K_α transition probabilities for platinum and uranium ions for possible X-ray biomedical applications[1]

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Abstract: Platinum compounds, such as cisplatin and other high-*Z* materials, are increasingly common in biomedical applications. The absorption and emission of high-energy X-rays can occur via the 1s–2p K_α transitions in ions of heavy elements involving deep inner-shells. Oscillator strengths (*f*), line strengths (*S*), and radiative decay rates (*A*), for the 1s–2p transitions for the nine ionic states from hydrogen-like to fluorine-like, are presented for platinum and uranium. For platinum ions the K_α transitions are found to be in the hard X-ray region, 64–71 keV (0.18–0.17 Å), and for uranium ions they are in the range 94–105 keV (0.12–0.13 Å). Since the number of electrons in each ionic state of the element is different, the number of K_α transitions varies considerably. While there are two 1s–2p transitions ($1s\ ^2S_{1/2}$–$2p\ ^2P^o_{1/2,3/2}$) in H-like ions, there are 2, 6, 2, 14, 35, 35, and 14 transitions in He-like, Li-like, Be-like, B-like, C-like, N-like, and O-like ions, respectively, for a total of 112 K_α transitions for each element. These include both types of electric dipole (E1) allowed transitions, same-spin multiplicity and intercombination. The former dipole allowed transitions are in general strong; their radiative decay rates are of the order of $A \sim 10^{16}$ s^{-1}. However, there are also many weaker transitions. We demonstrate the importance of these K_α transitions, as they appear as resonances in photo-ionization, which is relevant to the enhanced production of Auger electrons for possible radiation diagnostics and therapy.

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Résumé : Les composés de platine comme le cisplatine et d'autres composés d'éléments de *Z* élevé sont de plus en plus utilisés dans les applications biomédicales. L'absorption et l'émission de rayons-X de haute énergie peuvent se produire via les transitions 1s–2p K_α, impliquant les couches internes dans les ions d'éléments lourds. Nous présentons ici, pour les ions de platine et d'uranium, les forces d'oscillateur (*f*), les intensités de raie (*S*) et les taux de désintégration (*A*) des transitions 1s–2p pour les neuf états ioniques qui vont du type hydrogène jusqu'au type fluor. Pour les ions de platine, les transitions K_α sont dans la région des rayons-X durs, 64–71 keV (0,18–0,17 Å) et pour l'uranium, dans la région 94–105 keV (0,12–0,13 Å). Parce que le nombre d'électrons dans chaque état ionique des deux éléments est différent, le nombre de transitions K_α varie considérablement. Alors qu'il y a deux transitions 1s–2p ($1s\ ^2S_{1/2}$–$2p\ ^2P^o_{1/2,3/2}$) dans les ions de type H, il y a 2, 6, 2, 14, 35, 35 et 14 transitions dans les ions de type He, Li, Be, B, C, N, et O respectivement, pour un total de 112 transitions K_α pour chaque élément. Elles incluent les deux sortes de transitions E1 permises : même multiplicité de spin et intercombinaison. Les transitions permises des premières sont intenses et leur taux de désintégration est de l'ordre de $A \sim 10^{16}$ s^{-1}. Cependant, il y a aussi des transitions moins intenses. Nous démontrons l'importance de ces dernières transitions K_α qui apparaissent comme des résonances dans la photoionisation et sont importantes, parce qu'elles augmentent la production d'électrons Auger, qui peuvent être utiles dans le diagnostique et la thérapie par radiation.

[Traduit par la Rédaction]

1. Introduction

In previous works [1–4], a new methodology called *resonant theranostics* has been proposed, employing resonant X-ray irradiation of high-*Z* materials for potential usage as diagnostic and therapeutic agents. Compounds of heavy high-*Z* elements are common in biomedicine, especially in cancer therapy and diagnostics (theranostics). Radiation therapy is also advancing along with usage of nanoparticles embedded in malignant tumors, which is found to be more effective than direct irradiation. X-rays interact more efficiently with high-*Z* elements in the nanoparticles, involving inner-shell ionization and photo-absorption, in general, absorption and emission of photons and electrons through the Auger process. These emissions could play an important role in destroying the surrounding malignant cells.

In medical facilities, conventional machines use intense and high-energy *broadband* X-rays in radiation therapy and diagnostics to ensure sufficient tissue penetration. The radiation is still produced in the Roentgen X-ray tube via the well-known Bremsstrahlung process. To avoid collateral damage

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Table 1. Sets of configurations used in the atomic structure calculations for energies and oscillator strengths of various ionic states, from H-like to F-like, of Pt and U.

H-like
1s(1), 2s(2), 2p(3), 3s(4), 3p(5), 3d(6), 4s(7), 4p(8), 4d(9), 4f(10)
He-like
$1s^2$ (1), 1s2s(2), 1s2p(3), 1s3s(4), 1s3p(5), 1s3d(6), 1s4s(7), 1s4p(8), 1s4d(9), 1s4f(10), $2s^2$(11), $2p^2$(12), $3s^2$(13), $3p^2$(14), $3d^2$(15), 2s2p(16), 2s3s(17), 2s3p(18), 2s3d(19), 2s4s(20), 2s4p(21), 2s4d(22), 2s4f(23), 2p3s(24), 2p3p(25), 2p3d(26), 2p4s(27), 2p4p(28)
Li-like
$1s^22s$(1), $1s^22p$(2), $1s^23s$(3), $1s^23p$(4), $1s^23d$(5), $1s^24s$(6), $1s^24p$(7), $1s^24d$(8), $1s^24f$(9), $1s2s^2$(10), 1s2s2p(11), 1s2s3s(12), 1s2s3p(13), 1s2s3d(14), 1s2s4s(15), 1s2s4p(16), 1s2s4d(17), 1s2s4f(18), 1s2p3s(19), 1s2p3p(20), 1s2p3d(21), 1s2p4s(22), 1s2p4p(23), $1s2p^2$(24), $1s3s^2$ (25), $1s3p^2$(26), $1s3d^2$(27)
Be-like
$1s^22s^2$(1), $1s^22s2p$(2), $1s^22p^2$(3), $1s^22s3s$(4), $1s^22s3p$(5), $1s^22s3d$(6), $1s^22s4s$(7), $1s^22s4p$(8), $1s^22s4d$(9), $1s^22s4f$(10), $1s^22p3s$(11), $1s^22p3p$(12), $1s^22p3d$(13), $1s^22p4s$(14), $1s^22p4p$(15), $1s^22p4d$(16), $1s^22p4f$(17), $1s^22s5s$(18), $1s^22s5p$(19), $1s^22s5d$(20), $1s^22s5f$(21), $1s^22s5g$(22), $1s^22p5s$(23), $1s^22p5p$(24), $1s^22p5d$(25), $1s^22p5f$(26), $1s^22p5g$(27), $1s2s^22p$(28), $1s^23s^2$(29), $1s^23p^2$(30), $1s^23d^2$(31)
B-like
$1s^22s^22p$(1),$1s^22s2p^2$(2), $1s^22p^3$ (3), $1s^22s^23s$(4), $1s^22s^23p$(5), $1s^22s^23d$(6), $1s^22s2p3s$(7), $1s^22s2p3p$(8), $1s^22s2p3d$(9), $1s^22s^24s$(10), $1s^22s^24p$(11), $1s^22s^24d$(12), $1s^22s^24f$(13), $1s^22s2p4s$(14), $1s^22s2p4p$(15), $1s^22s2p4d$(16), $1s^22s3d^2$(17), $1s^22p^23s$(18), $1s^22p^23p$(19), $1s^22p^23d$(20), $1s^22p^24s$(21), $1s^22p^24p$(22), $1s2s^22p^2$ (23), $1s2s^22p3p$(24), $1s2s^22p3d$(25)
C-like
$1s^22s^22p^2$(1), $1s^22s2p^3$(2), $1s^22p^4$ (3), $1s^22s^22p3s$(4), $1s^22s^22p3p$(5), $1s^22s^22p3d$(6), $1s^22s^22p4s$(7), $1s^22s^22p4p$(8), $1s^22s^22p4d$(9), $1s^22s^22p4f$(10), $1s^22s2p^23s$(11), $1s^22s2p^23p$(12), $1s^22s2p^23d$(13), $1s^22s2p^24s$(14), $1s^22s2p^24p$(15), $1s^22s2p^24d$(16), $1s2s^22p^3$(17)
N-like
$1s^22s^22p^2$(1), $1s^22s2p^4$(2), $1s^22s^22p^23s$(3), $1s^22s^22p^23p$(4), $1s^22s^22p^23d$(5), $1s^22s^22p^24s$(6), $1s^22s^22p^24p$(7), $1s^22s^22p^24d$(8), $1s^22s^22p^24f$(9), $1s^22p^5$(10), $1s^22s2p^33s$(11), $1s^22s2p^33p$(12), $1s^22s2p^33d$(13), $1s2s^22p^4$(14)
O-like
$1s^22s^22p^4$(1), $1s^22s2p^5$(2), $1s^22p^6$(3), $1s^22s^22p^33s$(4), $1s^22s^22p^33p$(5), $1s^22s^22p^33d$(6), $1s^22s^22p^34s$(7), $1s^22s^22p^34p$(8), $1s^22s^22p^34d$(9), $1s^22s^22p^34f$(10), $1s^22s2p^43s$(11), $1s^22s2p^43p$(12), $1s^22s2p^43d$(13), $1s^22s2p^44s$(14), $1s^22s2p^44p$(15), $1s^22s2p^44d$(16), $1s^22s^22p^23s^2$ (17), $1s2s^22p^5$(18)
F-like
$1s^22s^22p^5$(1), $1s^22s2p^6$(2), $1s^22s^22p^43s$(3), $1s^22s^22p^43p$(4), $1s^22s^22p^43d$(5), $1s^22s^22p^44s$(6), $1s^22s^22p^44p$(7), $1s^22s^22p^44d$(8), $1s^22s^22p^44f$(9), $1s^22s2p^53s$(10), $1s^22s2p^53p$(11), $1s^22s2p^53d$(12), $1s^22s2p^54s$(13), $1s^22s2p^54p$(14), $1s^22s2p^54d$(15), $1s2s^22p6^6$(16)

Note: The configurations are numbered, within parentheses, for convenience.

incurred by the exposure to broadband radiation, resonant theranostics [1–4] aims to focus on narrow energy regions that correspond to resonant transitions, a new method, for enhanced absorption and emission of radiation via the Auger process and Coster–Kronig or Super Coster–Kronig cascades [5]. We show that (*i*) at the resonant energies, the attenuation or absorption coefficients κ are orders of magnitude higher than the background, including at the K-shell ionization energy E_K and (*ii*) such energy bands lie below the K-shell ionization energy and are thereby potentially of higher utility than the ionization edge at E_K itself.

The physical properties of high-Z heavy elements are largely unknown. For improvement and development, it is important to understand the precise interaction of X-rays as a function of incident energy and the target atomic structure. Here we study the atomic transitions in Pt and U ions and predict the energy range and strengths of the transitions most suitable for enhanced emission of electrons and photons. K-shell ionization and K-shell transitions of both these elements occur at sufficiently high energies where X-rays can penetrate the body tissue sufficiently to enable radiation imaging or treatment of ordinary tumors, especially if embedded with high-Z material(s). We will illustrate that resonances are formed during X-ray interaction through inner shell transitions and that these resonances represent higher absorption coefficients than at background energies by orders of magnitude.

2. Theory and computations

Interaction between an atomic species X^{+z} of charge z and an X-ray photon can lead to two processes. One is photo-excitation, where an electron absorbs the photon and jumps to a higher excited level,

$$X^{+z} + h\nu \rightarrow X^{+z*}$$

where the asterisk (*) denotes an excited state. The oscillator strength f represents the strength of the transition. De-excitation occurs as an excited electron drops down to a lower state by emitting a photon. The atomic parameter for this process is the radiative decay rate, or Einsteins A-coefficient. The second process is the photo-ionization – photo-dissociation – photoelectric effect, where an electron absorbs a photon and exits to continuum,

$$X^{+z} + h\nu \rightarrow X^{+z+1} + e$$

This direct ionization gives the background feature of the process. Photo-ionization can also occur via an intermediate doubly excited auto-ionizing state, as given below. The auto-ionizing state can lead to auto-ionization (AI) when an elec-

Table 2. Transition parameters, f_{ij}, S, A_{ij}, and cross section σ_{PI} for 1s–2p K_α transitions for Pt and U ions.

Z	Ne	slpc:i	slpc:j	gi	gj	wl (Å)	E (kev)	E_i (Ry)	E_j (Ry)	f_{ij}	S	A_{ji} (s-1)	σ_{PI} (Mb)
Pt Ions													
H-like: $C_i(1)$ = 1s, $C_j(3)$ = 2p													
78	1	2Se 1	2Po 3	2	2	0.185	67.019	0.00	4914.41	9.94×10^{-2}	1.21×10^{-4}	1.93×10^{16}	8.02×10^{-1}
78	1	2Se 1	2Po 3	2	4	0.181	68.500	0.00	5047.53	1.96×10^{-1}	2.33×10^{-4}	2.00×10^{16}	1.58
LS						5003.16	68.071	0.00	5003.16	2.95×10^{-1}	3.54×10^{-4}	1.98×10^{16}	2.38
Total:No of trans = 2							E = 68.071			f, σ_{PI}, κ =	2.95×10^{-1}	2.38	7.35×10^{3}
He-like: $C_i(1)$ = 1s1s, $C_j(3)$ = 1s2p													
78	2	1Se 1	1Po 3	1	3	0.183	67.751	0.00	4979.21	3.97×10^{-1}	2.39×10^{-4}	2.63×10^{16}	3.20
78	2	1Se 1	3Po 3	1	3	0.188	65.949	0.00	4848.80	1.87×10^{-1}	1.15×10^{-4}	1.18×10^{16}	1.51
LS						4979.21	67.746	0.00	4979.21	3.97×10^{-1}	2.39×10^{-4}	2.63×10^{16}	3.20
Total: No of trans = 2							E = 67.746			f, σ_{PI}, κ =	5.83×10^{-1}	4.71	1.45×10^{4}
Li-like: $C_i(1)$ = 1s1s2s, $C_j(11)$ = 1s2s2p													
78	3	2Se 1	2Po11	2	2	0.186	66.658	0.00	4890.34	5.09×10^{-2}	6.24×10^{-5}	9.77×10^{15}	4.10×10^{-1}
78	3	2Se 1	2Po11	2	4	0.183	67.751	0.00	4973.05	1.78×10^{-1}	2.15×10^{-4}	1.77×10^{16}	1.44
78	3	2Se 1	2Po11	2	2	0.183	67.751	0.00	4976.69	1.24×10^{-1}	1.50×10^{-4}	2.47×10^{16}	1.00
78	3	2Se 1	2Po11	2	4	0.182	68.123	0.00	5014.78	8.40×10^{-2}	1.00×10^{-4}	8.48×10^{15}	6.77×10^{-1}
78	3	2Se 1	4Po11	2	2	0.188	65.949	0.00	4843.56	1.43×10^{-2}	1.77×10^{-5}	2.69×10^{15}	1.15×10^{-1}
78	3	2Se 1	4Po11	2	4	0.188	65.949	0.00	4847.18	1.16×10^{-1}	1.44×10^{-4}	1.10×10^{16}	9.38×10^{-1}
LS						4973.78	67.672	0.00	4973.78	4.38×10^{-1}	5.28×10^{-4}	2.90×10^{16}	3.53
Total: No of trans = 6							E = 67.672			f, σ_{PI}, κ =	5.68×10^{-1}	4.58	1.41×10^{4}
Be-like: $C_i(1)$ = 1s1s2s2s, $C_j(28)$ = 1s2s2s2p													
78	4	1Se 1	1Po28	1	3	0.183	67.751	3.24	4987.22	3.50×10^{-1}	2.11×10^{-4}	2.33×10^{16}	2.82
78	4	1Se 1	3Po28	1	3	0.187	66.302	3.24	4871.11	1.68×10^{-1}	1.04×10^{-4}	1.07×10^{16}	1.36
LS						4983.98	67.811	3.24	4987.22	3.50×10^{-1}	2.11×10^{-4}	2.33×10^{16}	2.82
Total: No of trans = 2							E = 67.811			f, σ_{PI}, κ =	5.19×10^{-1}	4.18	1.29×10^{4}
B-like: $C_i(1)$ = 1s1s2s2s2p, $C_j(23)$ = 1s2s2s2p2p													
78	5	2Po 1	2De23	2	4	0.184	67.383	0.00	4963.48	4.78×10^{-4}	5.78×10^{-7}	4.73×10^{13}	3.86×10^{-3}
78	5	2Po 1	2De23	4	4	0.188	65.949	119.56	4963.48	1.94×10^{-2}	4.80×10^{-5}	3.65×10^{15}	1.56×10^{-1}
78	5	2Po 1	2De23	4	6	0.188	65.949	119.56	4966.55	9.32×10^{-2}	2.31×10^{-4}	1.17×10^{16}	7.51×10^{-1}
78	5	2Po 1	2Pe23	2	2	0.183	67.751	0.00	4967.55	1.24×10^{-1}	1.49×10^{-4}	2.45×10^{16}	9.97×10^{-1}
78	5	2Po 1	2Pe23	4	2	0.188	65.949	119.56	4967.55	3.10×10^{-2}	7.68×10^{-5}	1.17×10^{16}	2.50×10^{-1}
78	5	2Po 1	2Pe23	2	4	0.179	69.265	0.00	5086.94	1.22×10^{-5}	1.44×10^{-8}	1.27×10^{12}	9.83×10^{-5}
78	5	2Po 1	2Pe23	4	4	0.183	67.751	119.56	5086.94	1.79×10^{-1}	4.33×10^{-4}	3.56×10^{16}	1.45
78	5	2Po 1	2Se23	2	2	0.179	69.265	0.00	5088.99	1.10×10^{-5}	1.30×10^{-8}	2.29×10^{12}	8.89×10^{-5}
78	5	2Po 1	2Se23	4	2	0.183	67.751	119.56	5088.99	4.40×10^{-2}	1.06×10^{-4}	1.74×10^{16}	3.55×10^{-1}
78	5	2Po 1	4Pe23	2	2	0.188	65.949	0.00	4849.66	8.67×10^{-2}	1.07×10^{-4}	1.64×10^{16}	6.99×10^{-1}
78	5	2Po 1	4Pe23	4	2	0.193	64.241	119.56	4849.66	8.03×10^{-5}	2.04×10^{-7}	2.89×10^{13}	6.48×10^{-4}
78	5	2Po 1	4Pe23	2	4	0.183	67.751	0.00	4968.97	2.36×10^{-1}	2.85×10^{-4}	2.34×10^{16}	1.90
78	5	2Po 1	4Pe23	4	4	0.188	65.949	119.56	4968.97	4.20×10^{-2}	1.04×10^{-4}	7.92×10^{15}	3.38×10^{-1}
78	5	2Po 1	4Pe23	4	6	0.184	67.383	119.56	5083.08	4.68×10^{-2}	1.13×10^{-4}	6.18×10^{15}	3.78×10^{-1}
LS						4928.89	67.061	85.40	5014.29	2.86×10^{-1}	1.04×10^{-3}	3.35×10^{16}	2.31
Total: No of trans = 14							E = 67.061			f, σ_{PI}, κ =	9.03×10^{-1}	7.28	2.25×10^{4}
C-like: $C_i(1)$ = 1s1s2s2s2p2p, $C_j(17)$ = 1s2s2s2p2p2p													
78	6	3Pe 1	3Po17	3	5	0.188	65.949	117.95	4976.01	6.68×10^{-2}	1.24×10^{-4}	7.60×10^{15}	5.39×10^{-1}

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Table 2 (*continued*).

Z	Ne	slpc:i	slpc:j	gi	gj	wl (Å)	E (kev)	E_i (Ry)	E_j (Ry)	f_{ij}	S	A_{ji} (s-1)	σ_{PI} (Mb)
78	6	3Pe 1	3Po17	5	5	0.192	64.575	239.63	4976.01	2.97×10^{-5}	9.40×10^{-8}	5.35×10^{12}	2.39×10^{-4}
78	6	3Pe 1	3Po17	1	3	0.183	67.751	0.00	4979.11	3.39×10^{-1}	2.04×10^{-4}	2.25×10^{16}	2.73
78	6	3Pe 1	3Po17	3	3	0.187	66.302	117.95	4979.11	1.36×10^{-2}	2.52×10^{-5}	2.58×10^{15}	1.10×10^{-1}
78	6	3Pe 1	3Po17	5	3	0.192	64.575	239.63	4979.11	3.27×10^{-5}	1.03×10^{-7}	9.82×10^{12}	2.63×10^{-4}
78	6	3Pe 1	3Do17	5	7	0.188	65.949	239.63	5087.91	7.84×10^{-2}	2.42×10^{-4}	1.06×10^{16}	6.32×10^{-1}
78	6	3Pe 1	3So17	1	3	0.179	69.265	0.00	5089.05	2.26×10^{-5}	1.33×10^{-8}	1.57×10^{12}	1.82×10^{-4}
78	6	3Pe 1	3So17	3	3	0.183	67.751	117.95	5089.05	1.43×10^{-1}	2.60×10^{-4}	2.85×10^{16}	1.16
78	6	3Pe 1	3So17	5	3	0.188	65.949	239.63	5089.05	3.32×10^{-2}	1.03×10^{-4}	1.05×10^{16}	2.68×10^{-1}
78	6	1De 1	1Do17	5	5	0.183	67.751	120.14	5090.98	1.56×10^{-1}	4.69×10^{-4}	3.09×10^{16}	1.25
78	6	3Pe 1	3Po17	3	1	0.183	67.751	117.95	5091.07	2.78×10^{-2}	5.03×10^{-5}	1.66×10^{16}	2.24×10^{-1}
78	6	1De 1	1Po17	5	3	0.183	67.751	120.14	5092.57	4.33×10^{-2}	1.31×10^{-4}	1.43×10^{16}	3.49×10^{-1}
78	6	1Se 1	1Po17	1	3	0.188	65.949	243.88	5092.57	1.67×10^{-1}	1.03×10^{-4}	1.05×10^{16}	1.35
78	6	3Pe 1	3Do17	3	5	0.179	69.265	117.95	5200.85	2.17×10^{-7}	3.83×10^{-10}	2.70×10^{10}	1.75×10^{-6}
78	6	3Pe 1	3Do17	5	5	0.184	67.383	239.63	5200.85	8.82×10^{-2}	2.67×10^{-4}	1.74×10^{16}	7.11×10^{-1}
78	6	3Pe 1	3Do17	1	3	0.175	70.848	0.00	5203.80	7.74×10^{-8}	4.46×10^{-11}	5.61×10^{9}	6.24×10^{-7}
78	6	3Pe 1	3Do17	3	3	0.179	69.265	117.95	5203.80	1.45×10^{-5}	2.57×10^{-8}	3.02×10^{12}	1.17×10^{-4}
78	6	3Pe 1	3Do17	5	3	0.184	67.383	239.63	5203.80	8.54×10^{-2}	2.58×10^{-4}	2.82×10^{16}	6.88×10^{-1}
78	6	1De 1	3Po17	5	5	0.188	65.949	120.14	4976.01	3.81×10^{-2}	1.18×10^{-4}	7.22×10^{15}	3.08×10^{-1}
78	6	1De 1	3Po17	5	3	0.188	65.949	120.14	4979.11	3.99×10^{-2}	1.23×10^{-4}	1.26×10^{16}	3.21×10^{-1}
78	6	1Se 1	3Po17	1	3	0.192	64.575	243.88	4979.11	4.62×10^{-5}	2.92×10^{-8}	2.77×10^{12}	3.72×10^{-4}
78	6	3Pe 1	5So17	3	5	0.183	67.751	117.95	5084.48	4.77×10^{-2}	8.65×10^{-5}	5.67×10^{15}	3.85×10^{-1}
78	6	1De 1	5So17	5	5	0.184	67.383	120.14	5084.48	1.86×10^{-3}	5.61×10^{-6}	3.68×10^{14}	1.50×10^{-2}
78	6	3Pe 1	5So17	5	5	0.188	65.949	239.63	5084.48	1.92×10^{-2}	5.95×10^{-5}	3.62×10^{15}	1.55×10^{-1}
78	6	1De 1	3Do17	5	7	0.183	67.751	120.14	5087.91	4.11×10^{-2}	1.24×10^{-4}	5.82×10^{15}	3.31×10^{-1}
78	6	1De 1	3So17	5	3	0.183	67.751	120.14	5089.05	1.78×10^{-2}	5.38×10^{-5}	5.89×10^{15}	1.44×10^{-1}
78	6	1Se 1	3So17	1	3	0.188	65.949	243.88	5089.05	6.27×10^{-8}	3.88×10^{-11}	3.94×10^{9}	5.06×10^{-7}
78	6	3Pe 1	1Do17	3	5	0.183	67.751	117.95	5090.98	2.46×10^{-2}	4.44×10^{-5}	2.93×10^{15}	1.98×10^{-1}
78	6	3Pe 1	1Do17	5	5	0.188	65.949	239.63	5090.98	3.65×10^{-2}	1.13×10^{-4}	6.90×10^{15}	2.94×10^{-1}
78	6	3Pe 1	1Po17	1	3	0.179	69.265	0.00	5092.57	1.88×10^{-5}	1.11×10^{-8}	1.30×10^{12}	1.51×10^{-4}
78	6	3Pe 1	1Po17	3	3	0.183	67.751	117.95	5092.57	1.31×10^{-2}	2.36×10^{-5}	2.59×10^{15}	1.05×10^{-1}
78	6	3Pe 1	1Po17	5	3	0.188	65.949	239.63	5092.57	4.39×10^{-6}	1.36×10^{-8}	1.38×10^{12}	3.54×10^{-5}
78	6	1De 1	3Do17	5	5	0.179	69.265	120.14	5200.85	7.33×10^{-6}	2.16×10^{-8}	1.52×10^{12}	5.91×10^{-5}
78	6	1De 1	3Do17	5	3	0.179	69.265	120.14	5203.80	8.89×10^{-8}	2.62×10^{-10}	3.08×10^{10}	7.17×10^{-7}
78	6	1Se 1	3Do17	1	3	0.184	67.383	243.88	5203.80	1.77×10^{-1}	1.07×10^{-4}	1.17×10^{16}	1.43
LS						4916.39	66.891	173.51	5089.89	4.07×10^{-1}	2.24×10^{-3}	7.90×10^{16}	3.28
Total: No of trans = 35							E = 66.891			f, σ_{PI}, κ =	1.70	1.37×10^{1}	4.23×10^{4}
N-like: $C_i(1)$ = 1s1s2s2s2p2p2p, $C_j(14)$ = 1s2s2s2p2p2p2p													
78	7	4So 1	4Pe14	4	6	0.188	65.949	116.24	4959.29	6.48×10^{-2}	1.61×10^{-4}	8.14×10^{15}	5.22×10^{-1}
78	7	2Do 1	2Pe14	4	4	0.184	67.383	0.00	4963.05	1.67×10^{-1}	4.04×10^{-4}	3.31×10^{16}	1.35
78	7	2Do 1	2Pe14	6	4	0.188	65.949	118.99	4963.05	4.27×10^{-2}	1.59×10^{-4}	1.21×10^{16}	3.45×10^{-1}
78	7	2Po 1	2Pe14	2	4	0.188	65.949	122.07	4963.05	2.05×10^{-6}	2.54×10^{-9}	1.93×10^{11}	1.65×10^{-5}
78	7	2Po 1	2Pe14	4	4	0.193	64.241	238.87	4963.05	5.17×10^{-5}	1.31×10^{-7}	9.27×10^{12}	4.17×10^{-4}
78	7	2Po 1	2Se14	2	2	0.188	65.949	122.07	4964.94	7.96×10^{-2}	9.87×10^{-5}	1.50×10^{16}	6.42×10^{-1}
78	7	2Po 1	2Se14	4	2	0.193	64.241	238.87	4964.94	1.67×10^{-5}	4.23×10^{-8}	5.98×10^{12}	1.34×10^{-4}

Table 2 (*continued*).

Z	Ne	slpc:i	slpc:j	gi	gj	wl (Å)	E (kev)	E_i (Ry)	E_j (Ry)	f_{ij}	S	A_{ji} (s-1)	σ_{PI} (Mb)
78	7	2Do 1	2De14	4	4	0.180	68.880	0.00	5069.66	7.26×10^{-6}	1.72×10^{-8}	1.50×10^{12}	5.86×10^{-5}
78	7	2Do 1	2De14	6	4	0.184	67.383	118.99	5069.66	4.35×10^{-3}	1.58×10^{-5}	1.28×10^{15}	3.51×10^{-2}
78	7	2Po 1	2De14	2	4	0.184	67.383	122.07	5069.66	2.19×10^{-4}	2.66×10^{-7}	2.15×10^{13}	1.77×10^{-3}
78	7	2Po 1	2De14	4	4	0.189	65.600	238.87	5069.66	1.79×10^{-2}	4.45×10^{-5}	3.36×10^{15}	1.44×10^{-1}
78	7	2Do 1	2De14	4	6	0.180	68.880	0.00	5072.60	2.14×10^{-6}	5.07×10^{-9}	2.96×10^{11}	1.73×10^{-5}
78	7	2Do 1	2De14	6	6	0.184	67.383	118.99	5072.60	8.08×10^{-2}	2.94×10^{-4}	1.59×10^{16}	6.52×10^{-1}
78	7	2Po 1	2De14	4	6	0.189	65.600	238.87	5072.60	8.46×10^{-2}	2.10×10^{-4}	1.06×10^{16}	6.83×10^{-1}
78	7	2Do 1	2Pe14	4	2	0.180	68.880	0.00	5073.42	9.88×10^{-7}	2.34×10^{-9}	4.09×10^{11}	7.97×10^{-6}
78	7	2Po 1	2Pe14	2	2	0.184	67.383	122.07	5073.42	5.97×10^{-2}	7.24×10^{-5}	1.18×10^{16}	4.82×10^{-1}
78	7	2Po 1	2Pe14	4	2	0.188	65.949	238.87	5073.42	2.77×10^{-2}	6.88×10^{-5}	1.04×10^{16}	2.23×10^{-1}
78	7	4So 1	4Pe14	4	4	0.184	67.383	116.24	5074.86	1.05×10^{-2}	2.53×10^{-5}	2.07×10^{15}	8.44×10^{-2}
78	7	4So 1	4Pe14	4	2	0.180	68.880	116.24	5185.33	6.00×10^{-6}	1.42×10^{-8}	2.48×10^{12}	4.84×10^{-5}
78	7	2Do 1	4Pe14	4	6	0.184	67.383	0.00	4959.29	4.36×10^{-2}	1.06×10^{-4}	5.74×10^{15}	3.52×10^{-1}
78	7	2Do 1	4Pe14	6	6	0.188	65.949	118.99	4959.29	3.58×10^{-2}	1.33×10^{-4}	6.74×10^{15}	2.89×10^{-1}
78	7	2Po 1	4Pe14	4	6	0.193	64.241	238.87	4959.29	1.15×10^{-5}	2.92×10^{-8}	1.37×10^{12}	9.25×10^{-5}
78	7	4So 1	2Pe14	4	4	0.188	65.949	116.24	4963.05	1.69×10^{-2}	4.19×10^{-5}	3.19×10^{15}	1.36×10^{-1}
78	7	2Do 1	2Se14	4	2	0.184	67.383	0.00	4964.94	4.14×10^{-2}	1.00×10^{-4}	1.64×10^{16}	3.34×10^{-1}
78	7	4So 1	2Se14	4	2	0.188	65.949	116.24	4964.94	1.56×10^{-6}	3.85×10^{-9}	5.88×10^{11}	1.26×10^{-5}
78	7	4So 1	2De14	4	4	0.184	67.383	116.24	5069.66	8.06×10^{-2}	1.95×10^{-4}	1.59×10^{16}	6.50×10^{-1}
78	7	4So 1	2De14	4	6	0.184	67.383	116.24	5072.60	8.04×10^{-3}	1.95×10^{-5}	1.06×10^{15}	6.49×10^{-2}
78	7	4So 1	2Pe14	4	2	0.184	67.383	116.24	5073.42	6.90×10^{-2}	1.67×10^{-4}	2.72×10^{16}	5.56×10^{-1}
78	7	2Do 1	4Pe14	4	4	0.180	68.880	0.00	5074.86	1.14×10^{-5}	2.71×10^{-8}	2.37×10^{12}	9.23×10^{-5}
78	7	2Do 1	4Pe14	6	4	0.184	67.383	118.99	5074.86	8.69×10^{-2}	3.16×10^{-4}	2.57×10^{16}	7.01×10^{-1}
78	7	2Po 1	4Pe14	2	4	0.184	67.383	122.07	5074.86	1.14×10^{-1}	1.38×10^{-4}	1.12×10^{16}	9.19×10^{-1}
78	7	2Po 1	4Pe14	4	4	0.188	65.949	238.87	5074.86	3.87×10^{-2}	9.59×10^{-5}	7.26×10^{15}	3.12×10^{-1}
78	7	2Do 1	4Pe14	4	2	0.176	70.446	0.00	5185.33	1.98×10^{-8}	4.59×10^{-11}	8.57×10^{9}	1.60×10^{-7}
78	7	2Po 1	4Pe14	2	2	0.180	68.880	122.07	5185.33	8.93×10^{-6}	1.06×10^{-8}	1.84×10^{12}	7.20×10^{-5}
78	7	2Po 1	4Pe14	4	2	0.184	67.383	238.87	5185.33	8.65×10^{-2}	2.10×10^{-4}	3.40×10^{16}	6.98×10^{-1}
LS						4909.95	66.803	125.55	5035.50	6.36×10^{-1}	1.55×10^{-3}	4.10×10^{16}	5.13
Total: No of trans = 35							E = 66.803			f, σ_{PI}, κ =	1.26	1.02×10^{1}	3.14×10^{4}
O-like: $C_i(1)$ = 1s1s2s2s2p2p2p2p, $C_j(18)$ = 1s2s2s2p2p2p2p2p													
78	8	3Pe 1	3Po18	5	5	0.184	67.383	0.00	4962.32	8.18×10^{-2}	2.47×10^{-4}	1.62×10^{16}	6.60×10^{-1}
78	8	3Pe 1	3Po18	3	5	0.188	65.949	114.76	4962.32	6.57×10^{-2}	1.22×10^{-4}	7.44×10^{15}	5.30×10^{-1}
78	8	1Se 1	1Po18	1	3	0.184	67.383	4.11	4965.17	1.64×10^{-1}	9.91×10^{-5}	1.08×10^{16}	1.32
78	8	1De 1	1Po18	5	3	0.188	65.949	116.95	4965.17	3.90×10^{-2}	1.21×10^{-4}	1.23×10^{16}	3.14×10^{-1}
78	8	3Pe 1	3Po18	3	1	0.184	67.383	114.76	5069.51	5.39×10^{-2}	9.79×10^{-5}	3.19×10^{16}	4.34×10^{-1}
78	8	3Pe 1	3Po18	5	3	0.180	68.880	0.00	5070.99	4.60×10^{-6}	1.36×10^{-8}	1.58×10^{12}	3.71×10^{-5}
78	8	3Pe 1	3Po18	3	3	0.184	67.383	114.76	5070.99	2.62×10^{-2}	4.76×10^{-5}	5.17×10^{15}	2.11×10^{-1}
78	8	3Pe 1	3Po18	1	3	0.188	65.949	233.36	5070.99	1.64×10^{-1}	1.02×10^{-4}	1.03×10^{16}	1.32
78	8	1De 1	3Po18	5	5	0.188	65.949	116.95	4962.32	3.80×10^{-2}	1.18×10^{-4}	7.16×10^{15}	3.06×10^{-1}
78	8	3Pe 1	1Po18	5	3	0.184	67.383	0.00	4965.17	7.92×10^{-2}	2.39×10^{-4}	2.61×10^{16}	6.38×10^{-1}
78	8	3Pe 1	1Po18	3	3	0.188	65.949	114.76	4965.17	1.39×10^{-2}	2.57×10^{-5}	2.62×10^{15}	1.12×10^{-1}
78	8	3Pe 1	1Po18	1	3	0.193	64.241	233.36	4965.17	5.86×10^{-5}	3.72×10^{-8}	3.52×10^{12}	4.73×10^{-4}
78	8	1Se 1	3Po18	1	3	0.180	68.880	4.11	5070.99	1.76×10^{-5}	1.04×10^{-8}	1.21×10^{12}	1.42×10^{-4}

Table 2 (*continued*).

Z	Ne	slpc:i	slpc:j	gi	gj	wl (Å)	E (kev)	E_i (Ry)	E_j (Ry)	f_{ij}	S	A_{ji} (s-1)	σ_{PI} (Mb)
78	8	1De 1	3Po18	5	3	0.184	67.383	116.95	5070.99	8.33×10^{-2}	2.52×10^{-4}	2.74×10^{16}	6.72×10^{-1}
LS						4933.37	67.122	71.35	5004.72	1.53×10^{-1}	8.36×10^{-4}	2.99×10^{16}	1.23
Total: No of trans = 14							E = 67.122			f, σ_{PI}, κ =	8.09×10^{-1}	6.52	2.01×10^{4}
F-like: $C_i(1)$ = 1s1s2s2s2p2p2p2p2p, $C_j(16)$ = 1s2s2s2p2p2p2p2p2p													
78	9	2Po 1	2Se16	4	2	0.184	67.383	0.00	4944.70	8.33×10^{-2}	2.02×10^{-4}	3.27×10^{16}	6.71×10^{-1}
78	9	2Po 1	2Se16	2	2	0.189	65.600	117.22	4944.70	8.16×10^{-2}	1.01×10^{-4}	1.53×10^{16}	6.58×10^{-1}
LS						4905.62	66.744	39.07	4944.70	8.27×10^{-2}	3.03×10^{-4}	4.80×10^{16}	6.67×10^{-1}
Total: No of trans = 2							E = 66.744			f, σ_{PI}, κ =	1.65×10^{-1}	1.33	4.10×10^{3}
U ions													
H-like: $C_i(1)$ = 1s, $C_j(3)$ = 2p													
92	1	2Se 1	2Po 3	2	2	0.129	96.112	0.00	7037.27	8.41×10^{-2}	7.17×10^{-5}	3.34×10^{16}	6.78×10^{-1}
92	1	2Se 1	2Po 3	2	4	0.125	99.187	0.00	7301.33	1.67×10^{-1}	1.37×10^{-4}	3.58×10^{16}	1.35
LS						7213.31	98.142	0.00	7213.31	2.51×10^{-1}	2.09×10^{-4}	3.50×10^{16}	2.03
Total: No of trans = 2							E = 98.142			f, σ_{PI}, κ =	2.51×10^{-1}	2.03	5.13×10^{3}
He-like: $C_i(1)$ = 1s1s, $C_j(3)$ = 1s2p													
92	2	1Se 1	1Po 3	1	3	0.126	98.166	0.00	7215.97	3.36×10^{-1}	1.40×10^{-4}	4.69×10^{16}	2.71
92	2	1Se 1	3Po 3	1	3	0.131	94.644	0.00	6957.72	1.62×10^{-1}	6.97×10^{-5}	2.09×10^{16}	1.30
LS						7215.97	98.178	0.00	7215.97	3.36×10^{-1}	1.40×10^{-4}	4.69×10^{16}	2.71
Total: No of trans = 2							E = 98.178			f, σ_{PI}, κ =	4.98×10^{-1}	4.02	1.02×10^{4}
Li-like: $C_i(1)$ = 1s1s2s, $C_j(11)$ = 1s2s2p													
92	3	2Se 1	2Po11	2	2	0.129	96.112	0.00	7075.07	4.34×10^{-2}	3.68×10^{-5}	1.74×10^{16}	3.50×10^{-1}
92	3	2Se 1	2Po11	2	4	0.126	98.400	0.00	7240.28	1.45×10^{-1}	1.20×10^{-4}	3.06×10^{16}	1.17
92	3	2Se 1	2Po11	2	2	0.126	98.400	0.00	7244.50	1.08×10^{-1}	8.93×10^{-5}	4.54×10^{16}	8.69×10^{-1}
92	3	2Se 1	2Po11	2	4	0.124	99.987	0.00	7327.23	7.93×10^{-2}	6.49×10^{-5}	1.71×10^{16}	6.40×10^{-1}
92	3	2Se 1	4Po11	2	2	0.131	94.644	0.00	6982.28	1.27×10^{-2}	1.09×10^{-5}	4.98×10^{15}	1.02×10^{-1}
92	3	2Se 1	4Po11	2	4	0.130	95.372	0.00	6986.54	1.03×10^{-1}	8.87×10^{-5}	2.02×10^{16}	8.33×10^{-1}
LS						7242.43	98.538	0.00	7242.43	3.76×10^{-1}	3.12×10^{-4}	5.28×10^{16}	3.03
Total: No of trans = 6							E = 98.538			f, σ_{PI}, κ =	4.92×10^{-1}	3.97	1.00×10^{4}
Be-like: $C_i(1)$ = 1s1s2s2s, $C_j(28)$ = 1s2s2s2p													
92	4	1Se 1	1Po28	1	3	0.126	98.635	22.09	7269.23	2.89×10^{-1}	1.20×10^{-4}	4.06×10^{16}	2.33
92	4	1Se 1	3Po28	1	3	0.130	95.519	22.09	7043.33	1.46×10^{-1}	6.23×10^{-5}	1.92×10^{16}	1.17
LS						7247.15	98.602	22.09	7269.23	2.89×10^{-1}	1.20×10^{-4}	4.06×10^{16}	2.33
Total: No of trans = 2							E = 98.602			f, σ_{PI}, κ =	4.34×10^{-1}	3.50	8.87×10^{3}
B-like: $C_i(1)$ = 1s1s2s2s2p, $C_j(23)$ = 1s2s2s2p2p													
92	5	2Po 1	2De23	4	6	0.131	95.007	258.26	7239.28	8.45×10^{-2}	1.45×10^{-4}	2.20×10^{16}	6.81×10^{-1}
92	5	2Po 1	2Pe23	2	2	0.126	98.322	14.93	7240.36	1.04×10^{-1}	8.65×10^{-5}	4.37×10^{16}	8.40×10^{-1}
92	5	2Po 1	2Pe23	4	2	0.131	95.007	258.26	7240.36	2.82×10^{-2}	4.84×10^{-5}	2.21×10^{16}	2.27×10^{-1}
92	5	2Po 1	2De23	2	4	0.126	98.322	14.93	7242.10	2.02×10^{-1}	1.68×10^{-4}	4.24×10^{16}	1.63
92	5	2Po 1	2De23	4	4	0.131	95.007	258.26	7242.10	3.80×10^{-2}	6.53×10^{-5}	1.49×10^{16}	3.07×10^{-1}
92	5	2Po 1	2Pe23	2	4	0.122	101.626	14.93	7481.58	4.28×10^{-6}	3.44×10^{-9}	9.59×10^{11}	3.45×10^{-5}
92	5	2Po 1	2Pe23	4	4	0.126	98.244	258.26	7481.58	1.53×10^{-1}	2.53×10^{-4}	6.39×10^{16}	1.23
92	5	2Po 1	2Se23	2	2	0.122	101.626	14.93	7484.05	6.38×10^{-6}	5.13×10^{-9}	2.86×10^{12}	5.15×10^{-5}
92	5	2Po 1	2Se23	4	2	0.126	98.322	258.26	7484.05	3.74×10^{-2}	6.21×10^{-5}	3.14×10^{16}	3.02×10^{-1}

Table 2 (*continued*).

Z	Ne	slpc:i	slpc:j	gi	gj	wl (Å)	E (kev)	E_i (Ry)	E_j (Ry)	f_{ij}	S	A_{ji} (s-1)	σ_{PI} (Mb)
92	5	2Po 1	4Pe23	2	2	0.130	95.080	14.93	7001.38	7.75×10^{-2}	6.65×10^{-5}	3.04×10^{16}	6.25×10^{-1}
92	5	2Po 1	4Pe23	4	2	0.135	91.772	258.26	7001.38	1.55×10^{-4}	2.75×10^{-7}	1.13×10^{14}	1.25×10^{-3}
92	5	2Po 1	4Pe23	2	4	0.126	98.244	14.93	7235.57	4.30×10^{-4}	3.57×10^{-7}	8.99×10^{13}	3.46×10^{-3}
92	5	2Po 1	4Pe23	4	4	0.131	94.934	258.26	7235.57	1.80×10^{-2}	3.09×10^{-5}	7.04×10^{15}	1.45×10^{-1}
92	5	2Po 1	4Pe23	4	6	0.126	98.244	258.26	7477.01	3.91×10^{-2}	6.50×10^{-5}	1.09×10^{16}	3.15×10^{-1}
LS						7148.69	97.263	188.74	7337.42	3.29×10^{-1}	8.29×10^{-4}	8.11×10^{16}	2.65
Total: No of trans = 14							E = 97.263			f, σ_{PI}, κ =	7.82×10^{-1}	6.31	1.60×10^{4}
C-like: $C_i(1)$ = 1s1s2s2s2p2p, $C_j(17)$ = 1s2s2s2p2p2p													
92	6	3Pe 1	3Po17	3	5	0.130	95.519	238.01	7256.88	5.53×10^{-2}	7.09×10^{-5}	1.31×10^{16}	4.46×10^{-1}
92	6	3Pe 1	3Po17	5	5	0.135	92.182	481.08	7256.88	3.13×10^{-5}	6.93×10^{-8}	1.15×10^{13}	2.52×10^{-4}
92	6	3Pe 1	3Po17	1	3	0.126	98.792	0.00	7260.43	2.80×10^{-1}	1.16×10^{-4}	3.95×10^{16}	2.26
92	6	3Pe 1	3Po17	3	3	0.130	95.519	238.01	7260.43	1.12×10^{-2}	1.44×10^{-5}	4.45×10^{15}	9.06×10^{-2}
92	6	3Pe 1	3Po17	5	3	0.134	92.250	481.08	7260.43	3.33×10^{-5}	7.36×10^{-8}	2.05×10^{13}	2.68×10^{-4}
92	6	3Pe 1	3Do17	5	7	0.130	95.153	481.08	7476.79	6.52×10^{-2}	1.40×10^{-4}	1.83×10^{16}	5.26×10^{-1}
92	6	3Pe 1	3So17	1	3	0.122	101.710	0.00	7478.03	7.26×10^{-6}	2.91×10^{-9}	1.09×10^{12}	5.85×10^{-5}
92	6	3Pe 1	3So17	3	3	0.126	98.478	238.01	7478.03	1.18×10^{-1}	1.47×10^{-4}	4.98×10^{16}	9.54×10^{-1}
92	6	3Pe 1	3So17	5	3	0.130	95.226	481.08	7478.03	2.79×10^{-2}	5.98×10^{-5}	1.83×10^{16}	2.25×10^{-1}
92	6	1De 1	1Do17	5	5	0.126	98.478	240.66	7480.34	1.28×10^{-1}	2.66×10^{-4}	5.41×10^{16}	1.04
92	6	3Pe 1	3Po17	3	1	0.126	98.557	238.01	7480.54	2.30×10^{-2}	2.86×10^{-5}	2.91×10^{16}	1.86×10^{-1}
92	6	1De 1	1Po17	5	3	0.126	98.557	240.66	7482.28	3.54×10^{-2}	7.33×10^{-5}	2.48×10^{16}	2.85×10^{-1}
92	6	1Se 1	1Po17	1	3	0.130	95.153	486.20	7482.28	1.40×10^{-1}	5.99×10^{-5}	1.83×10^{16}	1.13
92	6	3Pe 1	3Do17	3	5	0.122	101.460	238.01	7697.95	3.72×10^{-7}	4.49×10^{-10}	9.98×10^{10}	3.00×10^{-6}
92	6	3Pe 1	3Do17	5	5	0.126	98.166	481.08	7697.95	7.21×10^{-2}	1.50×10^{-4}	3.02×10^{16}	5.82×10^{-1}
92	6	3Pe 1	3Do17	1	3	0.118	104.805	0.00	7701.39	1.91×10^{-8}	7.43×10^{-12}	3.03×10^{9}	1.54×10^{-7}
92	6	3Pe 1	3Do17	3	3	0.122	101.543	238.01	7701.39	5.49×10^{-6}	6.61×10^{-9}	2.45×10^{12}	4.42×10^{-5}
92	6	3Pe 1	3Do17	5	3	0.126	98.244	481.08	7701.39	7.08×10^{-2}	1.47×10^{-4}	4.94×10^{16}	5.71×10^{-1}
92	6	1De 1	3Po17	5	5	0.130	95.446	240.66	7256.88	3.22×10^{-2}	6.89×10^{-5}	1.28×10^{16}	2.60×10^{-1}
92	6	1De 1	3Po17	5	3	0.130	95.519	240.66	7260.43	3.32×10^{-2}	7.08×10^{-5}	2.19×10^{16}	2.67×10^{-1}
92	6	1Se 1	3Po17	1	3	0.135	92.182	486.20	7260.43	5.68×10^{-5}	2.52×10^{-8}	6.98×10^{12}	4.58×10^{-4}
92	6	3Pe 1	5So17	3	5	0.126	98.400	238.01	7472.74	3.84×10^{-2}	4.77×10^{-5}	9.67×10^{15}	3.09×10^{-1}
92	6	1De 1	5So17	5	5	0.126	98.400	240.66	7472.74	1.51×10^{-3}	3.14×10^{-6}	6.36×10^{14}	1.22×10^{-2}
92	6	3Pe 1	5So17	5	5	0.130	95.153	481.08	7472.74	1.65×10^{-2}	3.55×10^{-5}	6.49×10^{15}	1.33×10^{-1}
92	6	1De 1	3Do17	5	7	0.126	98.478	240.66	7476.79	3.35×10^{-2}	6.95×10^{-5}	1.01×10^{16}	2.70×10^{-1}
92	6	1De 1	3So17	5	3	0.126	98.478	240.66	7478.03	1.45×10^{-2}	3.01×10^{-5}	1.02×10^{16}	1.17×10^{-1}
92	6	1Se 1	3So17	1	3	0.130	95.153	486.20	7478.03	9.13×10^{-8}	3.92×10^{-11}	1.20×10^{10}	7.36×10^{-7}
92	6	3Pe 1	1Do17	3	5	0.126	98.557	238.01	7480.34	2.09×10^{-2}	2.60×10^{-5}	5.29×10^{15}	1.69×10^{-1}
92	6	3Pe 1	1Do17	5	5	0.130	95.226	481.08	7480.34	3.00×10^{-2}	6.43×10^{-5}	1.18×10^{16}	2.42×10^{-1}
92	6	3Pe 1	1Po17	1	3	0.122	101.793	0.00	7482.28	9.73×10^{-6}	3.90×10^{-9}	1.46×10^{12}	7.84×10^{-5}
92	6	3Pe 1	1Po17	3	3	0.126	98.557	238.01	7482.28	1.11×10^{-2}	1.38×10^{-5}	4.69×10^{15}	8.98×10^{-2}
92	6	3Pe 1	1Po17	5	3	0.130	95.226	481.08	7482.28	9.00×10^{-7}	1.93×10^{-9}	5.91×10^{11}	7.26×10^{-6}
92	6	1De 1	3Do17	5	5	0.122	101.460	240.66	7697.95	3.27×10^{-6}	6.57×10^{-9}	1.46×10^{12}	2.63×10^{-5}
92	6	1De 1	3Do17	5	3	0.122	101.543	240.66	7701.39	1.63×10^{-7}	3.27×10^{-10}	1.21×10^{11}	1.31×10^{-6}
92	6	1Se 1	3Do17	1	3	0.126	98.166	486.20	7701.39	1.46×10^{-1}	6.06×10^{-5}	2.03×10^{16}	1.18
LS						7130.56	97.016	348.54	7479.10	3.36×10^{-1}	1.27×10^{-3}	1.37×10^{17}	2.71

Table 2 (*continued*).

Z	Ne	slpc:i	slpc:j	gi	gj	wl (Å)	E (kev)	E_i (Ry)	E_j (Ry)	f_{ij}	S	A_{ji} (s-1)	σ_{PI} (Mb)
Total: No of trans = 35							E = 97.016			f, σ_{PI}, κ =	1.40	1.13×10^{1}	2.87×10^{4}
N-like: $C_i(1)$ = 1s1s2s2s2p2p2p, $C_j(14)$ = 1s2s2s2p2p2p2p													
92	7	4So 1	4Pe14	4	6	0.130	95.372	235.47	7228.84	5.33×10^{-2}	9.15×10^{-5}	1.40×10^{16}	4.30×10^{-1}
92	7	2Do 1	2Pe14	4	4	0.126	98.400	0.00	7233.19	1.39×10^{-1}	2.30×10^{-4}	5.82×10^{16}	1.12
92	7	2Do 1	2Pe14	6	4	0.130	95.372	238.77	7233.19	3.55×10^{-2}	9.13×10^{-5}	2.09×10^{16}	2.86×10^{-1}
92	7	2Po 1	2Pe14	2	4	0.130	95.372	242.51	7233.19	3.25×10^{-7}	2.79×10^{-10}	6.38×10^{10}	2.62×10^{-6}
92	7	2Po 1	2Pe14	4	4	0.135	91.840	479.17	7233.19	6.61×10^{-5}	1.17×10^{-7}	2.42×10^{13}	5.33×10^{-4}
92	7	2Po 1	2Se14	2	2	0.130	95.372	242.51	7235.52	6.61×10^{-2}	5.68×10^{-5}	2.60×10^{16}	5.33×10^{-1}
92	7	2Po 1	2Se14	4	2	0.135	91.840	479.17	7235.52	1.84×10^{-5}	3.27×10^{-8}	1.35×10^{13}	1.48×10^{-4}
92	7	4So 1	4Pe14	4	4	0.126	98.400	235.47	7446.55	6.57×10^{-2}	1.09×10^{-4}	2.75×10^{16}	5.30×10^{-1}
92	7	2Do 1	2De14	4	6	0.122	101.626	0.00	7450.00	1.42×10^{-6}	2.28×10^{-9}	4.21×10^{11}	1.14×10^{-5}
92	7	2Do 1	2De14	6	6	0.126	98.400	238.77	7450.00	6.62×10^{-2}	1.65×10^{-4}	2.76×10^{16}	5.33×10^{-1}
92	7	2Po 1	2De14	4	6	0.131	94.644	479.17	7450.00	7.04×10^{-2}	1.21×10^{-4}	1.83×10^{16}	5.68×10^{-1}
92	7	2Do 1	2Pe14	4	2	0.122	101.626	0.00	7450.92	1.48×10^{-7}	2.38×10^{-10}	1.32×10^{11}	1.19×10^{-6}
92	7	2Po 1	2Pe14	2	2	0.126	98.400	242.51	7450.92	4.85×10^{-2}	4.04×10^{-5}	2.02×10^{16}	3.91×10^{-1}
92	7	2Po 1	2Pe14	4	2	0.131	94.644	479.17	7450.92	2.33×10^{-2}	4.01×10^{-5}	1.82×10^{16}	1.88×10^{-1}
92	7	2Do 1	2De14	4	4	0.122	101.626	0.00	7452.63	4.58×10^{-6}	7.37×10^{-9}	2.04×10^{12}	3.69×10^{-5}
92	7	2Do 1	2De14	6	4	0.126	98.400	238.77	7452.63	7.15×10^{-2}	1.78×10^{-4}	4.48×10^{16}	5.77×10^{-1}
92	7	2Po 1	2De14	2	4	0.126	98.400	242.51	7452.63	9.43×10^{-2}	7.85×10^{-5}	1.97×10^{16}	7.61×10^{-1}
92	7	2Po 1	2De14	4	4	0.131	94.644	479.17	7452.63	3.17×10^{-2}	5.45×10^{-5}	1.24×10^{16}	2.55×10^{-1}
92	7	4So 1	4Pe14	4	2	0.123	100.800	235.47	7670.50	2.03×10^{-6}	3.28×10^{-9}	1.80×10^{12}	1.64×10^{-5}
92	7	2Do 1	4Pe14	4	6	0.126	98.400	0.00	7228.84	3.54×10^{-2}	5.88×10^{-5}	9.92×10^{15}	2.86×10^{-1}
92	7	2Do 1	4Pe14	6	6	0.130	95.372	238.77	7228.84	3.01×10^{-2}	7.76×10^{-5}	1.18×10^{16}	2.43×10^{-1}
92	7	2Po 1	4Pe14	4	6	0.135	91.840	479.17	7228.84	1.54×10^{-5}	2.73×10^{-8}	3.75×10^{12}	1.24×10^{-4}
92	7	4So 1	2Pe14	4	4	0.130	95.372	235.47	7233.19	1.37×10^{-2}	2.35×10^{-5}	5.40×10^{15}	1.11×10^{-1}
92	7	2Do 1	2Se14	4	2	0.126	98.400	0.00	7235.52	3.42×10^{-2}	5.67×10^{-5}	2.88×10^{16}	2.76×10^{-1}
92	7	4So 1	2Se14	4	2	0.130	95.372	235.47	7235.52	2.75×10^{-7}	4.71×10^{-10}	2.16×10^{11}	2.21×10^{-6}
92	7	2Do 1	4Pe14	4	4	0.122	101.626	0.00	7446.55	2.85×10^{-6}	4.60×10^{-9}	1.27×10^{12}	2.30×10^{-5}
92	7	2Do 1	4Pe14	6	4	0.126	98.400	238.77	7446.55	3.55×10^{-3}	8.87×10^{-6}	2.22×10^{15}	2.87×10^{-2}
92	7	2Po 1	4Pe14	2	4	0.126	98.400	242.51	7446.55	1.50×10^{-4}	1.25×10^{-7}	3.14×10^{13}	1.21×10^{-3}
92	7	2Po 1	4Pe14	4	4	0.131	94.644	479.17	7446.55	1.53×10^{-2}	2.64×10^{-5}	5.98×10^{15}	1.24×10^{-1}
92	7	4So 1	2De14	4	6	0.126	98.400	235.47	7450.00	6.77×10^{-3}	1.13×10^{-5}	1.89×10^{15}	5.46×10^{-2}
92	7	4So 1	2Pe14	4	2	0.126	98.400	235.47	7450.92	5.75×10^{-2}	9.56×10^{-5}	4.81×10^{16}	4.64×10^{-1}
92	7	4So 1	2De14	4	4	0.126	98.400	235.47	7452.63	9.11×10^{-3}	1.51×10^{-5}	3.81×10^{15}	7.35×10^{-2}
92	7	2Do 1	4Pe14	4	2	0.119	104.188	0.00	7670.50	4.71×10^{-9}	7.37×10^{-12}	4.45×10^{9}	3.80×10^{-8}
92	7	2Po 1	4Pe14	2	2	0.123	100.800	242.51	7670.50	5.01×10^{-6}	4.05×10^{-9}	2.22×10^{12}	4.04×10^{-5}
92	7	2Po 1	4Pe14	4	2	0.127	97.625	479.17	7670.50	7.13×10^{-2}	1.19×10^{-4}	5.92×10^{16}	5.75×10^{-1}
LS						7126.08	96.955	251.99	7378.07	7.47×10^{-1}	1.26×10^{-3}	1.02×10^{17}	6.02
Total: No of trans = 35							E = 96.955			f, σ_{PI}, κ =	1.04	8.41	2.13×10^{4}
O-like: $C_i(1)$ = 1s1s2s2s2p2p2p2p, $C_j(18)$ = 1s2s2s2p2p2p2p2p													
92	8	3Pe 1	3Po18	5	5	0.126	98.400	0.00	7240.45	6.73×10^{-2}	1.39×10^{-4}	2.83×10^{16}	5.42×10^{-1}
92	8	3Pe 1	3Po18	3	5	0.130	95.372	231.63	7240.45	5.39×10^{-2}	6.93×10^{-5}	1.28×10^{16}	4.35×10^{-1}
92	8	1Se 1	1Po18	1	3	0.126	98.400	4.99	7243.79	1.36×10^{-1}	5.62×10^{-5}	1.90×10^{16}	1.09
92	8	1De 1	1Po18	5	3	0.130	95.372	234.26	7243.79	3.23×10^{-2}	6.91×10^{-5}	2.12×10^{16}	2.60×10^{-1}

Table 2 (*concluded*).

Z	Ne	slpc:i	slpc:j	gi	gj	wl (Å)	E (kev)	E_i (Ry)	E_j (Ry)	f_{ij}	S	A_{ji} (s-1)	σ_{PI} (Mb)
92	8	3Pe 1	3Po18	3	1	0.126	98.400	231.63	7452.44	4.47×10^{-2}	5.57×10^{-5}	5.62×10^{16}	3.60×10^{-1}
92	8	3Pe 1	3Po18	5	3	0.122	101.626	0.00	7454.15	1.54×10^{-6}	3.10×10^{-9}	1.14×10^{12}	1.24×10^{-5}
92	8	3Pe 1	3Po18	3	3	0.126	98.400	231.63	7454.15	2.20×10^{-2}	2.74×10^{-5}	9.22×10^{15}	1.77×10^{-1}
92	8	3Pe 1	3Po18	1	3	0.130	95.372	468.39	7454.15	1.35×10^{-1}	5.81×10^{-5}	1.77×10^{16}	1.09
92	8	1De 1	3Po18	5	5	0.130	95.372	234.26	7240.45	3.17×10^{-2}	6.78×10^{-5}	1.25×10^{16}	2.55×10^{-1}
92	8	3Pe 1	1Po18	5	3	0.126	98.400	0.00	7243.79	6.60×10^{-2}	1.37×10^{-4}	4.64×10^{16}	5.33×10^{-1}
92	8	3Pe 1	1Po18	3	3	0.130	95.372	231.63	7243.79	1.11×10^{-2}	1.43×10^{-5}	4.40×10^{15}	8.98×10^{-2}
92	8	3Pe 1	1Po18	1	3	0.134	92.526	468.39	7243.79	7.12×10^{-5}	3.15×10^{-8}	8.75×10^{12}	5.74×10^{-4}
92	8	1Se 1	3Po18	1	3	0.122	101.626	4.99	7454.15	9.16×10^{-6}	3.69×10^{-9}	1.36×10^{12}	7.39×10^{-5}
92	8	1De 1	3Po18	5	3	0.126	98.400	234.26	7454.15	6.84×10^{-2}	1.42×10^{-4}	4.77×10^{16}	5.51×10^{-1}
LS						7179.91	97.688	143.44	7323.35	1.26×10^{-1}	4.75×10^{-4}	5.23×10^{16}	1.02
Total: No of trans = 14							$E = 97.688$			f, σ_{PI}, κ =	6.68×10^{-1}	5.39	1.36×10^{4}
1F-like: $C_i(1) = 1s1s2s2s2p2p2p2p2p$, $C_f(16) = 1s2s2s2p2p2p2p2p$													
92	9	2Po 1	2Se16	4	2	0.126	98.166	0.00	7217.00	6.88×10^{-2}	1.14×10^{-4}	5.76×10^{16}	5.55×10^{-1}
92	9	2Po 1	2Se16	2	2	0.131	95.007	235.40	7217.00	6.69×10^{-2}	5.75×10^{-5}	2.62×10^{16}	5.39×10^{-1}
LS						7138.54	97.125	78.47	7217.00	6.82×10^{-2}	1.72×10^{-4}	8.37×10^{16}	5.50×10^{-1}
Total: No of trans = 2							$E = 97.125$			f, σ_{PI}, κ =	1.36×10^{-1}	1.09	2.77×10^{3}

tron goes free or to dielectronic recombination (DR) when a photon is emitted. The inverse of DR is photo-ionization,

$$e + X^{+z} \Leftrightarrow (X^{+z-1})^{**} \Leftrightarrow \begin{cases} e + X^{+z} & \text{AI} \\ X^{+z-1} + h\nu & \text{DR} \end{cases}$$

The photo-ionization cross section is designated as σ_{PI}.

The atomic parameters are obtained from atomic structure calculations or the *R*-matrix method. In the relativistic Breit–Pauli approximation, we write the Hamiltonian H as (e.g., [6]),

$$H^{BP} = H^{NR} + H^{mass} + H^{Dar} + H^{so} + \frac{1}{2}\sum_{i\neq j}^{N}\left[g_{ij}(so + so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}(oo')\right] \quad (1)$$

where H_{NR} is the nonrelativistic Hamiltonian,

$$H^{NR} = \sum_{i=1}^{N}\left(-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N}\frac{2}{r_{ij}}\right) \quad (2)$$

and the relativistic one-body terms are the mass correction,

$$H^{mass} = -\frac{\alpha^2}{4}\sum\nolimits_i p_i^4$$

the Darwin term,

$$H^{Dar} = \frac{\alpha^2}{4}\sum\nolimits_i \nabla^2\left(\frac{Z}{r_i}\right)$$

and the spin-orbit interaction,

$$H^{so} = \left[\frac{Ze^2\hbar^2}{2m^2c^2r^3}\right]\mathbf{L}.\mathbf{S}.$$

The rest of the terms are two-body terms, where the Breit interaction is [6, 7],

$$H^{B} = \sum_{i>j}\left[g_{ij}(so + so') + g_{ij}(ss')\right] \quad (3)$$

The transition matrix elements are obtained with the dipole operator $\boldsymbol{D} = \Sigma_i\, r_i$, where the sum is over all electrons, giving the generalized line strength as,

$$S = \left|\left\langle \Psi_f \left| \sum_{j=1}^{N} r_j \right| \Psi_i \right\rangle\right|^2 \quad (4)$$

The oscillator strengths f_{ij}, radiative decay rates A_{ji}, photo-ionization cross section (σ_{PI}), and mass attenuation coefficient can then be expressed as,

$$f_{ij} = \left(\frac{E_{ji}}{3g_i}\right)S$$

$$A_{ji}(\text{sec}^{-1}) = \left(0.8032\times10^{10}\frac{E_{ji}^3}{3g_j}\right)S$$

$$\sigma_{PI}(K_\alpha, \nu) = \left(\frac{4\pi^2a_o^2\alpha}{3}\frac{E_{ij}}{g_k}\right)S \quad (5)$$

and

$$\kappa(\nu, \mathrm{K}_\alpha) = \frac{\sigma_{\mathrm{PI}}(\nu, \mathrm{K}_\alpha)}{uW_{\mathrm{A}}} \quad (6)$$

where u is 1 amu = 1.66054×10^{-24} g, and W_{A} is the atomic weight. The resonant structures of the K_α complex in photo-ionization cross sections σ_{PI} can be obtained from Auger line strengths by convolving the resonant cross sections over a normalized Gaussian function $\phi(\nu)$ as $\sigma_{\mathrm{PI}}(\mathrm{K}_\alpha)\phi(\nu)$ where,

$$\phi(\nu) = \frac{1}{\sqrt{2\pi}\Delta E}\exp\left(-\frac{E^2}{2\Delta E^2}\right)$$

The energies and oscillator strengths for the resonant 1s–2p transitions were obtained from configuration-interaction atomic structure calculations using the Thomas–Fermi approximation, as implemented in the program SUPERSTRUCTURE (SS) [5, 8]. The 1s–2p transitions can occur for all ionic states of hydrogen-like through fluorine-like ions. The states of each ion, such as, H-, He-, Li-, Be-, B-, C-, N-, O-, and F-like, were represented by a set of configurations as listed in Table 1. The sets are similar to those used earlier by Nahar et al. [9] for gold ions. The later version of SS [6], which includes relativistic effects in Breit–Pauli approximations discussed above, was used for the computations. Each set was optimized by the inclusion of additional configurations and by changing the values of the Thomas–Fermi parameters of the orbitals to obtain the lowest energies and correct order of states expected for these ions. The number of configurations and orbitals vary for each ions The calculated values of f and A were then processed to obtain other parameters using code PRCSS [7].

3. Results and discussion

We present atomic parameters for all possible allowed E1 fine-structure transitions $1s^p$–$2p^q$, where $p \leq 2$ and $q \leq 6$, in the following subsection. The resonances corresponding to these transitions in photo-ionization and attenuation coefficients relevant to biomedical applications are discussed in separate subsections.

3.1. 1s–2p K_α transitions of Pt and U ions

Oscillator strengths f_{ij}, line strength S, radiative decay rates A_{ij} in sec^{-1}, and the corresponding cross section (σ_{PI}) for various resonant K_α transitions for all ionic states, from hydrogen-like to fluorine-like, of platinum and uranium are presented in Table 2. The table also gives the symmetries (slp) with configuration numbers (ci and cj), the transition wavelength (wl) in Å and energy E in keV, and individual level energies E_i and E_j in Ry of transitional levels i and j. The numbers within parentheses of the transitional configurations C_i and C_j corresponds to configuration numbers, that is, their positions in the set of configurations used in the calculations (Table 1). For an estimate of the average strength of the transitions, the LS multiplet values calculated from transitions of same-spin multiplicity are also given. The last line includes the total oscillator strength, cross section (Megabarns), and absorption coefficient (cm^2/g). It can be noted that the number of 1s–2p or K_α transitions varies considerably, 2 to 35, with number of electrons in the 2p subshell, as the possible number of states formation also changes with them. Hence, in case of ionic breakdown due to cascades of electron droppings and ejections initiated by an Auger process, a total sum of 112 K_α transitions are possible.

Radiative decay rates of intercombination transitions are usually two to three orders of magnitude weaker than those with same-spin multiplicity. However, for these transitions, the A-values for intercombination transitions are often as strong as those with same-spin multiplicity. For example, the E1 transitions for Li-like Pt with same-spin multiplicity, $^2\mathrm{S}$ – $^2\mathrm{P^o}$, are of the same order of magnitude as those of the intercombination transitions, $^2\mathrm{S}$–$^4\mathrm{P^o}$.

To the best of our knowledge these are the first calculations for these elements and ions. While experimental data are available for ionization edges of elements, excitation data are rare. As such, it is not possible to compare with existing values. However, we adopt our earlier calculations for levels and excitation energies for iron ions as the benchmark [5] to ascertain the order of levels of higher Z elements.

For all ionic states, the states of the ground configuration are found to be in the expected right order, except for the nitrogen-like ions. The expected order of states of the ground configuration of a nitrogen-like ion is $2s^22p^3(^4\mathrm{S^o})$, $2s^22p^3$ $(^2\mathrm{D^o})$, and $2s^22p^3(^2\mathrm{P^o})$. The present computation using SS yields the right order in LS coupling. However, relativistic Breit–Pauli calculations for fine structure shifts the levels such that $2s^22p^3\left(^2\mathrm{D^o_{3/2}}\right)$ lies lower than the level $2s^22p^3\left(^4\mathrm{S^o_{3/2}}\right)$. We expect the N-like configuration to be more sensitive to relativistic effects compared with other ions, since it has a half-filled subshell. That is because of not only relativistic effects, but also more electron correlation than for other ions with lesser number of active electrons in the 2p subshell. The Breit–Pauli Hamiltonian (1) implies that both the relativistic and electron correlation effects are important in determining the energies and transition probabilities. But, while higher order Breit–Pauli corrections may play a role, it is unlikely that the order of levels would change from what is obtained at lower Z, such as for N-like iron and other similar ions. Since no other experimental or calculated values are available, it is difficult to determine the exact accuracy in the present results. We expect that with the exception of N-like Pt and U, our results should be accurate to 1%–5% for energies and 10%–30% for radiative transition probabilities of strong E1 transitions. However, we note that there are 112 K_α transitions and many of them are exceedingly weak. For those transitions, the uncertainty in transition probabilities would likely be much higher, perhaps a factor of two or more.

The main purpose of the present work is to obtain reasonably accurate values and line strengths to indicate approximate positions of K_α resonance complexes that may potentially participate in Auger processes upon X-ray irradiation.

3.2. Resonant energies and strengths in X-ray photo-ionization

The 1s–2p transition arrays from H-like to F-like ionization states of the high-Z elements of Pt and U correspond to auto-ionizing resonances, since the excitation energy of 1s into the 2p lies above the ionization limit. Thus these transi-

Fig. 1. Photo-absorption coefficient κ of Pt background (blue online, line on the left-hand side in print) and K_α resonances (red online, right-hand side in print). Photo-absorption is enhanced by orders of magnitude by the K_α resonances below the K-shell ionization threshold.

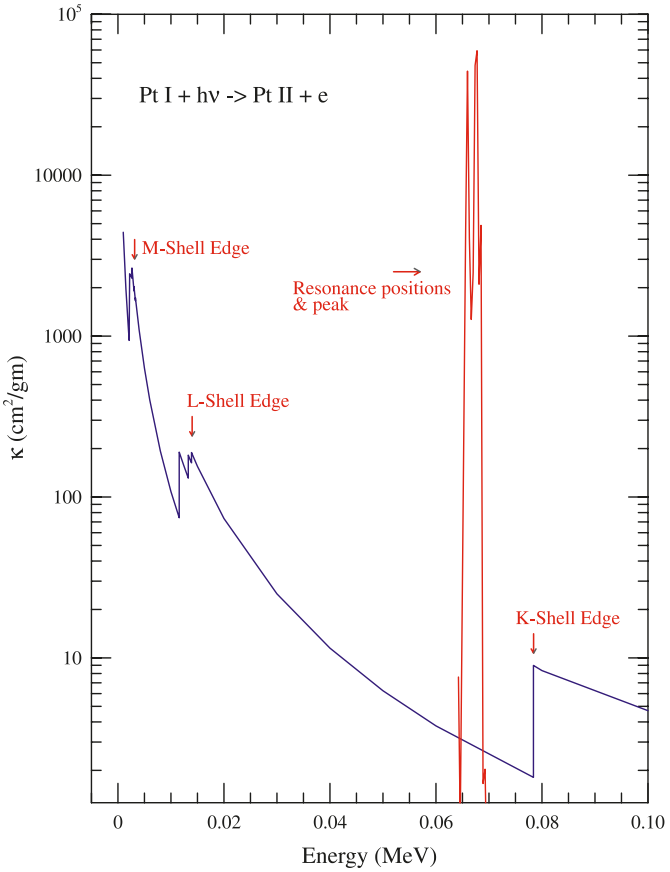
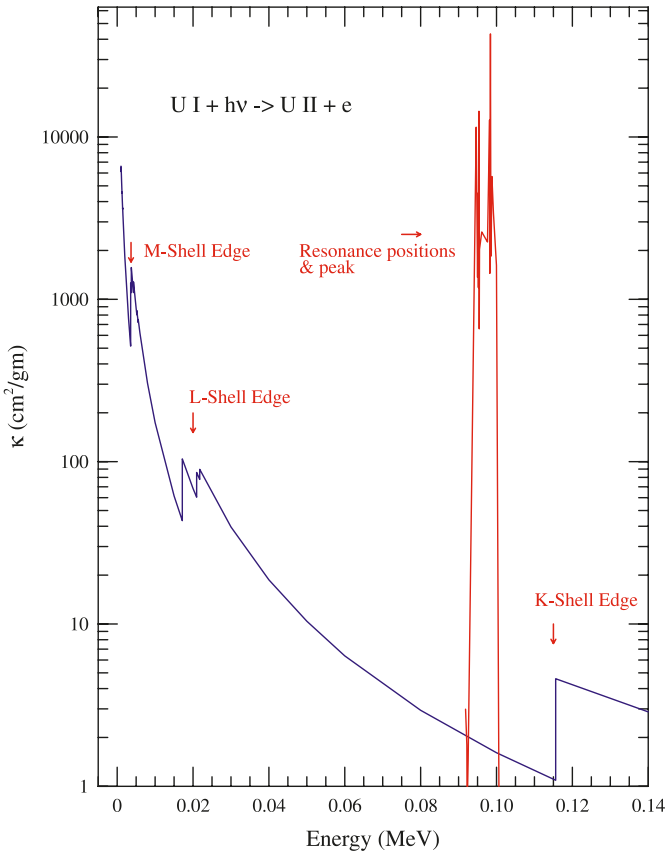


Fig. 2. Photoabsorption coefficient κ of U background (blue online; line on the left-hand side in print) and K_α resonances (red online, right-hand side in print). Photo-absorption is enhanced by orders of magnitude by the K_α resonances below the K-shell ionization threshold.



tions appear as resonances in photo-ionization cross sections. The background photo-ionizaton cross section (σ_{PI}) without auto-ionization decreases monotonically with photon energy. As the photon energy reaches the ionization threshold of an inner orbital or shell, the cross section jumps at the energy in a step-wise manner, and again decreases until the threshold energy of the next orbital or deeper inner shell.

For platinum ions the K_α transitions are found to be in the hard X-ray region 64–71 keV (0.18–0.17 Å), and for uranium ions they are in the range 94–105 keV (0.12–0.13 Å).

The curves in Figs. 1 and 2 are plots of the background mass absorption coefficient ($\kappa = \sigma_{PI}/m$) of neutral Pt and U [10]. The features in κ are the same as for σ_{PI}. The jumps in Figs. 1 and 2 are at the ionization thresholds of electronic shells K, L, and M. The auto-ionizing resonances due to 1s–2p transitions for all hydrogen to fluorine ionic states lie below the K-shell ionization edge. It is clear that the peaks of these resonances are far higher, differing by orders of magnitude, than the jump at the K-shell edge in the background cross section. The physical consequence is that the X-ray photo-absorption probability over the spread of the K_α resonances is considerably higher than at the K-shell ionization edge. Such an absorption of radiation, if possible, would further lead to Auger processes, and a resulting cascade of Coster–Kronig and Super Coster–Kronig transitions.

4. X-ray irradiation with Bremsstrahlung and monochromatic sources

As mentioned earlier, conventional X-ray machines in medical facilities produce broadband Bremsstrahlung radiation using technology, which, from a basic physics point of view, has *not* changed since Roentgen invented the X-ray tube. A beam of electrons is accelerated across the potential difference between the cathode and the anode, striking a high-Z target such as tungsten ($Z = 74$), producing characteristic Bremsstrahlung radiation at all energies from zero to the peak value of the potential, denoted as kVp. Typical X-ray sources are divided into two groups, one up to 100–250 kVp (peak voltage), and the other, employing linear accelerators, up to about 10–15 MVp. Exposure to such a wide range of radiation is inefficient in the extreme. That is because low-energy X-rays below a few tens of keV are absorbed by the body tissue without any significant penetration. On the other hand, much of high-energy X-ray flux (in the MeV range) range passes through the body without significant attenuation. Therefore, for both the low- energy and high-energy X-ray sources it becomes necessary to increase radiation dosage to high levels for diagnostics (imaging), or even more so for therapy.

To address this fundamental problem in medical X-ray devices, the resonant theranostics (RT) methodology [1, 3, 4]

aims to generate and employ *monochromatic* radiation. The advantage of monochromatic over Bremsstrahlung radiation is manifestly clear. From a physical viewpoint, we may control and target specific features in X-ray photo-ionization cross sections for maximal radiation absorption.

To implement the RT mechanism, it is necessary to build monochromatic radiation sources. One particular technique is based on partial conversion of Bremsstahlung radiation into monochromatic K_α energy according to the following expression,

$$I(K_\alpha) \propto N(X) \int_{E \geq E_K}^{E=E(kVp)} f_B(E)\sigma_K(E)\,dE \quad (7)$$

where $N(X)$ is number density of atoms of element X, f_B is the Bremsstahlung flux from an ordinary X-ray source, and σ_K is the K-shell photo-ionization cross section. It may be assumed, to a good approximation, that each K-shell ionization leads to the production of a K_α photon. The K-fluorescence yield may be expressed as,

$$\omega_K = \frac{A_r(L-K)}{A_r(L-K) + A_a(L)} \quad (8)$$

where A_r and A_a are the radiative and auto-ionization decay rates, respectively. For high-Z elements such as Pt or U, $\omega_K > 0.95$, approaching unity. It follows that all photons from the Bremsstrahlung source above the K-shell ionization energy, with $E > E_K$, may be *converted* into monochromatic K_α radiation with high efficiency. Moreover, such monochromatic deposition of X-ray energy may be localized using high-Z material, such as nanoparticles, embedded in cancerous tumors [3]. Monte Carlo simulations using the Geant4 computational package have shown [4] that the RT scheme would enhance the rate of Auger processes via Coster–Kronig and Super Coster–Kronig branching transitions [5] and result in significant production of electron ejections and photon emission.

5. Conclusion

Energies and transition strengths of K_α transitions are presented for all ionic states from the hydrogen-like to the fluorine-like of two high-Z elements, Pt and U. The transition strengths have been converted into cross sections to illustrate that these represent strong resonances with much higher probability of ionization than at the K-shell ionization threshold. Hence, these resonant energies could be the focus for potential biomedical applications using monochromatic X-ray sources.

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