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# Ionization Energies of Cu-like ions with $Z \leq 92$

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The overview of the experimental and theoretical data on the ionization energies (IE) of the Cu-like ions is presented. In various works data are obtained by interpolation and extrapolation the parameters of model potentials for Dirac equations. In other approaches, the function of the dependence of the ionization energy on  $Z$  ( $Z$  is nuclear charge) is approximated by a polynomial with power-law dependence on  $Z$  in order to achieve a minimum difference between theoretical and experimental data. The compilation of ionization energies is in database of the National Institute of Standards and Technology (USA), where the typical uncertainty is several units in the fourth significant digit. This means that for heavy ions the error can reach several tens of thousands  $\text{cm}^{-1}$ . In this work, the ionization energies of Cu-like ions are refined to achieve accuracy to the fifth significant digit. Two methods have been developed for the interpolation and extrapolation. Scaling ionization energies along  $Z$ : scaling results in the function of the dependence of ionization energies on  $Z$  to the form of a quasi-line, i.e., weakly varying function on interval of 10–15  $Z$  values. This allows the function to be interpolated up to the fifth significant numbers. The scaled refined function of the dependence of the ionization energy on  $Z$  is approximated by analytical functions that allow extrapolation with good accuracy to the  $Z \sim 92$  region. The relativistic model potential is used to interpolate and extrapolate ionization energies. The parameter of the relativistic model potential for the  $4s_{1/2}$  orbital turned out to be almost linear function of  $Z$  for  $Z > 70$ , which made it possible to extrapolate with high accuracy to the  $4s_{1/2}$  region of 92. The results of both methods are in good agreement up to  $Z \sim 92$ .

**Keywords:** atomic spectroscopy, ionization energies, Cu-like isoelectronic sequence, relativistic model potential.

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## 1. Introduction

The ionization energy (IE) and spectra of highly charged ions provide important information for the development of X-ray lasers, for the study of thermonuclear plasmas, and for testing relativistic calculations of atomic ion structures with a large value of the nuclear charge. Copper isoelectron sequence ions (Cu-like ions) are of particular interest: these ions have a single  $nlj$  electron over tightly bound  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$  filled shells (the core), and their spectra remain simple even for ions with very high ionization rates. Therefore, intense lines of Cu-like ions are often used as reference points in studies of complex spectra of heavy ions. They also serve as an indicator of impurities in the high-temperature plasma. Although the structure of Cu-like ions is mostly determined by a single electron over the core, their theoretical interpretation is very difficult for the lowest members of the isoelectron series with a core charge  $Z < 36$  because of the strong interaction with more complex configurations corresponding to the electron excitation from the core. Compilations are often used for various purposes, it is important to establish erroneous and inaccurate data in order to correct them.

Spectra of Cu-like ions Mo XIV [1], Rb IX [2], Y XI [3], Zr XII [4], Nb XIII [5], Sr X [6] were observed in the low inductance spark and laser produced plasma in the region 70–630 Å on the 10/7 m grazing-incidence spectrograph.

The energy levels of Cu-like ions included series  $ns$  ( $n = 4 - 6$ ),  $np$  ( $n = 4 - 6$ ),  $nd$  ( $n = 4, 5$ ),  $nf$  ( $n = 4 - 6$ ),  $ng$  ( $n = 5 - 7$ ). The observed energy levels were compared with the Hartree-Fock calculations [7,8]. Ionization energies were determined using the series  $ng$ .  $ng$ -series limit was taken as the ionization energy. The limit uncertainty was estimated from the uncertainties of the wavelength measurements. For the above ions, it was 200–300  $\text{cm}^{-1}$ . The spectra of Cu-like ions  $\text{Ru}^{15+}$ ,  $\text{Rh}^{16+}$ ,  $\text{Pd}^{17+}$ ,  $\text{Ag}^{18+}$ ,  $\text{Cd}^{19+}$ ,  $\text{In}^{20+}$  and  $\text{Sn}^{21+}$  were observed in laser plasma using a 10.7 m [9] grazing-incidence spectrograph. Wavelengths, energy levels, and ionization energies were established for each of these ions. For these ions, the ionization energies were calculated using  $5g$  and  $6g$  configuration energies and quantum defect  $\Delta n^*(6g - 5g)$ . The ionization energy of the Cu-like xenon was determined in a similar way in [10], but here the uncertainty was  $\sim 3000 \text{ cm}^{-1}$ .

The spectra of Cu-like ions  $\text{Ba}^{27+}$ ,  $\text{La}^{28+}$ ,  $\text{Nd}^{31+}$ ,  $\text{Sm}^{33+}$ ,  $\text{Gd}^{35+}$ ,  $\text{Dy}^{37+}$ ,  $\text{Er}^{39+}$ ,  $\text{Yb}^{41+}$ ,  $\text{Ta}^{44+}$ ,  $\text{W}^{45+}$  were studied with a laser produced plasma on a 2.2 m grazing incidence spectrograph [11]. Wavelengths, energy levels, and ionization energies were determined for each of these ions. Although series like  $nf$  ( $n = 4 - 6$ ) were observed for some ions, the large uncertainty in energy levels with  $n = 5, 6$  led to large uncertainties in the  $n = 5$  and  $n = 6$  energy levels produced very large uncertainties in the derived limits. Therefore, the ionization energies were obtained using the theoretical

binding energies for the  $4f$ ,  $5g$  and  $6h$ , configurations calculated in [12]. The uncertainty increased from 900, 1000  $\text{cm}^{-1}$  (for  $\text{Ba}^{27+}$ ,  $\text{La}^{28+}$ ) to 15,000  $\text{cm}^{-1}$  (for  $\text{Ta}^{44+}$ ,  $\text{W}^{45+}$ ). The spectra of highly charged Au, Pb, Bi, Th, U ions ( $Z = 79-92$ ) were observed in laser plasma at the OMEGA facility at the University of Rochester [13]. Lines in the 9–110 Å area were identified for the isoelectronic sequences Fe I, Co I, Cu I, and Zn I. For these ions, the energy levels were calculated by the multi-configuration Dirac – Fock method, taking into account Breit and quantum electrodynamic (QED) corrections using the programs [14,15]. Comparison of experimental and theoretical wavelengths of Cu-like ions showed that taking into account QED corrections significantly improves the accuracy of the calculated wavelengths of  $4s-4p$  transitions. However, significant differences between the observed and calculated values remain. For Cu-like ions, the QED corrections have a noticeable effect only on the  $4s-4p$  [13] transitions.

The spectra of Cu-like ions in the [16] experiment were observed in laser plasma with a two-meter grazing incidence spectrograph with a 1152 grooves/mm lattice. The transition wavelengths of  $4-5$  and  $4-4$  were studied experimentally for Cu-like ions  $\text{Ag}^{18+} - \text{Sn}^{21+}$  ( $Z = 47-50$ ). To extrapolate and interpolate the  $4lj$  and  $5lj$  ( $l = 0-3$ ) energy levels in the  $Z = 36-80$  range, the relativistic model potential (RMP) method was used. Two variants of calculations were carried out. In the first version, the known experimental energies for  $Z = 36, 42, 56, 63$  [1,9,11] were used as reference points. The energy levels obtained by interpolation and extrapolation by the RMP method agree well with the new experimental results [16]. In the second — new experimental energy levels [16] were used to extrapolate in order to obtain more accurate smoothed values for large  $Z$ .

In experiment [17], the gold laser plasma spectrum in the Cu-like ion  $\text{Au}^{50+}$  identified transitions from configuration levels  $3d^{10}nf$  ( $n = 7, 8$ ) on  $3d^94d$ , from  $3d^{10}nd$  ( $n = 6, 7$ ) and  $3d^{10}7s$  on  $3d^{10}4p$  and from  $3d^{10}6p$  on  $3d^{10}4s$ . The resulting ionization energy agrees well with the assessments *ab initio* using the RMP [17] interpolation method. Small deviations between experimental and theoretical ionization energies are consistent for the entire copper sequence and predictions are given for unobserved elements. The accuracy of the ionization energy obtained by the RMP method was checked. This central-field model is well applicable to Cu-like ions, and due to the new identification of the upper levels in  $\text{Au}^{50+}$ , consistency in the deviations  $[\text{IE}(Z)_{\text{exp}} - \text{IE}(Z)]_{\text{theor}}$  for a wide range of elements has been established.

The excitation energies, ionization energies and dipole polarizabilities for the whole copper isoelectronic sequence have been compiled in [18]. The calculated lifetimes for  $4p$  and  $4d$  levels in Cu-like ions are presented for atomic numbers  $Z = 29-92$ . These calculations agree well with recent qualitative measurements of lifetimes. Note that the

results for the level  $4d$  were obtained by simple curve-fitting methods [19–22]. In the study, the authors combined semi-empirical parameterizations of existing databases with Dirac – Fock calculations to obtain a set of IE values and excitation energies  $4p$  and  $4d$  for all stable ions in this sequence. IE [18] compilation is fully included in the National Institute of Standards and Technology (NIST) [23] database. The ionization energies in square brackets in [23] were obtained from semi-empirical (corrected) Dirac – Fock calculations. For each ion, an uncertainty estimate IE is given. For some heavy ions, the claimed error is several tens of thousands  $\text{cm}^{-1}$ .

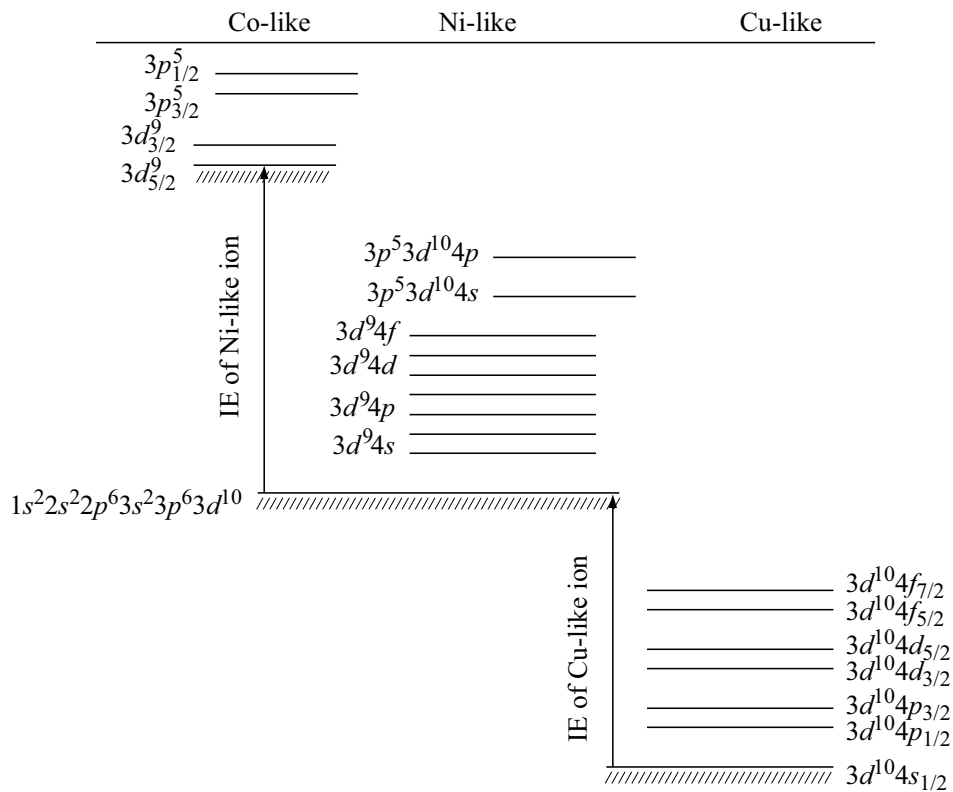
The compilation of NIST ionization energies from He- to Xe-like ions has been reviewed in papers [24,25]. The preliminary paper [26,27] showed that the NIST data for the IE of atomic ions [23] as well as the correlation energies of atomic ions can be placed on the same universal curve. A simple model was developed to identify problematic IE values in a particular isoelectronic sequence [24]. For each isoelectronic sequence, a regularized perturbation theory series based on the IE behavior for  $Z \gg N$  and  $Z \sim N-1$  ( $N$  — the number of electrons in the atomic system) is constructed. A comparison of the NIST data with this series reveals problematic values in the data presented.

In various papers, the data are obtained by interpolation and extrapolation of parameters of model potentials for Dirac equations or by IE approximation by a polynomial with power dependence on  $Z$  in order to achieve a minimal difference between theoretical and experimental values. The [24] model for IE is a smooth interpolation that fits areas with both large  $Z$  (heavy ion) and  $Z \sim N-1$  (anion).

The claimed error in the NIST database is a few units in the fourth significant digit. This means that for some heavy ions, the error can reach several tens of thousands  $\text{cm}^{-1}$ . The present paper proposes new methods for determining high-precision spectroscopic data along isoelectronic sequences. Two interpolation and extrapolation methods were developed to achieve accuracy to the fifth significant digit in IE values for Cu-like ions.

## 2. Ionization energies for constructing the model potential of an atom

Multi-charged ions with one electron above the filled shell as well as with one vacancy in the filled shell are of interest for the construction of one-quasi-particle basis functions for calculations of spectroscopic characteristics of atomic systems with one, two and three quasi-particles (quasi-particle — electron or vacancy). The energies of one electron and one vacancy are counted from the energy of the filled shell (core). As an example, Fig. 1 shows a diagram of the energy structure of Ni-like ions. The diagram also shows the energy levels of ions of neighboring ionization



**Figure 1.** Schematic of energy levels of the Ni-like ion, as well as ions of adjacent ionization stages: Cu- and Co-like. The first ionization potentials of the Cu- and Ni-like ions are shown.

stages: Cu-like ion with one electron above the core and Co-like ion with one vacancy in the core. The energy matrix element of an excited Ni-like ion with total momentum  $J$  and projection  $M_J$  is represented as a perturbation theory (PT) [28] series:

$$E(n_1 l_1 j_1 n_2 l_2 j_2 [JM_J]) = E_{\text{el}}^0(n_1 l_1 j_1) + E_{\text{vac}}^0(n_2 l_2 j_2) + \Delta E^{(1)} + \Delta E^{(2)} + \dots \quad (1)$$

In calculations of Ni-like ions,  $E_{\text{el}}^0(n_1 l_1 j_1)$  is determined by the first ionization energy of the Cu-like ion, and the energy structure of this ion (Fig. 1),  $E_{\text{vac}}^0(n_2 l_2 j_2)$  is determined by the first ionization energy from the filled shell of the Ni-like ion and the energy structure of the Co-like ion. The  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$  core is taken as the energy reference level. The zero-approximation energies  $E_{\text{el}}^0(n_1 l_1 j_1)$ ,  $E_{\text{vac}}^0(n_2 l_2 j_2)$  are empirical high-precision values of the electron energy above the core and the vacancy in the core, respectively.  $E_{\text{el}}^0(n_1 l_1 j_1)$ ,  $E_{\text{vac}}^0(n_2 l_2 j_2)$  contribute only to the diagonal matrix elements. In Ni-like ions, for almost all states, their sum is 80–95% of the total transition energy from the ground state  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$  to the excited state  $E(n_1 l_1 j_1 n_2 l_2 j_2 [JM_J])$ .

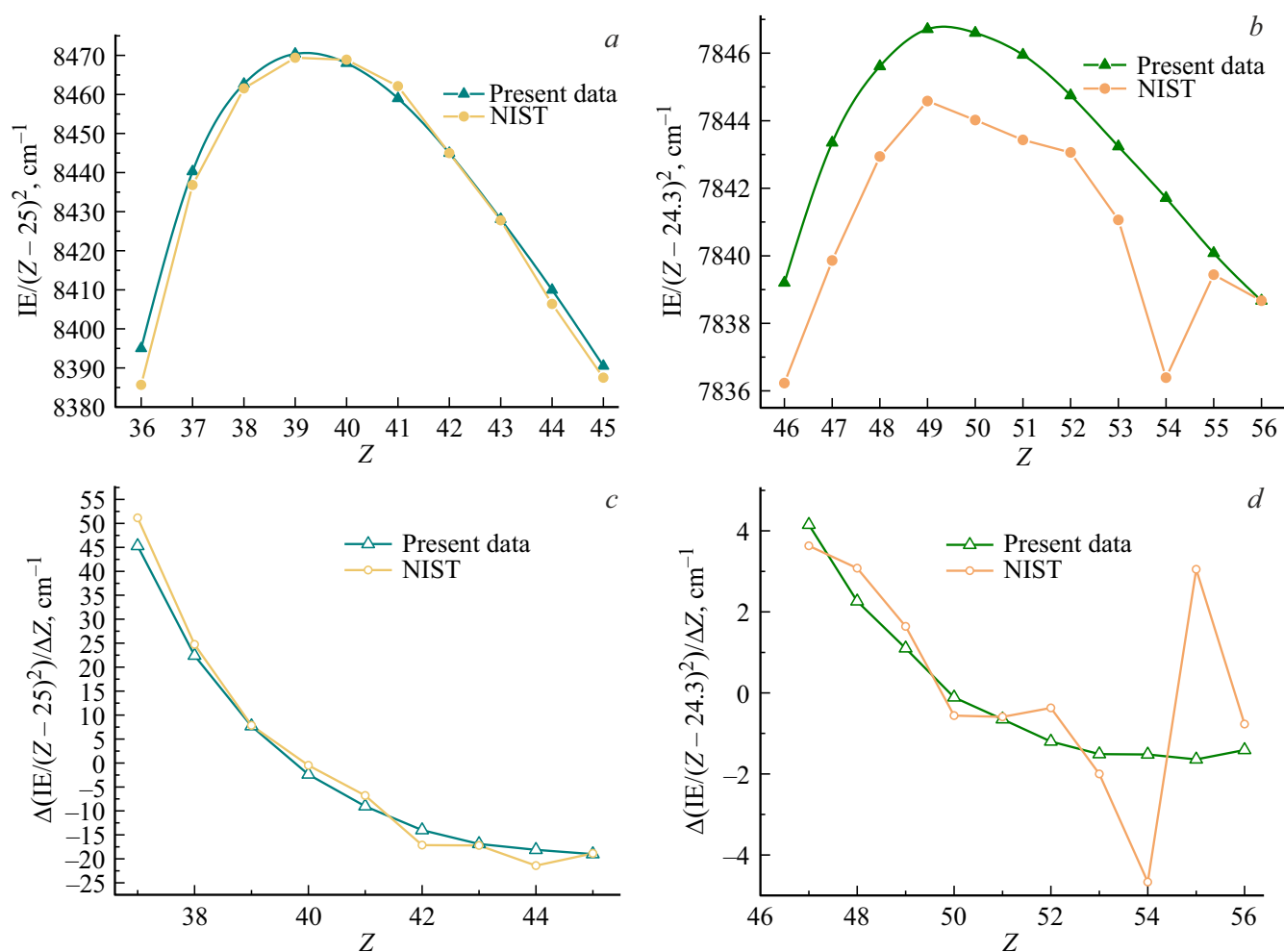
Precisely defined one-particle energies allow taking into account the vast majority of correlation, relativistic, and electrodynamic effects already in the zero order PT. Within

the first order PT only the matrix elements of the electron-vacancy interaction  $\Delta E^{(1)}$  [28] need to be calculated. The basis of one-particle wave functions is found by solving the Dirac equation using one-particle energies  $E_{\text{el}}^0(n_1 l_1 j_1)$ ,  $E_{\text{vac}}^0(n_2 l_2 j_2)$ . The high accuracy of the wave function basis results in rather high accuracy in calculating the probabilities of radiative transitions as well as the probabilities of transitions caused by electron-ion collisions. These values are the rate coefficients in the kinetic equations for calculating the amplification factors of X-ray lasers. In our calculations, we take most of the  $\Delta E^{(2)}$  and part of the higher-order PT corrections into account in the way outlined in [29,30].

In the present paper, we analyze and refine the ionization energies of Cu-like ions with  $Z \leq 92$  in order to achieve an accuracy of one or two units in the fifth significant digit, i.e. 1000–2000  $\text{cm}^{-1}$  for heavy ions.

### 3. Ionization energy scaling

IE values are known with high accuracy for Cu-like ions with  $Z \leq 53$  [16,23]. The  $IE(Z)$  function for  $36 \leq Z \leq 53$  Cu-like ions is a smooth curve to the fifth significant digit. This can be seen in Figs. 2, *a*, *b*, which show the scaled IE of Cu-like ions for  $Z = 36 - 56$  obtained in this paper and the NIST [23] data. The scaled functions  $IE(Z)$  on the interval



**Figure 2.** Scaled  $IE(Z)$  of Cu-like ions as function of  $Z$ ; (a)  $Z = 36 - 45$ , (b)  $Z = 46 - 56$ . Differentials of scaled functions  $IE(Z)$  of Cu-like ions: (c)  $Z = 37 - 45$ , (d)  $Z = 47 - 56$ .

10–15 values  $Z$  show smoothness up to the fourth to fifth significant digits.

The difference between the data obtained in this paper and the NIST data is  $\sim 1000\text{--}1500\text{ cm}^{-1}$ . Such a good match demonstrates the high accuracy of both compilations. To demonstrate the smoothness of the curves in Fig. 2, *c, d* the differentials of the scaled functions  $IE(Z)$  are given. The non-smoothness can be observed at  $Z = 54$  for both the scaled function constructed from NIST [23] data and its differential (Fig. 2, *b, d*).

A two-step methodology has been developed to interpolate and extrapolate known ionization energies:

- scaling the function  $IE(Z)$  to make it look like a slowly changing function,

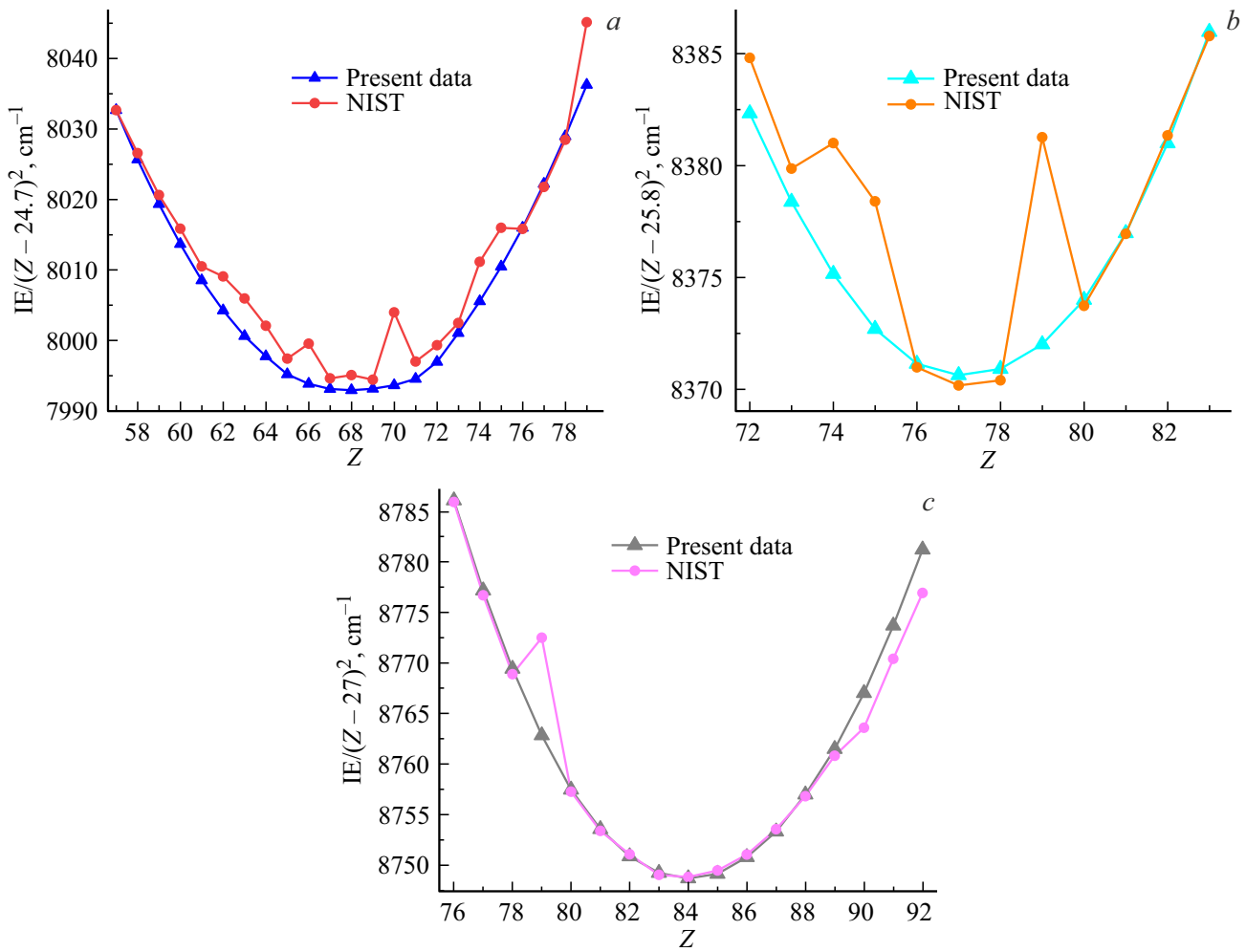
- polynomial approximation of the scaled function, which allows highly accurate interpolation and extrapolation of the scaled  $IE(Z)$ .

Fig. 3 *a, b* shows the scaled smoothed  $IE(Z)$  for intervals  $Z = 57 - 79$ ,  $Z = 72 - 83$ . Fig. 3, *c* shows the extrapolation of the scaled  $IE(Z)$  on the interval  $Z = 76 - 92$ .

The scaled functions  $IE(Z)$  from the compilation [16] had small outliers. Here, they are fitted to a smooth curve in the same way as, for instance, in papers [21,22]. Fig. 3, *a - c* also shows the corresponding scaled  $IE$  values from the NIST [23] database, for which significant outliers are observed. Smoothness is checked by the first differentials of the scaled functions  $IE(Z)$ . The differentials of the scaled functions  $IE(Z)$  are shown in Fig. 4, *a - c*.

#### 4. Model potential parameter $b(nlj|Z)$ for interpolation and extrapolation $IE(Z)$

The basic statements of relativistic perturbation theory with model potential of zero approximation (RPTMP) are presented in [28]. One-particle wave functions are determined by solving the Dirac equations. The model potential of the  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$  core includes the



**Figure 3.** Scaled ionization energies of Cu-like ions: (a)  $Z = 57 - 79$ , (b)  $Z = 72 - 83$ , (c)  $Z = 76 - 92$ .

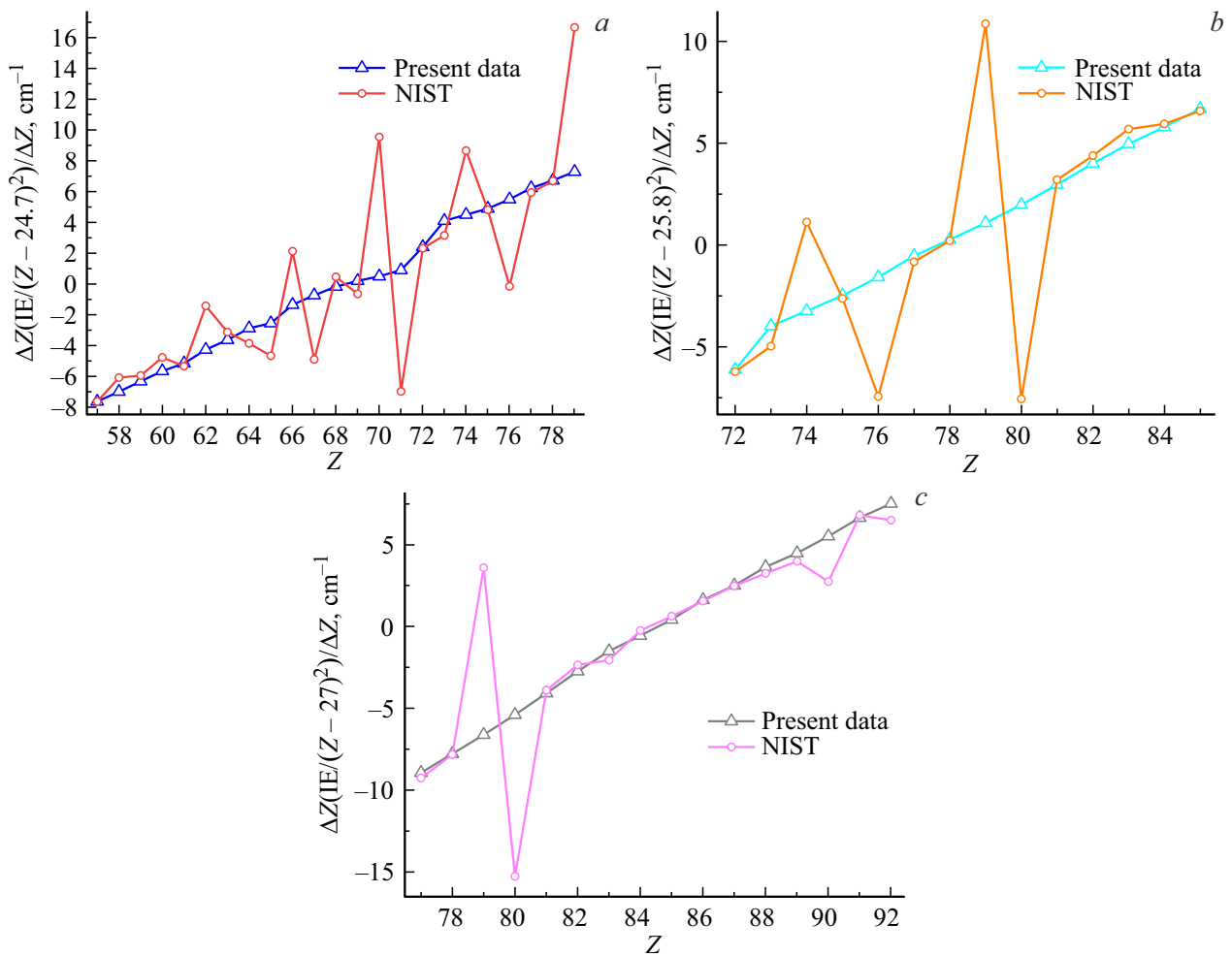
nuclear potential and the shell potentials with  $n = 1, 2, 3$ :

$$\begin{aligned}
 V(r|b(Z)) = & - \left( \frac{1}{Zr} \right) \left\{ Z - 2[1 - \exp(-2r)(1 + r)] \right. \\
 & - 8 \left[ 1 - \exp(-b_2 r) \left( 1 + \frac{3}{4}b_2 r + \frac{1}{4}b_2^2 r^2 + \frac{1}{16}b_2^3 r^3 \right) \right] \\
 & \left. - 18 \left[ 1 - \exp(-b_3 r) \left( 1 + \frac{5}{6}b_3 r + \frac{1}{3}b_3^2 r^2 + \frac{5}{54}b_3^3 r^3 \right) \right] \right\}. \quad (2)
 \end{aligned}$$

The first term represents the Coulomb potential of a point nucleus. The second and third terms — the potentials of the core shells  $K$  and  $L$ . The last term — the shell potential  $M$ , for which one common parameter  $b_3(nlj|Z)$  is introduced). The parameter  $b_2(nlj|Z)$  was determined earlier in the calculations of the isoelectronic sequence energies of neon [31]. Thus, the zero approximation model potential (2) is more developed than the one used in [16]. The parameter  $b_3(nlj|Z)$  describes the orbital state  $4lj$ , from now on we will refer to it as  $b(nlj|Z)$ .

The shell potentials  $K$ ,  $L$  and  $M$  remain unchanged when calculating shell-excited ions  $N$  as, for example, for Pd-like ions, whose spectroscopic constants have been calculated in [32]. Here, as well as in all previous RPTMP calculations (see, for example, [28], as well as references in [28] to the seminal papers [11,12]), instead of atomic units (AU), Coulomb (CU) units of length and energy are introduced: for length  $1 \text{ CU} = 1 \text{ AU} \times Z$ ; for energy  $1 \text{ CU} = 2 \text{ Ry} \times Z^2$ , for Rydberg constant, we use  $\text{Ry} = 109743 \text{ cm}^{-1}$ .

The parameter  $b(4s_{1/2}|Z)$  is adjusted so as to reproduce the value of the known empirical energy  $E(4s_{1/2}|Z)$ , i.e. the first ionization energies of the Cu-like ion, by solving the Dirac equation. A similar (inverse) procedure is used to reproduce  $b(4s_{1/2}|Z)$ ; namely, the energy  $E(4s_{1/2}|Z)$  is adjusted to reproduce the value of the extrapolated  $b(4s_{1/2}|Z)$  by solving the Dirac equation. In both cases, the adjustment is carried out until the fifth significant digit is stabilized. Fig. 5 shows the dependence of the parameter  $b(4s_{1/2}|Z)$  on  $Z$  along the isoelectronic sequence. The  $b(4s_{1/2}|Z)$  parameters for  $Z = 36 - 80$  are found using the corrected (smoothed)  $IE(Z)$  values from paper [16];



**Figure 4.** Scaled IE( $Z$ ) differentials of Cu-like ions: (a)  $\Delta Z(\text{IE}/(Z - 24.7)^2)/\Delta Z$  for  $Z = 57 - 79$ , (b)  $\Delta Z(\text{IE}/(Z - 25.8)^2)/\Delta Z$  for  $Z = 72 - 83$ , (c)  $\Delta Z(\text{IE}/(Z - 27)^2)/\Delta Z$  for  $Z = 76 - 92$ .

the  $b(4s_{1/2}|Z)$  parameters for  $Z = 81 - 92$  are found by extrapolation. From Fig. 5, *c* it can be seen that the function  $b(4s_{1/2}|Z)$  is almost straightforward; the parameter  $b(4s_{1/2}|Z)$  can be extrapolated to the fourth-fifth significant digit to  $Z = 92$ . Note, that if the value  $b(4s_{1/2}|Z)$  is defined to the fourth significant digit, then, the value of  $E(4s_{1/2}|Z)$  can be defined to the fourth – fifth significant digit.

## 5. Ionization energies of Cu-like ions

Table 1 shows the interpolated and extrapolated IE results for Cu-like ions with  $Z = 36 - 92$ , which are compared with the NIST [23] database. From Fig. 2 –4, it follows that the scaled IE( $Z$ ) functions are smooth curves. Mostly, the data of the two compilations differ by  $1000 - 3000 \text{ cm}^{-1}$ , which is a sign of high accuracy, especially for ions with charges  $Z \geq 80$ . The symbol \* denotes ions, for which the discrepancy is  $5000 - 8000 \text{ cm}^{-1}$ . The symbol \*\* denotes ions, for which the discrepancy is more than  $14000 \text{ cm}^{-1}$ . The NIST database contains IE for the complete Cu-like

isoelectronic sequence from the compilation [18], except for the 7 ions shown in Table 2.

## Conclusion

In theoretical simulations of X-ray lasers by RPTMP, knowledge of the IE with high accuracy is crucial to achieve reasonably accurate gain values [33,34]. The presented IE analysis for Cu-like ions is based on the assumption that the states of the ion with an electron above the  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s$  closed-shell core rather weakly interact with the states corresponding to the electron excitation from the closed shell. This statement is true for ions with  $Z \geq 36$ , which follows from Figs. 2, *a, b, 3* which show the smoothness of IE( $Z$ ) for Cu-like ions with  $Z \geq 36$  to the fifth significant digit.

The analysis carried out here shows that the errors of the IE values from the NIST database are much smaller than those stated in the NIST database itself. The plots of the scaled functions IE( $Z$ ) and their differentials plotted

**Table 1.** Corrected and extrapolated Cu-like ionization energies ( $\text{cm}^{-1}$ ) (PRESENT) compared to the NIST [23] database

Z	Ion	PRESENT	NIST	Z	Ion	PRESENT	NIST
36	Kr VIII	1015800	1014665	65	Tb XXXVII	12985600	12988600
37	Rb IX	1215400	1214900	66	Dy XXXVIII	13635100	13644800
38	Sr X	1430200	1430000	67	Ho XXXXIX	14302100	14304800
39	Y XI	1660200	1660000	68	Er XL	14986000	14990000
40	Zr XII	1905300	1905500	69	Tm XLI	15686600	15689100
41	Nb XIII	2165500	2166300	70	Yb XLII	16403800	16425000 **
42	Mo XIV	2440600	2440600	71	Lu XLIII	17137900	17143200 *
43	Tc XV	2730700	[2730600]	72	Hf XLIV	17891600	17896900 *
44	Ru XVI	3036000	3034700	73	Ta XLV	18665700	18669000
45	Rh XVII	3356200	3355000	74	W XLVI	19457500	19471100 **
46	Pd XVIII	3691400	3690000	75	Re XLVII	20267300	20281100 **
47	Ag XIX	4041600	4039800	76	Os XLVIII	21095600	21095200
48	Cd XX	4406800	4405300	77	Ir XLIX	21942000	21941900
49	In XXI	4787200	4785900	78	Pt L	22809400	22808000
50	Sn XXII	5182600	5180900	79	Au LI	23694800	23721000 **
51	Sb XXIII	5593300	5591500	80	Hg LII	24599800	24599000
52	Te XXIV	6019200	6017900	81	Tl LIII	25525400	25524900
53	I XXV	6460400	6458600	82	Pb LIV	26471400	26472000
54	Xe XXVI	6917100	6912400 *	83	Bi LV	27437600	27437000
55	Cs XXVII	7389200	7388600	84	Po LVI	28425500	28424900
56	Ba XXVIII	7877000	7877000	85	At LVII	29432100	29433200
57	La XXIX	8380400	8380800	86	Rn LVIII	30461500	30462400
58	Ce XXX	8899600	8900600	87	Fr LIX	31512000	31512800
59	Pr XXXI	9434700	9436200	88	Ra LX	32584800	32584200 *
60	Nd XXXII	9985800	9988500	89	Ac LXI	33679300	33676700 *
61	Pm XXXIII	10552800	10555400	90	Th LXII	34796500	34782800 **
62	Sm XXXIV	11136300	11143000 *	91	Pa LXIII	35937300	35923800 **
63	Eu XXXV	11736100	11743900 *	92	U LXIV	37101000	37082800 **
64	Gd XXXVI	12352600	12359200 *				

**Table 2.** Compilation data comparison [18] with the NIST database ( $\text{cm}^{-1}$ )

Z	Ion	[18]	NIST
62	Sm XXXIV	11138200	11143000
63	Eu XXXV	11736000	11743900
64	Gd XXXVI	12352400	12359200
70	Yb XLII	16396000	16425000
74	W XLVI	19460000	19471100
75	Re XLVII	20267630	20281100
79	Au LI	23697500	23721000

from NIST data show several scatters, which are shown in Fig. 2–4.

Compilations [17,18,24–26] check the accuracy by approximating the  $IE(Z)$  function by different polynomials for the whole sequence. Figs. 2, *a–c* show that the functional dependencies  $IE(Z)$  for the three intervals  $Z$  are very different. It follows that over the entire interval  $Z = 30–92$ , the function  $IE(Z)$  can be represented as a power polynomial with a sufficiently large error in the fourth significant digit. Our approach investigates the smoothness of the function  $IE(Z)$  approximated by a quadratic polynomial on sections

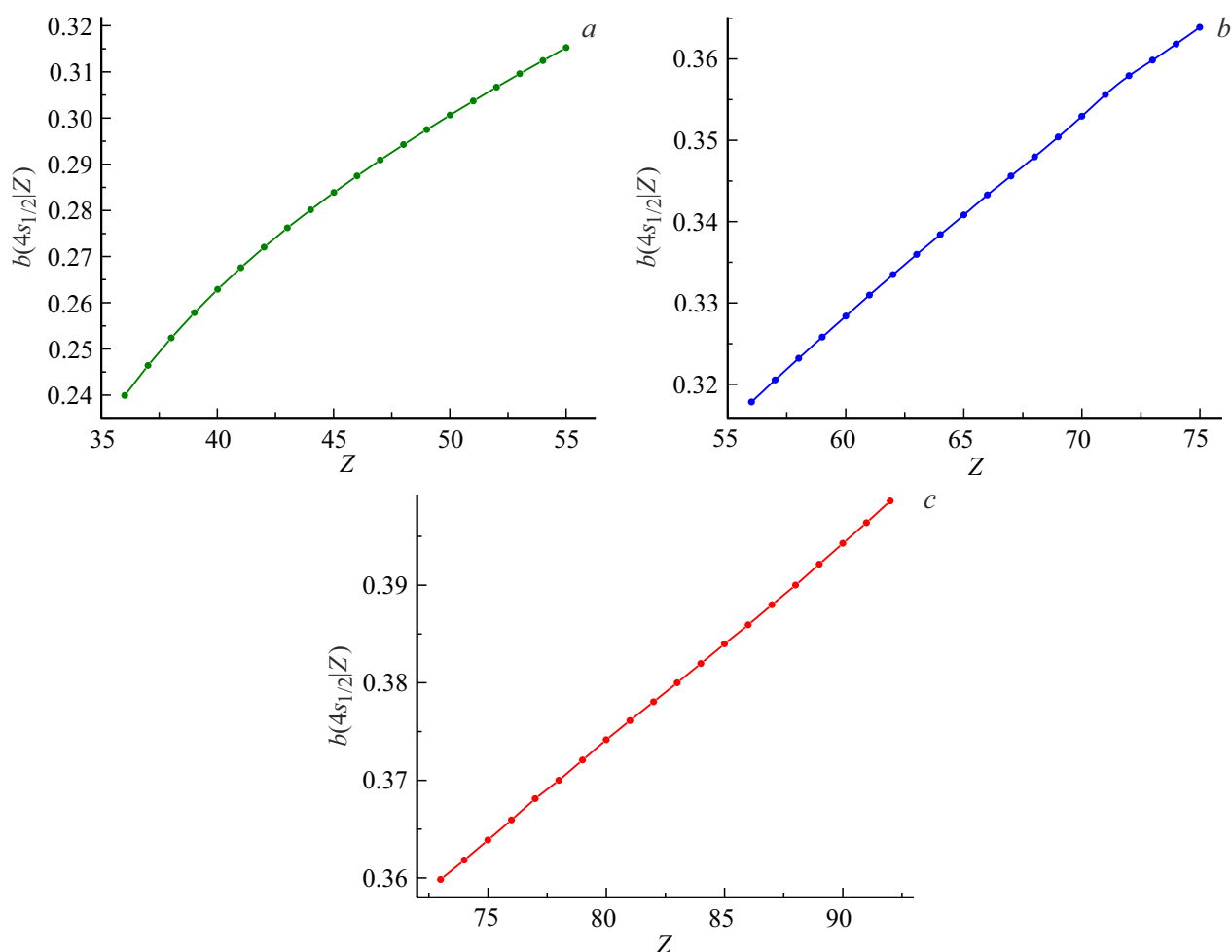
of 10–15 values  $Z$ . The scaled function  $IE(Z)$  varies on a segment of  $\sim 15$  values  $Z$  in the fourth significant digit, allowing confident interpolation to the fifth significant digit. The scaled function  $IE(Z)$  can be extrapolated with high accuracy to the area  $Z = 92$ . The quality of the extrapolation is controlled by the behavior of the differential function  $IE(Z)$ . In another method of our paper, the model potential of the Dirac equation was used to interpolate and extrapolate  $IE$  in the range  $Z = 36–92$ . The model potential parameter  $b(4s_{1/2}|Z)$  for the  $4s_{1/2}$  orbital proved to be a nearly linear function in the  $Z > 70$  area, and extrapolation of the relativistic model potential parameter proved to be an effective method for determining  $IE$  in the  $Z \sim 92$  area. The extrapolation results from both methods match up to the fifth significant digit.

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**Conflict of interest**

There are no conflicts of interest in this paper.



**Figure 5.** Model potential parameter  $b(4s_{1/2}|Z)$  for the  $4s_{1/2}$ -orbitals of Cu-like ions (dimensionless): (a)  $Z = 36–55$ , (b)  $Z = 56–75$ , (c)  $Z = 73–92$ .

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