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Theoretical Study on K, L, and M X-ray Transition Energies and Rates of Am and Its Ions Am^{q+}(q=1∼6)

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Abstract: Transition energies and rates of K, L, and M X-ray lines from electric-dipole transition of americium have been calculated using GRASP2K code based on the Dirac-Hartee-Fock method. The effects of the Breit interaction, vacuum polarization and self energy were taken into account. It is found that the present results agree within 0.04% with other experimental and theoretical values. Furthermore, we also calculated transition energies and rates of the K-, L-, and M-shell hole states of americium ions with charge states Am^{1+}–Am^{6+} for the first time. It is found that the transition energies and rates change slightly relative to the corresponding results of americium atoms, which indicates that the outermost electrons can hardly affect inner-shell transition properties.

Key words: Americium; K, L, and M X-rays; transition energy; transition rate
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1 Introduction

Americium (Am) is one of the transuranium elements, which is very important in nuclear industry. ^{241}Am, for example, has been employed as a target material in reactors to produce ^{238}Pu and other actinides. In addition, ^{241}Am is also used in nuclear industry for numerous applications such as in location sensing devices, in smoke detectors, and in many other aspects[1].

Although the basic nuclear properties of Am have been known well, the electronic properties are still a subject of intense interests of studies due to the rich and peculiar phenomena of it[2–4] and to the complication of 5f-shell electronic states[5]. Theoretical studies on K, L, and M X-ray properties of americium atoms and ions are of fundamental interest in atomic physics and could provide valuable information on the electronic structures and electron correlation effects in complex atoms.

Up to the present, theoretical calculations of level structure of atoms and ions have been considerably improved. The single-particle Dirac-Fock theory including the Breit interaction (BI) and quantum-electrodynamic (QED) effect could predict transition energies within the accuracy of experimentally measured values, for instance, a few eV in the range of actinide elements[6]. In the last several decades, many pieces of theoretical and experimental work have been performed on X-ray transition properties of Am atoms[7–10]. For example, Barreau *et al.*[6] measured K X-rays of Am atoms in order to determine accurately the transition energies, natural linewidths and line intensities with Dumond-type curved crystal spectrometers. Indelicato *et al.*[11] calculated the $K\alpha$ transition energies of Am by using the Dirac-Fock method with self-consistent magnetic interactions and full relaxation. Jaffe *et al.*[12] measured $L\beta1$ X-ray of Am emitted from the decay of ^{241}Am. Nelson *et al.*[13–14] determined K-shell binding energies of Am as well as the $K\alpha1$ and $K\alpha2$ X-ray photon energies with a Cauchois-type bent-crystal transmission spectrometer. Furthermore, Lu *et al.*[15] calculated the radiative transition rates of filling a K-shell vacancy from electrons

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in the L, M, O, and P shells by using a relativistic Hartree-Fock Slater method. Scofield[16] investigated the X-ray emission rates for the filling of the K- and L-shell vacancies with the use of a relativistic Hartree-Slater theory.

In the present work, K, L, and M X-ray transition energies and rates of Am atoms and its ions Am^{1+}–Am^{6+} have been calculated with the use of a general-purpose relativistic atomic structure package, GRASP2K[17], based on the Dirac-Hartee-Fock (DHF) method[18–20].

2 Theoretical methods

In the DHF method, the Dirac-Coulomb Hamiltonian of an atom or ion with N electrons is given by

$$H_{\rm DC}=\sum_{i=1}^{N}h_{\rm D}(r_i)+\sum_{i<j}^{N}(\frac{1}{r_{ij}}). \tag{1}$$

Here, while the second term is the electron-electron Coulomb interactions, $h_{\rm D}(r_i)$ denotes one-electron Dirac Hamiltonian, which consists of the kinetic energy and the interaction with the nucleus and is usually expressed as

$$h_{\rm D}(r)=c\alpha\cdot p+\beta c^2+V_{\rm nuc}(r), \tag{2}$$

in which α and β denote the 4×4 Dirac spin matrices, c is the speed of light, and $V_{\rm nuc}(r)$ represents the monopole part of the electron-nucleus Coulomb interaction. In this method, moreover, an atomic state function (ASF) of the system with angular momentum J and parity P is approximated by a linear combination of configuration state functions (CSFs) of the same symmetry,

$$|\psi_\alpha(PJM)\rangle=\sum_{r=1}^{n_c}c_r(\alpha)|\gamma_r PJM\rangle. \tag{3}$$

In this equation, n_c is the number of CSFs and $c_r(\alpha)$ denotes the configuration mixing coefficients corresponding to each individual CSF. The CSFs are expressed generally by antisymmetric linear combinations of the product of the relativistic spin-orbital wave functions as given by

$$\phi(r)=\frac{1}{r}\begin{pmatrix}P_{n\kappa}(r)\chi_{\kappa m}(\hat{r})\\ iQ_{n\kappa}(r)\chi_{-\kappa m}(\hat{r})\end{pmatrix}, \tag{4}$$

where n is the principle quantum number; κ and m are the relativistic angular quantum numbers and its z-components, respectively; $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ denote the large and small components of radial wave functions respectively, and $\chi_{\kappa m}(r)$ is the spinor spherical harmonic in the lsj coupling scheme.

According to the time-dependent perturbation theory, the Einstein spontaneous transition probability for the electric-dipole (E1) transition from an upper state β to a lower state α can be given by[21]

$$A_{\beta\alpha}=\frac{2\pi}{2j_\beta+1}\sum_{M_\beta}\sum_{M_\alpha}\left|\left\langle\alpha(P_\alpha J_\alpha M_\alpha)\left|O^{(1)}\right|\beta(P_\beta J_\beta M_\beta)\right\rangle\right|^2, \tag{5}$$

in which $O^{(1)}$ denotes the E1 transition operator, J_β is the total angular momentum of the upper state β, $|\beta(P_\beta J_\beta M_\beta)\rangle$ and $|\alpha(P_\alpha J_\alpha M_\alpha)\rangle$ represent the wave functions of the upper state β and the lower state α, respectively. The contributions of the Breit interaction will be included as a perturbation in the calculations. Apart from the Dirac-Coulomb Hamiltonian, the Breit interaction is given by[22]

$$V_{\rm Breit}=-\frac{\alpha_i\cdot\alpha_j}{r_{ij}}\cos(\omega_{ij}r_{ij})+(\alpha_i\cdot\nabla_i)(\alpha_j\cdot\nabla_j)\frac{\cos(\omega_{ij}r_{ij})-1}{\omega_{ij}^2r_{ij}}, \tag{6}$$

where α_i and α_j are the Dirac matrices of the i and j electrons, respectively, and ω_{ij} is the angular frequency of the exchanged virtual photon. The quantum electrodynamics (QED)contributions, *i.e.*, the self-energy and vacuum polarization corrections, are also included in the calculations of the transition energies and rates as suggested in Ref. [22].

3 Calculations and discussions

The calculation was performed from a single configuration Dirac-Fock solution with the nucleus described as an extended Fermi distribution. The trail radial wave functions are estimated by solving the Dirac equation for the orbitals either in the Thomas-Fermi potential or in the screened hydrogenic approximation, which can give rise to good starting wave functions for achieving self-consistency through the relativistic self-consistent field (RSCF) procedure and hence help overcome convergence problems or simply reduce the number of iterations needed for a given set of configurations. In the RSCF procedure of the DHF method, the extended optimization level (EOL) scheme has been used to optimize the radial wavefunction. In the present calculations, the configuration $[{\rm Rn}]5f^7 7s^2$ employed as the ground configuration of americium atom, and $[{\rm Rn}]5f^7 7s$, $[{\rm Rn}]5f^q (q=7,...,3)$ as the ground configurations of its ions with charge states Am^{1+}, Am^{2+}–Am^{6+}, respectively. For example, in order to calculate transition energy and rate of the $K\alpha 1$ X-ray of americium, we employ $1s_{1/2}^{-1}2s^2 2p^6...(5f^8 7s^2)$ as the excited state configuration and $1s^2 2s^2 2p_{3/2}^{-1}...(5f^8 7s^2)$ as the ground state configuration. Based on the wavefunctions, the contributions of the Breit interaction and

QED effect (including the vacuum polarization and self-energy) to the energy levels can be taken into account as perturbation by performing relativistic configuration interaction (RCI) calculations. Finally, the E1 transition properties are calculated by using the wavefunctions obtained by means of the biorthogonal transformation technique to include the relaxation effects.

The calculation here is based on single configuration Dirac-Fock method. It is worth to mention that, for the inner shell electrons such as $1s$ and $2p$ electrons in the $K\alpha1$ ($1s^{-1}$-$2p^{-1}$) radiative transition of americium atoms or ions, they are tightly bounded and highly localized and, thus, are hardly affected by the electrons from other subshells. The presently obtained results and conclusions for americium ions also support such a point. In the studies of linear polarization of $L\alpha1$ ($3d_{5/2} \rightarrow 2p_{3/2}$) and $L\alpha2$ ($3d^{3/2} \rightarrow 2p^{3/2}$) photons emitted from neutral tungsten atoms[23], although a single configuration approximation was employed to calculate the linear polarization, good agreement between the theoretical and experimental results were obtained. For this reason, we employed a single configuration approximation in the present work and think it can give rise to reasonable transition energies and rates.

Including the Breit interaction and QED effect, the transition energies and rates of strong K X-rays of Am are calculated and the results are presented in Table 1 along with other available experimental results[6, 24] and theoretical predictions[11, 26–27]. Overall, good agreements between the present results and these available ones are found. With respect to the transition energies, the maximum relative discrepancies between the present results and experimental values[6, 24] are less than 0.04% and 0.01%, respectively. Take the $K\alpha1$ X-ray for example, the presently calculated transition energy is 106 461.63 eV compared with the experimental value (106 465±20) eV of Porter *et al.*[24], which was measured by Ge(Li) detectors with a resolution (FWHM) of 600 eV. Also, an excellent agreement is found between the present results and the Dirac-Fock method results for $K\alpha1$ and $K\alpha2$ transition energies, which are calculated by Indelicato *et al.*[11]; and it is found that the maximum relative discrepancy is 0.01%. A comparison of our results with the transition energies from Ref. [26], in which were obtained using Dirac Hartree-Slater calculations it is found there are a maximum differences among them. In Ref. [26], they are using nonrelativistic method to investigate this ions. However, with respect to experimental values[6, 24], the present results are better. The presently calculated transition rates are convoluted to a Gaussian profile with the FWHM 600 eV and then plotted in Fig. 1. The FWHM is chosen as 600 eV since it is the typical resolution of K X-rays spectral with these wavelengths.

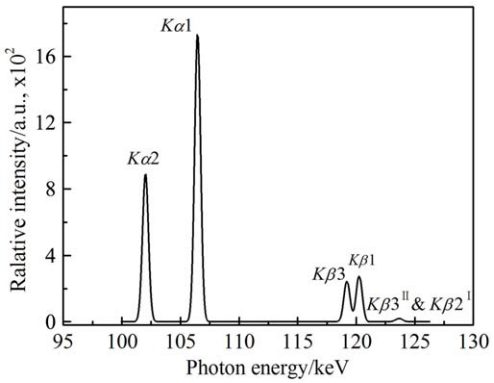

Fig. 1　The presently obtained K X-ray spectra of Am. The full width at half maximum (FWHM) utilized for the convolution is 600 eV.

The contributions of the Breit interaction and QED effect have been analyzed. The Breit interaction contributions to the transition energies ranges from 0.41%∼0.45% on K X-rays, from 0.28%∼0.55% and 0.20%–0.35% on L and M X-rays, respectively. Likewise, the QED contributions to the transition energies ranges from 0.09%∼0.10% on K X-rays, from 0.01%∼0.07% and 0.02%∼0.08% on L and M X-rays, respectively. It is found that the contributions of the Breit interaction and the QED effect on K X-rays are most pronounced, followed in turn by the L and M X-rays. For instance, $K\alpha1$ is 106 461.63 eV, as given in Table 1; its values without Breit interaction and QED effect are calculated as 106 941.09 eV and 106 352.18 eV, respectively. That means Breit and QED corrections contribute respectively by 479.50 eV and 109.41 eV, which reaches 0.45% and 0.10% respectively.

Besides the K X-rays of Am, the transition energies and rates of L X-rays are calculated, as shown in Table 2 together with other existing experimental results[7, 25] and theoretical ones[26–28]. As seen obviously from the table, the differences of the transition energies between the present calculations and the existing results are relatively small for most of the L X-rays, which are determined to be less than 8.25 eV. However, for a few L X-ray lines such as $L\beta1$, $L\gamma1$, and Ll, the absolute differences of their transition energies from the experimental measurements[7, 25] are found respectively to be 20.18, 14.62 and 11.65 eV. Nevertheless, the largest relative discrepancy from these measured results is determined to be less than 0.11%, which indicates further the reliability of the present calculations.

Table 1 The presently calculated transition energies (in eV) and rates (in atomic unit) of K X-rays of Am along with other experimental and theoretical results. The entries in parentheses refer to the power of ten, while those in square brackets denote to the reference numbers.

Lines	Trans.	Transition energies/eV			Transition rates/au
		This work	Expt.	Calc.	This work
$K\alpha1$	$K-L_{\rm III}$	106 461.63	106 474±3[6]	106 473.37[11]	4.873(-1)
			106 465±20[24]	107 043[26]	
				106 470.4±0.41[27]	
$K\alpha2$	$K-L_{\rm II}$	102 023.55	102 032±3[6]	102 033.31[11]	2.467(-1)
			102 024±20[24]	102 508[26]	
				102 030.7±0.42[27]	
$K\beta1$	$K-M_{\rm III}$	120 263.66	120 280±2[6]	120 884[26]	1.092(-1)
			120 274±30[24]	120 279.6±0.59[27]	
$K\beta3$	$K-M_{\rm II}$	119 223.20	119 240±2[6]	119 828[26]	4.899(-2)
			119 255±30[24]	119 237.9±0.58[27]	
$K\beta2^I$	$K-N_{\rm III}$	123 801.98	123 817±3[6]	124 423[26]	1.157(-2)
			123 817.5±2.9[24]	123 815.9±0.63[27]	
$K\beta2^{II}$	$K-N_{\rm II}$	123 523.62	123 548±3[6]	124 142[26]	2.392(-2)
			123 541.5±2.8[24]	123 542.0±0.78[27]	

Table 2 The same as Table 1 but for L X-rays of Am.

Lines	Trans.	Transition energies/eV				Transition rates/au
		This work	Expt.	Calc.	Calc.	This work
$L\alpha1$	$L_{\rm III}-M_{\rm V}$	14 617.08	14 629±3[7]	14 634.5[26]	14 617.2[28]	2.763(-2)
			14 617.33±0.23[25]	14 617.5±0.14[27]		
$L\alpha2$	$L_{\rm III}-M_{\rm IV}$	14 412.13	14 416±3[7]	14 423.4[26]	14 411.9[28]	1.413(-3)
			14 412.09±0.22[25]	14 411.9±0.14[27]		
$L\beta1$	$L_{\rm II}-M_{\rm IV}$	18 850.82	18 871±5[7]	18 958.4[26]	18 852.0[28]	1.806(-2)
			18 852.18±0.38[25]	18 851.6±0.17[27]		
$L\beta2$	$L_{\rm III}-N_{\rm V}$	17 674.21	17 676.66±0.34[25]	17 700.3[26]	17 676.5[28]	5.803(-3)
				17 678.2±0.26[27]		
$L\beta3$	$L_{\rm I}-M_{\rm III}$	19 104.90	19 105±8[7]	19 141.5[26]	19 105.9[28]	4.159(-3)
			19 106.24±0.87[25]	19 107.3±0.37[27]		
$L\beta4$	$L_{\rm I}-M_{\rm II}$	18 065.14	18 062.96±0.78[25]	18 085.4[26]	18 062.7[28]	1.201(-2)
				18 065.6±0.35[27]		
$L\beta5$	$L_{\rm III}-O_{\rm IV}$	18 399.75	18 408±8[7]	18 401.7[26]	18 399.6[28]	1.209(-4)
			18 399.60±0.50[25]			
$L\beta6$	$M_{\rm III}-N_{\rm I}$	16 883.29	16 887.52±0.65[25]	3 090.30[26]	16 887.0[28]	1.082(-3)
$L\gamma1$	$L_{\rm II}-N_{\rm IV}$	22 061.38	22 076±18[7]	22 184.1[26]	22 065.2[28]	7.265(-3)
			22 065.39±0.52[25]	22 067.0±0.29[27]		
$L\gamma2$	$L_{\rm I}-N_{\rm II}$	22 365.05	22 359±25[7]	22 398.8[26]	22 361[28]	3.228(-3)
			22 365.3±2.9[25]	22 370.3±0.56[27]		
$L\gamma3$	$L_{\rm I}-N_{\rm III}$	22 642.62	22 642.2±3.1[25]	22 680.0[26]		1.170(-3)
				22 643.5±0.40[27]		
$L\gamma4$	$L_{\rm I}-O_{\rm II}$	23 513.45		23 531.9[26]		1.249(-3)
$L\gamma5$	$L_{\rm II}-N_{\rm I}$	21 322.07	21 332.0±2.0[25]	21 466.8[26]		2.345(-4)
				21 330.9±0.33[27]		
$L\gamma6$	$L_{\rm II}-O_{\rm IV}$	22 833.78	22 828.20±0.80[25]	22 936.7[26]		1.276(-4)
$L\gamma8$	$L_{\rm II}-O_{\rm I}$	22 578.94		22 699.6[26]		1.582(-4)
$L\gamma13$	$L_{\rm I}-P_{\rm II}$	23 779.81		23 791.9[26]		2.822(-4)
Ll	$L_{\rm III}-M_{\rm I}$	12 371.35	12 383±7[7]	12 424.9[26]	12 384[28]	2.543(-3)
			12 378.2±1.4[25]	12 379.0±0.21[27]		
$L\eta$	$L_{\rm II}-M_{\rm I}$	16 809.40	16 819.2±1.3[25]	16 959.9[26]		1.055(-3)
				16 818.7±0.26[27]		

Furthermore, the presently obtained transition energies are much closer to these experimental results than the theoretical ones from Perkins *et al.*[26].

Apart from the K and L X-ray lines of Am, the transition energies and rates of several strong M X-rays are studied as well, which are listed in Table 3 and compared with the results from Zschornack[25] and Perkins *et al.*[26]. Generally, the present results are in reasonable agreements with the experimental values in Ref. [25], and the percentage discrepancies are determined to be 0.13%, 0.01%, 0.11%, 0.32%, 0.99% and, 1.04% for $M\alpha$, $M\beta$, $M\gamma$, $M\eta$, $M\delta$, and $M\zeta$, respectively. It is worth noting here that the transition energies of the M X-rays are much less than those of the K and L X-rays respectively by one and two orders of magnitude. Moreover, we also calculated energy differences between levels L_{II} and L_{III} as well as levels M_{II} and M_{III} in order to compare with the results from Bearden *et al.*[29], Hagström *et al.* [30], and Nelson *et al.*[13], as shown in Table 4.

Table 3　The same as Table 2 but for L X-rays of Am.

Lines	Trans.	Transition energies/eV			Transition rates/au
		This work	Expt.[25]	Calc.[26]	This work
$M\alpha1$	$M_{\rm V}-N_{\rm VII}$	3 445.54	3 442.70 ± 0.22	3 435.33	4.788(-4)
$M\alpha2$	$M_{\rm V}-N_{\rm VI}$	3 433.27	3 437.90 ± 1.70	3 421.47	6.234(-5)
$M\beta$	$M_{\rm IV}-N_{\rm VI}$	3 636.90	3 633.80 ± 0.25	3 632.57	5.024(-4)
$M\gamma$	$M_{\rm III}-N_{\rm V}$	3 871.39	3 867.30 ± 3.60	3 858.82	2.619(-4)
$M\zeta_1$	$M_{\rm V}-N_{\rm III}$	2 722.90	2 751.20	2 745.50	1.248(-4)
$M\zeta_2$	$M_{\rm IV}-N_{\rm II}$	2 650.14	2 680.30 ± 9.30	2 675.40	1.401(-4)
$M\eta$	$M_{\rm IV}-O_{\rm II}$	3 800.38	3 812.60 ± 3.50	3 808.54	1.094(-5)
$M\delta$	$M_{\rm IV}-N_{\rm III}$	2 926.96		2 956.60	1.064(-5)

Table 4　The presently calculated energy differences (keV) between levels $L_{\rm II}$ and $L_{\rm III}$ as well as levels $M_{\rm II}$ and $M_{\rm III}$ compared with the results from Bearden *et al.*[29], Hagström *et al.*[30], and Nelson *et al.*[13].

Trans.	This work	Calc.[29]	Calc.[30]	Expt.[13]
$L_{\rm II}-L_{\rm III}$	4.447	4.440	4.440	4.443 ± 0.008
$M_{\rm II}-M_{\rm III}$	1.040	1.043	1.043	1.061 ± 0.014

On the basis of the above comparisons of K, L, and M X-rays transition energies and rates of Am atom, further calculated transition energies and rates of the same radiative lines from the Am^{1+} ~Am^{6+} ions, for the first time, and the results are presented in Table 5. With respect to the transition energies, for a specific line, the difference in corresponding transition energies related with all Am ions are almost the same. For example, for the K-, L-, and M-shell, the largest differences between Am^{1+} to Am^{6+} ions are 4, 8 and 0.73 eV, respectively. While for the transition rates for these lines such differences are also near the same. Therefore, we conclude that the outermost electrons have a very small influence on the inner-shell transition properties.

Table 5　The presently calculated transition energies $\triangle E$ (eV) and rates A (au) of K, L, and M X-rays of Am^{1+}–Am^{6+} ions. The entries in parentheses refer to the power of ten.

Lines		Am^{1+}	Am^{2+}	Am^{3+}	Am^{4+}	Am^{5+}	Am^{6+}
$K\alpha1$	$\triangle E$	106 461.78	106 461.68	106 461.43	106 460.83	106 460.63	106 460.18
	A	5.294(-1)	4.881(-1)	5.823(-1)	7.786(-1)	1.168(-1)	6.288(-1)
$K\alpha2$	$\triangle E$	102 023.61	102 023.59	102 023.41	102 023.11	102 022.71	102 022.35
	A	3.30(-1)	2.434(-1)	2.075(-1)	1.374(-1)	3.777(-1)	1.272(-1)
$K\beta1$	$\triangle E$	120 263.49	120 263.15	120 262.15	120 262.11	120 261.67	120 260.00
	A	1.303(-2)	1.396(-1)	1.141(-1)	1.142(-1)	1.086(-1)	1.136(-1)
$K\beta3$	$\triangle E$	119 223.10	119 223.28	119 222.57	119 221.46	119 220.89	119 219.95
	A	4.939(-2)	4.858(-2)	9.396(-2)	3.332(-2)	6.159(-2)	2.948(-2)
$K\beta2^{\rm I}$	$\triangle E$	123 801.13	123 800.47	123 800.27	123 800.10	123 798.89	123 799.58
	A	2.166(-2)	2.016(-2)	2.206(-2)	3.611(-2)	1.860(-2)	3.237(-2)
$K\beta2^{\rm II}$	$\triangle E$	123 523.29	123 523.35	123 522.67	123 521.96	123 521.18	123 520.67
	A	1.641(-2)	1.606(-2)	2.382(-2)	1.090(-2)	2.087(-2)	5.085(-2)

Table 5 (Continued)

Lines		Am^{1+}	Am^{2+}	Am^{3+}	Am^{4+}	Am^{5+}	Am^{6+}
$L\alpha1$	$\triangle E$	14 616.44	14 617.11	14 616.17	14 616.12	14 615.83	14 615.76
	A	2.597(-2)	2.766(-2)	2.404(-2)	1.363(-2)	4.663(-2)	2.695(-2)
$L\alpha2$	$\triangle E$	14 411.80	14 412.16	14 412.07	14 411.53	14 410.02	14 4110.52
	A	2.430(-3)	1.418(-3)	1.475(-3)	1.275(-3)	2.196(-3)	2.959(-3)
$L\beta1$	$\triangle E$	18 850.88	18 850.09	18 849.86	18 849.55	18 848.36	18 848.26
	A	2.834(-2)	2.500(-2)	1.934(-2)	1.063(-2)	2.360(-2)	1.537(-2)
$L\beta2$	$\triangle E$	17 673.39	17 673.38	17 673.40	17 673.38	17 672.72	17 672.69
	A	4.203(-3)	1.365(-3)	5.770(-3)	3.565(-3)	9.132(-3)	1.101(-3)
$L\beta3$	$\triangle E$	19 104.85	19 104.02	19 103.91	19 103.36	19 103.49	19 102.53
	A	4.826(-3)	4.662(-3)	8.208(-3)	1.844(-3)	2.278(-3)	1.987(-3)
$L\beta4$	$\triangle E$	18 064.75	18 065.16	18 064.29	18 064.17	18 064.20	18 063.43
	A	1.508(-2)	1.191(-2)	1.048(-2)	2.324(-2)	1.038(-2)	3.326(-2)
$L\beta5$	$\triangle E$	18 400.01	18 399.97	18 400.36	18 400.65	18 404.32	18 405.42
	A	8.127(-4)	9.767(-4)	1.516(-4)	2.366(-4)	2.418(-4)	1.894(-3)
$L\beta6$	$\triangle E$	16 882.75	16 883.34	16 882.67	16 882.20	16 882.13	16 881.78
	A	1.187(-3)	1.077(-3)	1.273(-3)	1.191(-3)	1.365(-3)	1.315(-3)
$L\gamma1$	$\triangle E$	22 061.74	22 061.18	22 061.01	22 059.37	22 060.58	22 059.73
	A	6.582(-3)	2.424(-3)	1.165(-2)	1.564(-3)	3.934(-3)	1.027(-2)
$L\gamma2$	$\triangle E$	22 364.73	22 364.82	22 364.83	22 364.02	22 364.21	22 363.42
	A	1.068(-3)	6.247(-3)	1.730(-3)	1.274(-3)	2.912(-3)	1.551(-3)
$L\gamma3$	$\triangle E$	22 642.60	22 642.63	22 642.03	22 642.47	22 641.47	22 641.98
	A	1.874(-3)	1.194(-3)	2.574(-3)	4.392(-3)	1.353(-3)	1.983(-3)
$L\gamma4$	$\triangle E$	23 583.88	23 583.85	23 584.41	23 584.03	23 584.56	23 585.11
	A	3.466(-4)	3.402(-4)	1.013(-4)	1.825(-4)	2.164(-4)	3.302(-4)
$L\gamma5$	$\triangle E$	21 321.73	21 321.78	21 320.69	21 319.92	21 320.64	21 320.26
	A	1.293(-4)	2.331(-4)	1.610(-4)	3.216(-4)	3.410(-4)	1.299(-4)
$L\gamma6$	$\triangle E$	22 816.13	22 814.47	22 813.70	22 812.57	22 811.30	22 808.01
	A	2.383(-4)	1.703(-4)	1.506(-4)	1.505(-4)	3.350(-4)	4.375(-4)
$M\alpha1$	$\triangle E$	3 445.15	3 445.55	3 445.96	3 445.87	3 445.17	3 445.80
	A	1.276(-3)	4.812(-4)	2.465(-3)	4.122(-4)	1.726(-3)	2.909(-3)
$M\alpha2$	$\triangle E$	3 432.44	3 433.29	3 434.03	3 435.98	3 431.76	3 432.51
	A	1.136(-5)	1.463(-5)	1.138(-4)	1.372(-5)	1.484(-5)	1.081(-4)
$M\beta$	$\triangle E$	3 635.91	3 635.60	3 637.74	3 637.01	3 635.85	3 635.18
	A	2.012(-3)	3.295(-3)	2.493(-3)	5.224(-4)	2.056(-3)	1.034(-4)
$M\gamma$	$\triangle E$	3 872.24	3 872.26	3 872.78	3 871.71	3 871.90	3 872.78
	A	1.588(-4)	3.024(-4)	2.328(-4)	1.164(-4)	1.394(-3)	1.013(-4)

4 Conclusions

In this work, the electric-dipole transition energies and transition rates of K, L, and M X-ray lines of americium atoms have been systematically investigated by utilizing the GRASP2K package which is based on the Dirac-Hartee-Fock method. The contributions of the Breit interaction and the QED effect to the transition energies and rates are included throughout the calculations. It is found that the present results are in very good agreements with other available experimental and theoretical results. Moreover, we further calculated transition energies and rates of the same X-ray lines but radiated from Am^{1+}–Am^{6+} ions for the first time. We found that these transition energies and rates corresponding to the ions are nearly the same for particular X-ray lines, which indicates that outermost-shell electrons hardly affect inner-shell transition properties. Based on this fact, we expect that the transition properties of these X-ray lines emitted from americium oxides can be estimated likely to be the same as in the corresponding americium ions due to negligible effects of valence-shell electrons.

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Am原子及其离子$Am^{q+}(q=1\sim6)$的K, L, M-X射线跃迁能和跃迁几率的理论研究

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摘要： 使用基于Dirac-Hartree-Fock方法的Grasp2K程序包，计算了Am原子及离子的K,L,M-X射线的跃迁能和跃迁速率。在计算中，包括了Breit相互作用、真空极化和自能等重要效应。目前研究结果与已有的其他实验和理论结果相对误差约为0.04%。此外，我们还首次计算了从Am^{1+}到Am^{6+}离子的K, L, M-X射线的跃迁能和跃迁速率。相对于中性原子，来自低离化态的跃迁能相对于中性的相应跃迁线的能量仅有轻微的偏移，这反映出外层电子几乎不影响内壳层的跃迁性质。

关键词： 镅；K, L, M-X射线；跃迁能；跃迁速率

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