on the study of the TEOP process from doubly inner-shell K ionized atoms [21,22], and there are not any report for Ni-like ions in literature before. We hope the present study of the TEOP transition in Ni-like ions will contribute to well understand the TEOP process, and can be observed in experiment.

5. Conclusions

In summary, the 107 low-lying energy levels and the related transition probabilities connecting with these levels in the Ni-like ions from $Z = 31$ to 92 have been calculated by using the MCDF method. The comparison with some available experimental and theoretical results are made for energies and transition probabilities along the sequence. A good agreement can be obtained for both of them.

Based on the systematic calculations, all possible energy-crossings among the same J^P level groups have been found along the whole isoelectronic sequence. It is found that there are several level-crossings for some particular energy levels in different Z regions, those crossings can result in great changes of the transition probabilities even for some strong lines. Some of them are diminished and the others are enhanced accordingly. Especially the very strongly TEOP transition is observed for Ni-like ions, which is expected to be tested in experiment in the future.

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References

[1] U.I. Safronova, W.R. Johnson and J.R. Albritton, Skobelev, Phys. Rev. A **62**, 052505 (2000).

[2] J.F. Wyart, A.C. Bauche, J.C. Gauthier *et al.*, Phys. Rev. A **34**, 701 (1986).

[3] A. Zigler, H. Zmora, N. Spector, *et al.*, J. Opt. Soc. Am. **70**, 129 (1980).

[4] P. Beiersdorfer, A.L. Osterheld, J. Scofield *et al.*, Phys. Rev. Lett. **67**, 2272 (1991).

[5] P.L. Hagelstein, Phys. Rev. A **34**, 874 (1986).

[6] P. Quinet and E. Biemont, Physica Scripta. **43** 150 (1991), and references therein.

[7] P. Quinet and E. Biemont, Bull. Soc. Sci. Liege. **49**, 307 (1990).

[8] H.L. Zhang, D.H. Sampson and C.J. Fontes, At. Data Nucl. Data Tables. **48**, 91 (1991).

[9] E. Biemont, J. Phys. B: At. Mol. Opt. Phys. **30**, 4207 (1997).

[10] J.F. Wyart, Physica Scripta. **33**, 215 (1986).

[11] J.F. Wyart, Physica Scripta. **36**, 234 (1987).

[12] T. Brage and U. Litzen, Phys. Scr. **35**, 662 (1987).

[13] Y. Li, J. Nilsen, J. Dunn *et al.*, Phys. Rev. A **58**, R2668 (1998).

[14] J.H. Scofield and B.J. MacGowan, Physica Scripta. **46**, 361 (1992).

[15] W.H. Goldstein, J. Oreg, A. Zigler *et al.*, Phys. Rev. A **38**, 1797 (1988).

[16] F.A. Parpia, C. Fischer Froese and I.P. Grant, Compt. Phys. Commun. **94**, 249 (1996).

[17] S. Fritzsche, C. Fischer Froese and C.Z Dong, Compt. Phys. Commun. **124**, 340 (2000).

[18] F.K. Richtmyer, Phil. Mag. **6**, 64 (1928).

[19] J. Frank, Inst. **208**, 325 (1929).

[20] W. Wölfli, C. Stoller, G. Bonani *et al.*, Phys. Rev. Lett. **35**, 656 (1975).

[21] S.I. Salem, A. Kumar, B.L. Scott and R.D. Ayers, Phys. Rev. Lett. **49**, 1240 (1982).

[22] Y. Zou, J.R. Crespo López-Urrutia and J. Ullrich, Phys. Rev. A **67**, 042703 (2003).