Energies and Electric Dipole Transitions for Low-Lying Levels of Protactinium IV and Uranium V

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Z. Naturforsch. **67a,** 89 – 98 (2012) / DOI: 10.5560/ZNA.2011-0066
Received July 19, 2011

We have reported a relativistic multiconfiguration Dirac–Fock (MCDF) study on low-lying level structures of protactinium IV ($Z = 91$) and uranium V ($Z = 92$) ions. Excitation energies and electric dipole (E1) transition parameters (wavelengths, oscillator strengths, and transition rates) for these low-lying levels have been given. We have also investigated the influence of the transverse Breit and quantum electrodynamic (QED) contributions besides correlation effects on the level structure. A comparison has been made with a few available data for these ions in the literature.

Key words: MCDF Method; Energies; Wavelengths; Oscillator Strengths; Transition Rates.

1. Introduction

The investigation of the level structure of actinide atoms and ions is more complex because of the great experimental difficulties such as their short lifetimes and radioactivity and the difficulties in the assignment and interpretation of the enormous number of levels. The difficulty in observing of actinide elements arises from configuration interactions in their spectra. The spectra of actinides which may contain tens or hundreds of thousands of observable lines are tremendously complex. In many cases, a large amount of data is required for a correct interpretation of the spectra, and, hence, a large amount of sample material is needed. The problems occur such as the choice of coupling scheme, the evaluation of the matrix elements of the spin–orbit interaction and the Coulomb interaction, the estimation of the radial integrals, and the diagonalization of the energy matrices. Another problem is the capacity of computers for the test of theoretical studies.

Therefore, only few data are available for the protactinium IV ion. Studies on this ion are replaced by comprehensive studies about actinide and heavy atoms. Energy levels of only $5f^2$ configuration for this ion can be found in actinides web site [1]. Carlson et al. [2] calculated ionization potentials for all elements up to $Z = 103$ for all states of ionization. Brewer [3] described methods for estimating energies of the electronic configurations of the gaseous ions of the lanthanides and actinides. The relativistic local density functional with correlation energy has been used in conjunction with the concept of Slater transition state to calculated the ($ns \rightarrow np$) dipole oscillator strength in the isoelectronic series corresponding to beryllium ($n = 2$), magnesium ($n = 3$), calcium ($n = 4$), strontium ($n = 5$), barium ($n = 6$), and radium ($n = 7$) [4]. Both relativistic energy-consistent small-core ab initio pseudopotential and fully relativistic density functional all-electron calculations were carried out by exploiting the presently available highest computational capability for the first to fourth ionization potentials as well as the $df[\Delta_{df} = \mathrm{E}(f^{\mathrm{n}}d^1s^2) - \mathrm{E}(f^{\mathrm{n+1}}d^0s^2)$ ($n = 0-13$ for Ac–No)] and $fd[\Delta_{df} = \mathrm{E}(f^{\mathrm{n}}d^2s^2) - \mathrm{E}(f^{\mathrm{n+1}}d^1s^2)$ ($n = 0-13$ for Th–Lr)] excitation energies for the whole series of actinide atoms by Liu et al. [5]. Cao and Dolg [6] represented the theoretical prediction of the second to fourth actinides ionization potentials. A systematic study of atomic binding energies, in the Dirac–Fock approximation, was performed for lithium to dubnium isoelectronic series by Rodrigues et al. [7].

The spectrum of uranium V was observed from 2000 Å to 8 µm by Conway [8]. Optical spectra and paramagnetic resonance of uranium V ions in alcaline earth fluoride lattices was given by Title et al. [9]. Energy levels of uranium V in an octahedral cyristalline field were introduced by Satten et al. [10]. Johnson et al. [11] presented covalency effects in uranium V halide complexes. Prediction and interpretation of free-

ion and crystal-field spectra of the actinides was given by Varga et al. [12]. Hecht and Gruber investigated temperature-dependent polarized absorption spectra of single crystal UCl_4 in the range 4000 – 25 000 Å [13] and assigned and analyzed the uranium V ion in the field of D_{2d} point group symmetry as a model [14]. The photoreduction of the uranyl ion in sulfuric acid with laser light and ethanol was discussed by Bell and Buxton [15]. Crystal field calculations for energy levels of uranium V in $ZrSiO_4$ were made by Mackey et al. [16]. Desclaux and Freeman [17] reported results of accurate Dirac–Fock studies of some uranium, neptunium, plutonium, and americium ions. Thakur and Thakur [18] found the second to sixth ionization potentials of uranium, neptunium, and plutonium from a thermochemical procedure. Wyart et al. [19] reported wavelengths for 261 lines of four-times-ionized uranium between 443 Å and 2325 Å. Goldschmidt [20] investigated the effects of spin-dependent interactions on the energy-level scheme of uranium V. The $5f^2$ $^1S_0$ level of the uranium V ion has been found and a parametric analysis for this configuration has been made by Van Deurzen et al. [21]. A parametric model for lanthanide and actinide atomic and crystal energy levels was presented that correlates trends in Hartree–Fock calculations with empirically determined atomic parameters [22]. The orbital energies, total energies, and ionization energies for ground-state configurations of uranium ions from U I to U XCII was listed by Rashid et al. [23]. The energy levels of uranium V were analyzed using a ten parameter Hamiltonian and, in particular, the effect of magnetic and configuration interactions examined by Rahman [24]. Eliav et al. [25] applied the relativistic Fock-space coupled-cluster method for the direct calculation of ionization potentials and excitation energies (including fine structure) for the $4f^2$ levels of praseodymium IV and the $5f^2$ levels of uranium V. Kulagin [26] considered energy levels of singly, doubly, and triply charged ions, as well as lines of characteristic X-ray emission for transuranium elements. Morton extended his previous work [27] for resonance absorption lines adding technetium, thorium, and uranium [28]. Seth et al. [29] calculated f-f spectra of lanthanide and actinide ions by the multiconfiguration Dirac–Fock configuration interaction (MCDF-CI) method considering uranium V, praseodymium IV, neptunium IV, promethium IV, americium IV, and europium IV ions.

We have worked on protactinium IV and uranium V ions. Both of them have the same ground state $5f^2$ $^3H_4$ outside the [Rn] core. The excitation energies and the electric dipole transition parameters such as wavelengths, oscillator strengths, and transition probabilities for protactinium IV and uranium V ions have been calculated using the MCDF method [30]. In the calculations, it is considered also the transverse Breit and QED contributions besides correlation effects. The calculation of heavy atoms requires considering both relativistic effects and electron correlation, resulting in a large configuration state functions (CSF) expansion in the configuration interaction approaches. To investigate the effect of valence correlation, we took the $5f^2$, $6d5f$, $7s5f$, $6d^2$, $7s^2$, and $7p^2$ configurations outside the [Rn] core. The calculation has been performed using the general atomic structure package (GRASP) code which was developed by Dyall et al. [30]. The available data of triple ionized protactinium are so poor and although there are few data for uranium V in literature. The present work is a part of the studies continuing related to lanthanides and actinides ($4f$ and $5f$ elements) [31 – 39]. Reliable data on the energies and transition parameters are fundamental quantities for many scientific applications. These data will be useful especially to start predicting and interpreting the spectral output of uranium V and, especially protactinium IV.

2. Method of Calculation

We have used the multiconfiguration Dirac–Fock (MCDF) method [30] for obtaining some excited levels and electric dipole transition parameters for triply ionized protactinium and four times ionized uranium. We will here introduce this method briefly. In the MCDF method, an atomic state can be expanded as a linear combination of configuration state functions (CSFs),

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

and is optimized usually on the basis of the many-electron Dirac–Coulomb Hamiltonian in the form

$$H_{\mathrm{DC}} = \sum_{i=1}^{N} H_i + \sum_{i\neq j}^{N} \frac{1}{r_{ij}}, \tag{2}$$

where H_i is the one-electron Dirac Hamiltonian including the kinetic energy and the interaction with the

nucleus,

$$H_i = c\sum_{k=1}^{3}\boldsymbol{\alpha}_k\cdot\boldsymbol{p}_k + (\beta_i - 1)c^2 + \frac{Z}{r_i}. \tag{3}$$

In (1), n_c is the number of CSFs, J and P are total angular momentum and parity of the system, respectively; γ_r is a set of quantum numbers to specify CSFs additional to J and P, and $\{c_r(\alpha)\}$ are the mixing coefficients and denote the representation of the atomic state in this state. The CSFs $|\gamma_r PJM\rangle$ are constructed from a product of single electron wave functions through a proper angular momentum coupling and anti-symmetrization of the basis states. $c_r(\alpha)$ and radial orbitals are optimized simultaneously, based on the expectation values $\langle\psi_\alpha|H_{\rm DC}|\psi_\alpha\rangle$ of one or several atomic states in a self-consistent field (SCF) procedure.

Besides the Dirac–Coulomb Hamiltonian, the Breit interaction plays also an important role in understanding the electronic structure of heavy atoms. The Breit interaction arises from the relativistic retardation and the current–current interaction of fast-moving charges,

$$H_{\rm transverse} = -\sum_{i\neq j}^{N}\left(\frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j\cos(\omega_{ij}r_{ij})}{r_{ij}} + (\boldsymbol{\alpha}_i\cdot\nabla_i)\times(\boldsymbol{\alpha}_j\cdot\nabla_j)\frac{\cos(\omega_{ij}r_{ij})-1}{\omega_{ij}^2 r_{ij}}\right). \tag{4}$$

This Hamiltonian can be also interpreted on the exchange of a single transverse photon. Breit contributions are calculated in the low frequency limit ($\omega_{ij}\to 0$) by diagonalizing the Dirac–Coulomb–Breit Hamiltonian matrix.

Another important part are the quantum electrodynamic (QED) contributions. The dominant QED contributions, self-energy and vacuum polarization, are also included in the computations of the transition energy. The finite-nucleus effect is taken into account by assuming an extended Fermi distribution for the nucleus. Both Breit and QED contributions are treated as perturbation and are not included directly in the SCF procedure. Orbitals are here fixed but the mixing coefficients are calculated by diagonalizing the modified Hamiltonian.

The radiative matrix element can be obtained from

$$O_{if} = \langle\psi_{(i)}|\mathbf{O}^{(1)}|\psi_{(f)}\rangle \tag{5}$$

using the MCDF wavefunctions, where $\mathbf{O}^{(1)}$ is the electric dipole interaction operator. It is well known that the strongest transition is the electric dipole ($E1$) radiation.

For spontaneous emission, the transition probability from an upper state to a lower state is defined as

$$A_{if} = \frac{4e^2\omega^3}{3\hbar^3c^3}\left|\langle\psi_i|\sum_{r_j} r_j|\psi_f\rangle\right|^2, \tag{6}$$

where $\omega = (E_i - E_f)/\hbar$ is the angular frequency with the total energies E. This is called the dipole or $E1$ transition matrix element in the length form. The dipole oscillator strength is

$$f_{if} = \frac{mc^3 g_i}{2e^2\omega^2 g_f}A_{if}, \tag{7}$$

and the weighted oscillator strength or gf-value is given as

$$(gf)_{if} = g_f f_{fi} = -g_i f_{if}, \tag{8}$$

where g is the multiplicity of the respective state.

3. Results and Discussion

We have presented a multiconfiguration Dirac–Fock study on the low-lying level structure of protactinium IV and uranium V ions. The excitation energies and wavelengths, weighted oscillator strengths and transition probabilities of electric dipole (E^1) transitions for these ions have been calculated. The calculation has been performed using the widely-used atomic structure package GRASP [30] based on the multiconfiguration Dirac–Fock method [30, 40 – 42].

Triply ionized protactinium and four times ionized uranium have a rather simple electronic structure with two electrons moving in the resultant field of the nucleus and the 86 inner electrons. For this reason the electron correlation effect is important. In addition, relativistic effects must normally play a role. For heavy ions such as multiply ionized rare-earth (lanthanides and actinides), the consideration of both intervalence and core–valence correlation is essential for atomic structure calculations. In this study we investigated only the valence correlation and the transverse Breit and QED contributions.

In Tables 1 and 2, the level energies have been presented for protactinium IV and uranium V, respectively. In these tables, columns represent the MCDF energies E^0, the transverse Breit contribution E^1, the

Table 1. MCDF E^0, Breit contributions E^1, QED contributions E^2, other works values E^{Other}, and leading percentages of levels for protactinium IV.

Levels		E^0 [cm^{-1}]	E^1 [cm^{-1}]	E^2 [cm^{-1}]	E^{Other} [cm^{-1}]	Leading percentages	
$5f^2$	$^3H_4$	0.00	0.00	0.00	0.00[a,b]	$91.68+7.75$	$5f^2\ ^1G_4$
	$^3H_5$	3976.11	−225.87	$7.12\cdot10^{-5}$	4195[a]	100.00	
	$^3H_6$	7776.79	−420.61	$1.04\cdot10^{-4}$	7907[a]	$98.83+1.17$	$5f^2\ ^1I_6$
	$^3F_2$	4430.64	−47.37	$-1.35\cdot10^{-3}$	2878[a]	$91.33+6.17$	$5f^2\ ^1D_2$
	$^3F_3$	7440.63	−396.09	$-3.03\cdot10^{-2}$	6097[a]	$61.10+35.71$	$6d5f\ ^1G_4$
	$^3F_4$	12138.99	−459.45	$-7.66\cdot10^{-5}$	6573[a]	$55.92+40.75$	$5f^2\ ^1G_4$
	$^3P_0$	18534.09	−128.56	$-5.39\cdot10^{-3}$	11512[a]	$87.57+7.57$	$6d^2\ ^3P_0$
	$^3P_1$	20245.51	−240.20	$-2.56\cdot10^{-3}$	13124[a]	$92.85+7.15$	$6d^2\ ^3P_1$
	$^3P_2$	23091.13	−429.34	$-9.09\cdot10^{-4}$	16516[a]	$73.50+19.73$	$5f^2\ ^1D_2$
	$^1I_6$	22529.54	−293.19	$8.06\cdot10^{-5}$	15558[a]	$98.83+1.17$	$5f^2\ ^3H_6$
	$^1G_4$	7245.36	−220.10	$-4.50\cdot10^{-4}$	11513[a]	$49.91+42.02$	$5f^2\ ^3F_4$
	$^1D_2$	16434.91	−234.38	$-2.19\cdot10^{-3}$	11267[a]	$68.78+19.65$	$5f^2\ ^3P_2$
	$^1S_0$	39583.57	−446.02	$-3.23\cdot10^{-2}$	30274[a], 43613.58[c]	$74.34+19.71$	$6d^2\ ^1S_0$
$6d5f$	$^3H_4^o$	7287.73	−221.70	$-5.89\cdot10^{-4}$	20000[b]	$98.16+1.84$	$6d^2\ ^3F_3$
	$^3H_5^o$	13543.72	−568.31	$-1.65\cdot10^{-2}$	–	$99.88+0.08$	$6d5f\ ^1H_5$
	$^3H_6^o$	18853.04	−762.00	$-5.06\cdot10^{-3}$	–	100.00	
	$^3G_3^o$	15626.13	−406.33	$-4.30\cdot10^{-2}$	–	$87.27+7.21$	$6d5f\ ^1F_3$
	$^3G_4^o$	19841.54	−587.73	$-2.55\cdot10^{-2}$	–	$94.65+3.34$	$6d5f\ ^3F_4$
	$^3G_5^o$	23647.35	−710.03	$-9.32\cdot10^{-3}$	–	$97.84+2.13$	$6d5f\ ^1H_5$
	$^3F_2^o$	9175.74	−394.78	$-1.24\cdot10^{-1}$	–	$82.82+15.19$	$6d5f\ ^1D_2$
	$^3F_3^o$	12846.95	−541.26	$-1.80\cdot10^{-1}$	–	$92.61+3.33$	$6d5f\ ^3G_3$
	$^3F_4^o$	17436.79	−735.12	$-1.52\cdot10^{-1}$	–	$77.45+14.61$	$6d5f\ ^1G_4$
	$^3D_1^o$	20509.42	−436.44	$-2.14\cdot10^{-2}$	–	$92.25+5.20$	$6d5f\ ^1P_1$
	$^3D_2^o$	23358.29	−600.55	$-2.11\cdot10^{-2}$	–	$88.91+6.50$	$6d5f\ ^1D_2$
	$^3D_3^o$	26986.97	−665.41	−3.05	–	$41.25+23.42$	$7s5f\ ^1F_3$
	$^3P_0^o$	25534.70	−510.75	$-5.10\cdot10^{-3}$	–	100.00	
	$^3P_1^o$	25402.78	−503.00	$-9.81\cdot10^{-3}$	–	$90.20+5.28$	$6d5f\ ^1P_1$
	$^3P_2^o$	28367.26	−685.64	$-2.02\cdot10^{-1}$	–	$87.90+8.20$	$6d5f\ ^1D_2$
	$^1H_5^o$	36091.02	−629.79	$-1.37\cdot10^{-2}$	–	$97.79+2.11$	$6d5f\ ^3G_5$
	$^1G_4^o$	11673.04	−555.23	$-2.93\cdot10^{-2}$	–	$47.77+37.70$	$6d5f\ ^3H_4$
	$^1F_3^o$	22744.27	−571.43	$-5.20\cdot10^{-1}$	–	$41.16+45.40$	$6d5f\ ^3D_3^o$
	$^1D_2^o$	17961.14	−570.04	$-9.03\cdot10^{-2}$	–	$70.10+14.82$	$6d5f\ ^3F_2$
	$^1P_1^o$	38287.21	−695.72	$-8.44\cdot10^{-3}$	–	$89.52+7.24$	$6d5f\ ^3P_1$
$7s5f$	$^3F_2^o$	27402.63	−524.21	−8.05	37000[b]	$96.11+2.15$	$6d5f\ ^3P_2$
	$^3F_3^o$	28997.60	−621.33	−5.71	–	$59.59+23.44$	$6d5f\ ^1F_3$
	$^3F_4^o$	33116.17	−762.03	−8.25	–	$98.01+1.95$	$6d5f\ ^3F_4$
	$^1F_3^o$	34980.36	−745.82	−7.40	–	$67.28+20.69$	$7s5f\ ^3F_3$
$6d^2$	$^3F_2$	45804.80	−769.88	$-5.46\cdot10^{-2}$	45000[b]	$91.49+5.82$	$6d^2\ ^1D_2$
	$^3F_3$	50175.60	−899.39	$-3.39\cdot10^{-2}$	–	$98.16+1.84$	$5f^2\ ^3F_3$
	$^3F_4$	54196.13	−981.70	$-2.07\cdot10^{-2}$	–	$91.26+7.15$	$6d^2\ ^1G_4$
	$^3P_0$	58501.64	−762.83	$-9.60\cdot10^{-2}$	–	$89.06+6.41$	$5f^2\ ^3P_0$
	$^3P_1$	60300.62	−855.88	$-4.64\cdot10^{-2}$	–	$92.75+7.14$	$5f^2\ ^3P_1$
	$^3P_2$	65006.28	−1008.93	$-9.73\cdot10^{-3}$	–	$58.77+34.10$	$6d^2\ ^1D_2$

Table 1. Continued.

Levels		E^0 [cm^{-1}]	E^1 [cm^{-1}]	E^2 [cm^{-1}]	E^{Other} [cm^{-1}]	Leading percentages	
	$^1G_4$	63193.27	−967.08	$-2.34\cdot10^{-2}$	–	$91.25+7.16$	$6d^2\ {}^3F_4$
	$^1D_2$	58410.11	−854.67	$-5.01\cdot10^{-2}$	–	$54.67+34.26$	$6d^2\ {}^3P_2$
	$^1S_0$	82911.85	−899.97	−4.87	–	$54.38+28.35$	$7s^2\ {}^1S_0$
$7s^2$	$^1S_0$	99645.54	−1001.46	−12.13	–	$67.89+22.51$	$6d^2\ {}^1S_0$
$7p^2$	$^3P_0$	179654.75	−818.77	−25.23	–	$87.70+10.50$	$7p^2\ {}^1S_0$
	$^3P_1$	188715.02	−1001.87	−13.11	–	$99.89+0.11$	$6d^2\ {}^3P_1$
	$^3P_2$	192406.73	−1014.01	−12.30	–	$56.20+43.68$	$7p^2\ {}^1D_2$
	$^1D_2$	206415.51	−1209.77	$7.61\cdot10^{-1}$	–	$56.19+43.72$	$7p^2\ {}^3P_2$
	$^1S_0$	219800.68	−1185.78	$-7.96\cdot10^{-1}$	–	$85.02+11.79$	$7p^2\ {}^3P_0$

[a] http://www.lac.u-psud.fr/Database/Contents.html [1], [b] Brewer [3], [c] Van Deurzen et al. [21].

Table 2. MCDF E^0, Breit contributions E^1, QED contributions E^2, other works values E^{Other}, and leading percentages of levels for uranium V.

Levels		E^0 [cm^{-1}]	E^1 [cm^{-1}]	E^2 [cm^{-1}]	E^{Other} [cm^{-1}]	Leading percentages	
$5f^2$	$^3H_4$	0.00	0.00	0.00	0.00[a,b1,c,d,e,f], 24[b2]	$91.10+8.35$	$5f^2\ {}^1G_4$
	$^3H_5$	5539.99	−281.96	$6.30\cdot10^{-5}$	6136.88[a,b1,c,d,e], 6140[b2], 6145.0[c], 6145.2[d], 6145.5[d], 6233[e], 6029[e], 6137[f], 5831[f], 5872[f], 5963[f], 5945[f], 5998[f], 6206[f], 6139[f], 6026[f], 6005[f], 6167[f], 6084[f], 6062[f], 6223[f], 5944[f], 6012[f]	100.00	
	$^3H_6$	10709.35	−516.75	$1.07\cdot10^{-4}$	11513.58[a,b1,c,d,e], 11479[b2], 11508.1[c], 11512.6[d], 11518.1[d], 11711[e], 11354[e], 11514[f], 11240[f], 11270[f], 11332[f], 11280[f], 11382[f], 11459[f], 11574[f], 11375[f], 11357[f], 11380[f], 11433[f], 11414[f], 11406[f], 11097[f], 11116[f]	$98.09+1.91$	$5f^2\ {}^1I_6$
	$^3F_2$	5976.90	−33.36	$-1.77\cdot10^{-4}$	4160.65[a,b1,c,d,e], 4153[b2], 4156.7[c], 4157.1[d], 4163.1[d], 4084[e], 4090[e], 4161[f], 6249[f], 4837[f], 4154[f], 3803[f], 4111[f], 4449[f], 4542[f], 3610[f], 3971[f], 4370[f], 3198[f], 3777[f], 4244[f], 4213[f], 3844[f]	$92.33+7.23$	$5f^2\ {}^1D_2$
	$^3F_3$	9928.31	−259.95	$-2.65\cdot10^{-5}$	8983.53[a,b1,c,d,e], 8995[b2], 8986.3[c], 8984.6[d], 8980.5[d], 9025[e], 8848[e], 8984[f], 10401[f], 9235[f], 8738[f], 8442[f], 8801[f], 9255[f], 9273[f], 8313[f], 8717[f], 9170[f], 7985[f], 8611[f], 9112[f], 8857[f], 8624[f]	$99.82+0.18$	$6d^2\ {}^3F_3$

Table 2. Continued.

Levels		E^0 [cm^{-1}]	E^1 [cm^{-1}]	E^2 [cm^{-1}]	E^{Other} [cm^{-1}]	Leading percentages	
$5f^2$	$^3F_4$	16541.82	−558.76	$8.84 \cdot 10^{-5}$	9433.76[a,b1,c,d,e], 9451[b2], 9436.8[c], 9436.76[c], 9450.76[c], 9697.76[c], 9442.1[d], 9447.6[d], 9585[e], 9399[e], 9434[f], 10278[f], 9710[f], 9118[f], 9029[f], 9474[f], 9793[f], 9768[f], 8712[f], 9428[f], 9715[f], 8436[f], 9373[f], 9665[f], 9405[f], 9278[f]	56.63 + 41.31	$5f^2$ $^1G_4$
	$^3P_0$	24124.97	−86.82	$-7.41 \cdot 10^{-4}$	17128.16[a,b1,c,d,e], 17107[b2], 17128.2[c], 17119.9[d], 17127.3[d], 17471[e], 17460[e], 17128[f], 24963[f], 20475[f], 18060[f], 16627[f], 17249[f], 18353[f], 18902[f], 16352[f], 16761[f], 18066[f], 15266[f], 16163[f], 17690[f], 17609[f], 16199[f]	94.98 + 4.20	$5f^2$ $^1S_0$
	$^3P_1$	26288.51	−234.81	$-3.13 \cdot 10^{-4}$	19818.58[a,b1,c,d,e], 19817[b2], 19819.0[c], 19831.1[d], 19819.3[d], 20145[e], 20016[e], 19819[f], 27155[f], 22707[f], 20653[f], 19215[f], 19785[f], 21050[f], 21347[f], 19126[f], 19311[f], 20777[f], 18092[f], 18741[f], 20470[f], 20243[f], 18942[f]	99.32 + 0.68	$6d^2$ $^3P_1$
	$^3P_2$	30161.58	−490.63	$-2.96 \cdot 10^{-6}$	24652.91[a,b1,c,d,e], 24700[b2], 24651.4[c], 24641.5[d], 24653.4[d], 24979[e], 24648[e], 24652[f], 31219[f], 27010[f], 25080[f], 23858[f], 24658[f], 5617[f], 26093[f], 23628[f], 24211[f], 25317[f], 22676[f], 23796[f], 25060[f], 24576[f], 23379[f]	75.94 + 22.62	$5f^2$ $^1D_2$
$5f^2$	$^1I_6$	26803.60	−373.42	$7.76 \cdot 10^{-5}$	22276.05[a,b1,c,d,e], 22281[b2], 22276.4[c], 22276.2[d], 22276.3[d], 22581[e], 22319[e], 22276[f], 26954[f], 25439[f], 24762[f], 24025[f], 23433[f], 24053[f], 23138[f], 24221[f], 22651[f], 23452[f], 24030[f], 22086[f], 23103[f], 22730[f], 22131[f]	98.09 + 1.91	$5f^2$ $^3H_6$
	$^1G_4$	9807.47	−263.16	$-2.88 \cdot 10^{-5}$	16655.73[a,b1,c,d,e], 16640[b2], 16653.8[c], 16650.2[d], 16652.2[d], 6929[e], 6529[e], 6656[f], 17344[f], 16731[f], 16114[f], 16035[f], 16634[f], 16725[f], 16943[f], 15675[f], 16598[f], 16621[f], 15394[f], 16608[f], 16562[f], 16009[f], 15853[f]	50.12 + 42.66	$5f^2$ $^3F_4$

Table 2. Continued.

Levels		E^0 [cm^{-1}]	E^1 [cm^{-1}]	E^2 [cm^{-1}]	E^{Other} [cm^{-1}]	Leading percentages	
	$^1D_2$	21509.87	−241.29	$-3.55\cdot10^{-4}$	16465.30[a,b1,c,d,e], 16438[b2], 16467.1[c], 16462.8[d], 16454.4[d], 16554[e], 16407[e], 16465[f], 22281[f], 18652[f], 16853[f], 15909[f], 16601[f], 17573[f], 17801[f], 15572[f], 16185[f], 17293[f], 14722[f], 15764[f], 17041[f], 16808[f], 15816[f]	$69.59+23.20$	$5f^2\ ^3P_2$
	$^1S_0$	54131.71	−386.52	$-1.39\cdot10^{-3}$	43613.58[a,b1,d], 45812[b2], 45153.6[c], 43614.2[d], 43613.7[d], 46230[e], 46059[e], 43614[f], 57043[f], 51343[f], 41363[f], 43080[f], 46230[f], 47431[f], 47955[f], 40181[f], 45614[f], 46595[f], 38482[f], 45319[f], 46124[f], 45768[f], 43847[f]	$93.12+4.33$	$5f^2\ ^3P_0$
$6d5f$	$^3H_4^o$	48757.79	−482.99	$-4.02\cdot10^{-2}$	59183.36[a,b1], 59256[b2]	$61.96+34.56$	$6d5f\,^1G_4^o$
	$^3H_5^o$	57052.64	−702.12	$-2.33\cdot10^{-2}$	67606.40[a,b1], 67609[b2]	$99.78+0.18$	$6d5f\,^3G_5^o$
	$^3H_6^o$	64291.99	−942.57	$-7.00\cdot10^{-3}$	75272.66[a,b1], 75228[b2]	100.00	
	$^3G_3^o$	54832.85	−556.33	$-5.90\cdot10^{-2}$	63052.78[a,b1], 63047[b2]	$45.77+45.34$	$6d5f\,^3F_3^o$
	$^3G_4^o$	61035.02	−761.07	$-3.39\cdot10^{-2}$	69700.18[a,b1], 69720[b2]	$67.46+26.53$	$6d5f\,^3F_4^o$
	$^3G_5^o$	66794.74	−863.88	$-1.34\cdot10^{-2}$	75008.57[a,b1], 74996[b2]	$95.55+4.32$	$6d5f\,^1H_5^o$
	$^3F_2^o$	50245.14	−474.51	$-6.11\cdot10^{-2}$	59639.66[a,b1], 59582[b2]	$78.90+19.20$	$6d5f\,^1D_2^o$
	$^3F_3^o$	56653.82	−606.13	$-4.31\cdot10^{-2}$	67032.57[a,b1], 67055[b2]	$53.28+43.30$	$6d5f\,^3G_3^o$
	$^3F_4^o$	62749.23	−871.37	$-3.46\cdot10^{-2}$	73844.70[a,b1], 73853[b2]	$52.70+32.25$	$6d5f\,^3G_4^o$
	$^3D_1^o$	61965.88	−519.35	$-3.19\cdot10^{-2}$	68053.98[a,b1], 68035[b2]	$87.66+7.97$	$6d5f\,^1P_1^o$
	$^3D_2^o$	66125.03	−744.37	$-3.01\cdot10^{-2}$	72689.11[a,b1], 72715[b2]	$82.57+8.58$	$6d5f\,^1D_2^o$
	$^3D_3^o$	65343.31	−701.37	$-6.18\cdot10^{-2}$	72773.13[a,b1], 72741[b2]	$51.63+39.72$	$6d5f\,^1F_3^o$
	$^3P_0^o$	69278.37	−630.57	$-7.06\cdot10^{-3}$	75207.79[a,b1], 75183[b2]	100.00	
	$^3P_1^o$	68816.23	−618.03	$-1.25\cdot10^{-2}$	74740.33[a,b1], 74754[b2]	$85.21+8.08$	$6d5f\,^3D_1^o$
	$^3P_2^o$	73018.23	−863.67	$-1.67\cdot10^{-2}$	79219.37[a,b1], 79235[b2]	$84.19+12.15$	$6d5f\,^1D_2^o$
	$^1H_5^o$	79241.24	−790.71	$-1.79\cdot10^{-2}$	83416.15[a,b1], 83417[b2]	$95.64+4.28$	$6d5f\,^3G_5^o$
	$^1G_4^o$	54507.09	−686.24	$-2.89\cdot10^{-2}$	65538.11[a,b1], 65502[b2]	$46.48+36.39$	$6d5f\,^3H_4^o$
	$^1F_3^o$	72517.96	−927.98	$-1.00\cdot10^{-1}$	80997.23[a,b1], 81011[b2]	$47.92+47.31$	$6d5f\,^3D_3^o$
	$^1D_2^o$	61162.59	−690.89	$-2.72\cdot10^{-2}$	69277.42[a,b1], 69309[b2]	$60.04+19.69$	$6d5f\,^3F_2^o$
	$^1P_1^o$	83378.17	−877.89	$-1.03\cdot10^{-2}$	88914.24[a,b1], 88919[b2]	$85.31+10.43$	$6d5f\,^3P_1^o$
$7s5f$	$^3F_2^o$	85322.76	−653.23	−7.93	94069.63[a,b1], 94085[b2]	$99.50+0.47$	$6d5f\,^3F_2^o$
	$^3F_3^o$	86075.78	−660.56	−7.89	94614.33[a,b1], 94598[b2]	$68.95+29.96$	$7s5f\,^1F_3^o$
	$^3F_4^o$	92741.88	−949.88	−7.93	101611.74[a,b1], 101603[b2]	$99.47+0.52$	$6d5f\,^3F_4^o$
	$^1F_3^o$	93989.88	−943.30	−7.89	102407.49[a,b1], 102416[b2]	$68.40+30.56$	$7s5f\,^3F_3^o$
$6d^2$	$^3F_2$	128885.93	−954.56	$-7.87\cdot10^{-2}$	137608.14[a,b1], 137607.92[b1], 137667[b2]	$89.94+9.27$	$6d^2\ ^1D_2$
	$^3F_3$	135302.76	−1120.10	$-4.77\cdot10^{-2}$	145207.84[a,b1], 45200[b2]	$99.82+0.18$	$5f^2\ ^3F_3$
	$^3F_4$	140603.06	−1208.30	$-3.17\cdot10^{-2}$	151303.77[a,b1], 151227[b2]	$87.86+11.96$	$6d^2\ ^1G_4$
	$^3P_0$	141248.29	−988.320	$-1.19\cdot10^{-1}$	147608[b2]	$92.36+6.50$	$6d^2\ ^1S_0$
	$^3P_1$	144813.23	−1111.54	$-5.65\cdot10^{-2}$	152859[b2]	$99.27+0.68$	$5f^2\ ^3P_1$

Table 2. Continued.

Levels		E^0 [cm^{-1}]	E^1 [cm^{-1}]	E^2 [cm^{-1}]	E^{Other} [cm^{-1}]	Leading percentages	
	$^3P_2$	151957.14	−1291.95	$-1.43\cdot10^{-2}$	152992[b2]	$56.20+40.99$	$6d^2\ ^1D_2$
	$^1G_4$	150497.69	−1217.00	$-3.01\cdot10^{-2}$	159721.20[b1], 159669[b2]	$87.81+11.97$	$6d^2\ ^3F_4$
	$^1D_2$	143028.38	−1102.87	$-5.95\cdot10^{-2}$	163980[b2]	$49.12+42.59$	$6d^2\ ^3P_2$
	$^1S_0$	170544.04	−1217.85	$-5.84\cdot10^{-1}$	175883[b2]	$87.46+6.80$	$6d^2\ ^3P_0$
$7s^2$	$^1S_0$	217584.68	−1315.62	−15.68	–	$93.59+3.14$	$7p^2\ ^1S_0$
$7p^2$	$^3P_0$	316156.81	−986.77	−35.72	–	$84.88+13.65$	$7p^2\ ^1S_0$
	$^3P_1$	329600.30	−1240.18	−17.83	–	$99.95+0.05$	$6d^2\ ^3P_1$
	$^3P_2$	333808.56	−1250.92	−17.09	–	$51.87+48.08$	$7p^2\ ^1D_2$
	$^1D_2$	352543.35	−1518.18	1.87	–	$51.86+48.10$	$7p^2\ ^3P_2$
$7p^2$	$^1S_0$	366388.66	−1495.70	$3.78\cdot10^{-1}$	–	$83.03+14.77$	$7p^2\ ^3P_0$

[a] http://www.lac.u-psud.fr/Database/Contents.html [1] (The values compiled from [19]), [b1,b2] Wyart et al. [19], [c] Goldschmidt [20], [d] Van Deurzen et al. [21], [e] Eliav et al. [25], [f] Seth et al. [29].

Table 3. Wavelengths λ, weighted oscillator strengths gf-value, and transition rates A, for $E1$ transitions to the $5f^2\ ^3H_4$ ground level in protactinium IV and uranium V. Comparison values for wavelengths of uranium V ion are taken from reference [19].

Level	Pa IV			U V			
	λ [Å]	gf-value	A [s^{-1}]	λ [Å]	[19]	gf-value	A [s^{-1}]
$6d5f\ ^3H^o_4$	14 195.44	$5.20\cdot10^{-2}$	$1.91\cdot10^{5}$	2071.47	1689.662	$2.59\cdot10^{-1}$	$4.47\cdot10^{7}$
$6d5f\ ^3H^o_5$	7706.89	$3.64\cdot10^{-3}$	$3.72\cdot10^{4}$	1774.60	1479.153	$1.07\cdot10^{-2}$	$2.07\cdot10^{6}$
$6d5f\ ^3G^o_3$	6570.40	$4.25\cdot10^{-1}$	$9.38\cdot10^{6}$	1842.41	–	$5.42\cdot10^{-1}$	$1.52\cdot10^{8}$
$6d5f\ ^3G^o_4$	5193.78	$2.25\cdot10^{-2}$	$6.20\cdot10^{5}$	1659.09	1434.717	$2.18\cdot10^{-2}$	$5.89\cdot10^{6}$
$6d5f\ ^3G^o_5$	4359.70	$5.34\cdot10^{-5}$	$1.70\cdot10^{3}$	1516.74	–	$4.58\cdot10^{-5}$	$1.20\cdot10^{4}$
$6d5f\ ^3F^o_3$	8126.44	$1.58\cdot10^{-2}$	$2.28\cdot10^{5}$	1784.19	1491.809	$5.69\cdot10^{-1}$	$1.70\cdot10^{8}$
$6d5f\ ^3F^o_4$	5987.48	$1.14\cdot10^{-4}$	$2.36\cdot10^{3}$	1616.08	1354.191	$2.38\cdot10^{-2}$	$6.75\cdot10^{6}$
$6d5f\ ^3D^o_3$	3799.60	$4.66\cdot10^{-4}$	$3.08\cdot10^{4}$	1546.98	1374.131	$6.42\cdot10^{-3}$	$2.55\cdot10^{6}$
$6d5f\ ^1H^o_5$	2819.98	$3.29\cdot10^{-5}$	$2.51\cdot10^{3}$	1274.68	–	$1.25\cdot10^{-3}$	$4.68\cdot10^{5}$
$6d5f\ ^1G^o_4$	8994.60	$8.87\cdot10^{-3}$	$8.12\cdot10^{4}$	1858.01	1525.833	$2.48\cdot10^{-2}$	$5.33\cdot10^{6}$
$6d5f\ ^1F^o_3$	4510.12	$2.66\cdot10^{-3}$	$1.24\cdot10^{5}$	1396.84	–	$5.98\cdot10^{-4}$	$2.92\cdot10^{5}$
$7s5f\ ^3F^o_3$	3524.78	$1.39\cdot10^{-5}$	$1.06\cdot10^{3}$				
$7s5f\ ^3F^o_4$	3091.58	$3.31\cdot10^{-5}$	$2.57\cdot10^{3}$				
$7s5f\ ^1F^o_3$	2921.65	$5.41\cdot10^{-4}$	$6.04\cdot10^{4}$				

quantum electrodynamic contribution E^2, and comparison values in the available literature E^{Other}, respectively. The leading percentages to level have been placed into last column. In addition, only odd-parity levels are indicated with the superscript "o" in the tables.

We have taken the $5f^2$, $6d5f$, $7s5f$, $6d^2$, $7s^2$, and $7p^2$ configurations outside the [Rn] core for correlation. It can be seen from Table 1 that our results are somewhat in agreement with others, especially for some levels of $5f^2$ and $6d^2$ configurations. Of course, if we would have taken into account the core correlations, it is clear that the results would have been in better agreement. In Table 2, the E^0 results for uranium V are better than those of protactinium IV. For improving the results, it is necessary to select the configurations according to the core correlations (core–core and core–valence), and to include $5g$, $7p$, and $8s$ orbitals. In this case, the number of possible interacting configurations to be introduced in the model is rapidly increasing, and the computer limits quickly impose severe restrictions to that approach.

It is also required to consider the transverse Breit and QED contributions besides the correlations. Calculation of many-electron relativistic corrections is the most difficult problem to deal with in high-precision

energy level predictions in heavy ions. These corrections include two contributions: i) the vacuum polarization, for which effective potentials can be deduced from QED, ii) the self-energy, the first-order contribution of which is known exactly (i.e. to all orders in the external field strength $Z\alpha$) only for hydrogen-like ions. Some approximations are also known for very heavy atoms and for very light ions. None of these corrections can be neglected for a precise comparison with experimental results.

Spectroscopic parameters are fundamental characteristics of excited states of atoms and ions. They are very useful in the fields of quantum electronic, atomic physics, and laser spectroscopy, plasma physics and astrophysics. We have obtained 279 electric dipole transitions for both ions. Wavelengths λ, weighted oscillator strengths gf-value, and transition rates (or probabilities) A for $6d5f\ ^3H^o_{4,5}$, $^3G^o_{3,4,5}$, $^3F^o_{3,4}$, $^3D^o_3$, $^1H^o_5$, $^1G^o_4$, $^1F^o_3$, $7s5f\ ^3F^o_{3,4}$, $^1F^o_3$ – $5f^2\ ^3H_4$ for protactinium IV and $6d5f\ ^3H^o_{4,5}$, $^3G^o_{3,4,5}$, $^3F^o_{3,4}$, $^3D^o_3$, $^1H^o_5$, $^1G^o_4$, $^1F^o_3$ – $5f^2\ ^3H_4$ for uranium V are given in Table 3. These parameters include the transverse Breit and QED contributions. We did not find any values in the available literature for these transitions of the protactinium IV ion. The wavelength, obtained from this work, can be compared with experimental values in [19] for uranium V ion. And it is seen that the agreement is somewhat good (accurately $\lambda - \lambda_{[19]} \sim 200$ Å) for the most transitions.

4. Conclusion

In this work, the low-lying level structure of protactinium IV ($Z = 91$) and uranium V ($Z = 92$) has been calculated by using the MCDF atomic code, GRASP [30]. Excitation energies of levels and electric dipole transition parameters between these levels have been investigated in the framework of Breit and QED contributions and are presented in tables. It is clear that other calculations and experimental analysis are required for comparing our results. We think that the results obtained from this work, in particular for electric dipole transitions, will be useful for the theoretical and experimental studies for the level structure of these ions, especially protactinium IV, in future.

[1] http://www.lac.u-psud.fr/Database/Contents.html.
[2] T. A. Carlson, C. W. Nestor, N. Wasserman Jr., and J. D. McDowell, At. Data Nucl. Data Tables **63**, 2 (1970).
[3] L. Brewer, J. Opt. Soc. Am. **61**, 1666 (1971).
[4] K. D. Sen and A. Puri, Chem. Phys. Lett. **505**, 156 (1989).
[5] W. Liu, W. Küchle, and M. Dolg, Phys. Rev. A **58**, 1103 (1998).
[6] X. Cao and M. Dolg, Mol. Phys. **101**, 961 (2003).
[7] G. C. Rodrigues, P. Indelicato, J. P. Santos, P. Patté, and F. Parente, At. Data Nucl. Data Tables **86**, 117 (2004).
[8] J. G. J. Conway, J. Chem. Phys. **31**, 1002 (1959).
[9] R. S. Title, P. P. Sorokin, M. J. Stevenson, G. D. Pettit, J. E. Scardefield, and J. R. Lankard, Phys. Rev. **128**, 62 (1962).
[10] R. A. Satten, C. L. Schreiber, and E. Y. Wong, J. Chem. Phys. **42**, 162 (1965).
[11] D. R. Johnson, R. A. Satten, C. L. Schreiber, and E. Y. Wong, J. Chem. Phys. **44**, 3141 (1966).
[12] L. P. Varga, J. D. Brown, M. J. Reisfeld, and R. D. J. Cowan, J. Chem. Phys. **52**, 4233 (1970).
[13] H. G. Hecht and J. B. Gruber, J. Chem. Phys. **60**, 4872 (1974).
[14] H. G. Hecht and J. B. Gruber, J. Chem. Phys. **63**, 2773 (1975).
[15] J. T. Bell and S. R. Buxton, J. Inorg. Nucl. Chem. **36**, 1575 (1974).
[16] D. J. Mackey, W. A. Runciman, and E. R. Vance, Phys. Rev. B **11**, 211 (1975).
[17] J. P. Desclaux and A. J. Freeman, J. Magn. Magn. Mater. **8**, 119 (1978).
[18] L. Thakur and A. K. Thakur, Indian J. Pure Appl. Phys. **17**, 538 (1979).
[19] J. F. Wyart, V. Kaufman, and J. Sugar, Phys. Scr. **22**, 389 (1980).
[20] Z. B. Goldschmidt, Phys. Rev. A **27**, 740 (1983).
[21] C. H. H. Van Deurzen, K. Rajnak, and J. G. Conway, J. Opt. Soc. Am. B **1**, 45 (1984).
[22] H. M. Grosswhite and H. Crosswhite, J. Opt. Soc. Am. **1**, 246 (1984).
[23] K. Rashid, M. Z. Saadi, and M. Yasin, At. Data Nucl. Data Tables **40**, 365 (1988).
[24] H. U. Rahman, Il. Nuovo Cimento **17**, 1189 (1995).
[25] E. Eliav, U. Kaldor, and Y. Ishikawa, Phys. Rev. A **51**, 225 (1995).
[26] N. A. Kulagin, Opt. Spectrosc. **82**, 194 (1997).
[27] D. Morton, Astrophys. J. Suppl. Ser. **130**, 403 (2000).
[28] D. Morton, Astrophys. J. Suppl. Ser. **132**, 411 (2001).
[29] M. Seth, K. G. Dyall, R. Shepard, and A. Wagner, J. Phys. B: At. Mol. Opt. Phys. **34**, 2383 (2001).
[30] K. G. Dyall, I. P. Grant, C. T. Johnson, F. A. Parpia, and E. P. Plummer, Comput. Phys. Commun. **55**, 425 (1989).

[31] L. Özdemir and G. Ürer, Acta Phys. Pol. A **118**, 563 (2010).
[32] G. Ürer and L. Özdemir, Arab. J. Sci. Eng. A doi:10.1007/s13369-011-0154-5.
[33] G. Ürer and L. Özdemir, Chinese J. Phys. **49**, 1178 (2011).
[34] G. Ürer, L. Özdemir, and B. Karaçoban, Balkan Phys. Lett. **18**, 383 (2010).
[35] B. Karaçoban, L. Özdemir, and G. Ürer, Balkan Phys. Lett. **18**, 393 (2010).
[36] B. Karaçoban and L. Özdemir, J. Quant. Spectrosc. Radiat. Transf. **109**, 1968 (2008).
[37] B. Karaçoban and L. Özdemir, Acta. Phys. Pol. A **113**, 1609 (2008).
[38] B. Karaçoban and L. Özdemir, Cent. Eur. J. Phys. **9**, 800 (2011).
[39] B. Karaçoban and L. Özdemir, Arab. J. Sci. Eng. **36**, 635 (2011).
[40] I. P. Grant, Adv. Phys. **19**, 747 (1970).
[41] I. P. Grant, J. Phys. B **7**, 1458 (1974).
[42] I. P. Grant, Relativistic Quantum Theory of Atoms and Molecules, Springer, New York 2007.