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The excitation energies, ionization potentials and oscillator strengths of neutral and ionized species of Uub (Z = 112) and the homologue elements Zn, Cd and Hg

Y.J. Yu[1], J.G. Li[1], C.Z. Dong[1,2,a], X.B. Ding[1], S. Fritzsche[3], and B. Fricke[3]

[1] College of Physics and Electronic Engineering, Northwest Normal University, 730070 Lanzhou, P.R. China
[2] National Laboratory of Heavy Ion Accelerator of Lanzhou, 730000 Lanzhou, P.R. China
[3] Institut für Physik, Universität Kassel, 34132 Kassel, Germany

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Abstract. Multi-configuration Dirac-Fock method (MCDF) is employed to calculate excitation energies, ionization potentials and oscillator strengths for all neutral and up to 5 times ionized species of element Uub, as well as the homologue elements Zn, Cd and Hg. On the basis of not too extended MCDF calculations, we studied some peculiar properties of element Uub resulting from its stronger relativistic and electron correlation effects. Using an extrapolative scheme, improved ionization potentials of Uub were obtained with an uncertainty of less than 0.5 eV. Furthermore, we calculated the low-lying resonance excitation energies, absorption oscillator strengths and the first ionization potential for Hg and Uub using large scale MCDF calculations, which improved the uncertainty of the excitation energies to less than 0.25 eV for element Hg. We hope that such calculations yield good results for element Uub.

PACS. 31.25.Jf Electron correlation calculations for atoms and ions: excited states – 32.70.Cs Oscillator strengths, lifetimes, transition moments

1 Introduction

Nowadays some super-heavy elements and their isotopes were produced in “cold fusion” [1], or in “hot fusion” [2], however, identification of the new elements and their isotopes is an important problem at all times. Generally, the new elements are identified by measuring α-spectra from known decay products. But this method does not work when the α-decay chain of some super-heavy elements does not end in the region of known isotopes [3]. Another disadvantage is that the isotopes of super-heavy elements are close to proton drip-line making it increasingly more difficult to identify such new elements [4].

A second method for identification might be the chemical behaviour [4–7]. But this experimental work on the chemical properties of super-heavy elements is very difficult because of their short half-life and very low production rates. Therefore the chemistry of these elements (at least nowadays) is restricted to one atom at a time. Despite this difficulty one was able to get a first glance on the chemical properties of these elements up to $Z = 108$ [8]. It has been found that these elements fit into the periodic table, but do not follow completely the trends for lighter homologue in the chemical groups due to strong relativistic effects [9,10].

A third method might be an identification via spectroscopy either in the region of X-rays [11] or the observation of optical resonance lines [12]. In any case the prediction of chemical and physical properties for superheavy elements is highly desirable. The basic theories are quantum-chemical atomic structure calculations. Such theoretical predictions of the chemistry and structure of superheavy elements have been performed since the early 70s. The result was that the general behaviour continues as expected from the normal extension of the periodic system up to element $Z = 121$, whereas drastic changes appear in the region beyond [13,14].

First observation of element Uub ($Z = 112$) was made a few years ago by the GSI laboratory, Darmstadt [15]. Due to the already mentioned reasons and the necessity to confirm the recent observation of some decay chains and fission products associated with the production of elements 114 [2,16] and 116 [17], many experiments have been performed to search for their chemical and physical properties [8]. As mentioned above, the two possible methods are either chemistry or spectroscopy. Concerning the chemistry of this element Uub, several groups have tried to measure the adsorption enthalpy on a Au surface in a thermochromatographic column [5,6]. Recent results have been published in the references [18,19]. This still has to be confirmed. Theoretical predictions of the adsorption

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[a] e-mail: `dongcz@nwnu.edu.cn`

energy of element 112 on a Au surface are published in references [20–22].

However, a more direct approach to investigate the element Uub is to study the atomic level schemes, both by experimental and theoretical methods. Recently, great progress has been made in the experimental measurement of atomic structure for element Fm ($Z = 100$) [12,23], and the measurement for Lw ($Z = 101$) is in progress.

In this paper, we present our results of the ground state configurations with their weights, ionization potentials, excitation energies and oscillator strengths for neutral and ionized species of elements Zn, Cd, Hg and Uub using a medium-size multi-configuration Dirac-Fock (MCDF) method and predict some peculiar properties of element Uub. In addition, we calculate the resonance excitation energies, absorption oscillator strengths and the first ionization for Hg and Uub in sophisticated large MCDF calculations and hope that such calculations are helpful for the experimental investigation of the atomic structure of the element Uub. Of course in the literature there are several publications with a few results for these quantities [14,24,25], but this paper is a complete systematic study for all the interesting quantities of the element Uub.

2 Theoretical method

In this study, wave functions have been generated by the widely-used atomic structure package GRASP92 [26] which is an implementation of the multi-configuration Dirac-Fock (MCDF) method. In the MCDF method, an atomic state wavefunction (ASF) is approximated by a linear combination of configuration state functions (CSFs) of the same symmetry

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

where n_c is the number of CSFs and $\{c_r(\alpha)\}$ denotes the representation of the atomic state in this basis. In standard calculations, the CSFs are constructed from antisymmetrized products of a common set of *orthonormal* orbitals which are optimized on the basis of the Dirac-Coulomb Hamiltonian. Further relativistic contributions to the representation $\{c_r(\alpha)\}$ of the atomic states due to the (transverse) Breit interactions were also added by diagonal the Dirac-Coulomb-Breit Hamiltonian matrix [27].

According to the time-dependent perturbation theory, the Einstein spontaneous transition probability for the electric dipole transition from the upper state to the lower state can be given by [28],

$$A_{ik} = \frac{4e^2\omega_{ik}^3}{3\hbar c^3(2j_i+1)}|\langle\Psi_i(\alpha_i J_i P_i M_i)|O^{(1)}|\Psi_k(\alpha_k J_k P_k M_k)\rangle|^2$$

where $O^{(1)}$ is the electric dipole operator, j_i is the total angular momentum of the upper state i, $|\Psi_i(\alpha_i J_i P_i M_i)\rangle$ and $|\Psi_k(\alpha_k J_k P_k M_k)\rangle$ are the wave functions of the upper atomic state i and the lower atomic state k, respectively. Then, absorption oscillator strengths can be obtained from [28],

$$f_{ki} = \frac{\hbar\omega_{ki}}{3(2j_k+1)}|\langle\Psi_k(\alpha_k J_k P_k M_k)|O^{(1)}|\Psi_i(\alpha_i J_i P_i M_i)\rangle|^2$$

where j_k is the total angular momentum of the lower state k, ω_{ki} is frequency of the photon absorbed by an atom from the lower state k to the upper state i.

3 Calculations and discussions

It is well-known that the electron correlation effects are very important for calculating atomic structures of many-electron atoms, especially for the super-heavy elements. However, because the large scale calculations need much more time and are not necessary just for the prediction of fundamental properties for the elements, we calculated some fundamental properties first, including the ground states, ionization potentials and excitation energies for the element Uub, Zn, Cd and Hg within a medium-size MCDF method. Then we calculated the low-lying resonance excitation energies, absorption oscillator strengths and the first ionization potentials for neutral elements Hg and Uub using a large scale calculational model and hope that such calculations are helpful for the experimental investigation of the atomic structure of the element Uub.

3.1 Small-scale MCDF calculations

The atomic structure changes with increasing atomic number, which results in the different physical and chemical properties, especially for super-heavy elements. The major effects on the results come from the numbers of CSF, n_c, in equation (1) which reflects the extent to which electron correlation effects are taken into account. In our calculations, we have restricted ourselves to all possible configurations which can be constructed from the $\{(n-1)d, ns\}$ subshells with single, double, triple and quadruple excitations into $\{(n-1)d, ns, np\}$ ($n = 4$, 5, 6, 7 for Zn, Cd, Hg and Uub, respectively) single particle wave functions for a specific total angular momentum, parity and charge state, and the core of each element is kept fully occupied and the remaining electrons are distributed in all possible ways in the single particle wave functions given above. The cores of the elements Zn are given by the electronic configuration for [Ar], for the element Cd by [Kr], for the element Hg by [Xe]$4f^{14}$ and for the element Uub by [Rn]$5f^{14}$. It can be called SDTQ model. Table 1 lists the number of configurations which are possible and are taken into account in the calculations for the remaining k electrons outside the core for a given angular momentum and parity.

3.1.1 Ground states

In order to find the ground state of each element (Zn, Cd, Hg and Uub) in each charge state we have performed

Table 1. Number of CSF for a given angular momentum J and parity and number of electrons in the $\{(n-1)d, ns, np\}^k$ configurations for the group 12 elements.

J^P	k=12	k=10	k=8	J^P	k=11	k=9	k=7
$J=0^+$	91	188	194	$J=1/2^+$	241	355	255
$J=1^+$	194	430	440	$J=3/2^+$	406	606	429
$J=2^+$	281	628	644	$J=5/2^+$	469	710	497
$J=3^+$	254	605	618	$J=7/2^+$	414	640	437
$J=4^+$	212	523	536	$J=9/2^+$	308	489	325
$J=5^+$	124	336	342	$J=11/2^+$	178	293	186
$J=0^-$	86	170	170	$J=1/2^-$	253	359	253
$J=1^-$	228	466	466	$J=3/2^-$	433	624	433
$J=2^-$	298	629	629	$J=5/2^-$	490	714	490
$J=3^-$	294	639	639	$J=7/2^-$	441	656	441
$J=4^-$	227	525	525	$J=9/2^-$	317	492	317
$J=5^-$	140	352	352	$J=11/2^-$	189	303	189

Table 2. Calculated electronic ground states for Zn, Cd, Hg and Uub in the charge states 0 to 5+ with the dominant weights of their configurations.

Elements	Configurations	J^P	Weights (in %)
Zn	[Ar]$3d^{10}4s^2$	$J=0^+$	94.4
	[Ar]$3d^{10}4p^2$		4.3
Cd	[Kr]$4d^{10}5s^2$	$J=0^+$	94.2
	[Kr]$4d^{10}5p^2$		4.1
Hg	[Xe]$5d^{10}6s^2$	$J=0^+$	94.4
	[Xe]$5d^{10}6p^2$		2.6
	[Xe]$5d^9 6s6p^2$		1.7
Uub	[Rn]$6d^{10}7s^2$	$J=0^+$	94.4
	[Rn]$6d^9 6s7p^2$		2.0
	[Rn]$6d^{10}7p^2$		1.7
Zn^+	[Ar]$3d^{10}4s$	$J=1/2^+$	99.5
Cd^+	[Kr]$4d^{10}5s$	$J=1/2^+$	99.3
Hg^+	[Xe]$5d^{10}6s$	$J=1/2^+$	98.6
Uub^+	[Rn]$6d^9 7s^2$	$J=5/2^+$	95.7
	[Rn]$6d^9 7p^2$		1.7
Zn^{2+}	[Ar]$3d^{10}$	$J=0^+$	99.7
Cd^{2+}	[Kr]$4d^{10}$	$J=0^+$	99.6
Hg^{2+}	[Xe]$5d^{10}$	$J=0^+$	99.1
Uub^{2+}	[Rn]$6d^8 7s^2$	$J=4^+$	96.3
	[Rn]$6d^8 7p^2$		1.6
Zn^{3+}	[Ar]$3d^9$	$J=5/2^+$	99.8
Cd^{3+}	[Kr]$4d^9$	$J=5/2^+$	99.7
Hg^{3+}	[Xe]$5d^9$	$J=5/2^+$	98.9
Uub^{3+}	[Rn]$6d^9$	$J=5/2^+$	61.4
	[Rn]$6d^8 7s$		28.6
	[Rn]$6d^7 7s^2$		8.5
Zn^{4+}	[Ar]$3d^8$	$J=4^+$	99.9
Cd^{4+}	[Kr]$4d^8$	$J=4^+$	99.8
Hg^{4+}	[Xe]$5d^8$	$J=4^+$	99.5
Uub^{4+}	[Rn]$6d^8$	$J=4^+$	95.4
	[Rn]$6d^6 7s^2$		1.8
	[Rn]$6d^7 7s$		1.2
Zn^{5+}	[Ar]$3d^7$	$J=9/2^+$	99.9
Cd^{5+}	[Kr]$4d^7$	$J=9/2^+$	99.9
Hg^{5+}	[Xe]$5d^7$	$J=9/2^+$	99.7
Uub^{5+}	[Rn]$6d^7$	$J=9/2^+$	97.0
	[Rn]$6d^6 7s$		1.8

calculations for each angular momentum and parity with the number of configuration state functions given in Table 1. Table 2 presents our results, including the angular momentum and parity of the ground state for each atom and ion, and the dominant electronic configurations (in the nonrelativistic nomenclature) with their weights. For all calculations, the theoretically determined ground state configurations for the atoms and ions of Zn, Cd and Hg are in agreement with the experimental results given in the tables of Moore [29] as far as they were known. However, for the element Uub there exist some peculiar properties which already have been found in reference [13]. Firstly, for the neutral element Uub, though its ground state is analog to the homologue element, the orbital energies of $7s_{1/2}$ orbital and $6d_{5/2}$ orbital are reverse. This results from the stronger relativistic effects for the element Uub. Secondly, the ground state of Uub^+, which is $6d^4_{3/2}6d^5_{5/2}7s^2 (J = 5/2^+)$, is different from the $(n-1)d^4_{3/2}(n-1)d^6_{5/2}ns (J = 1/2^+)$ (n = 4, 5 and 6 for Zn, Cd and Hg, respectively) for Zn^+, Cd^+ and Hg^+. For Uub^{2+} the dominant configuration is $6d^4_{3/2}6d^4_{5/2}7s^2 (J = 4^+)$, rather than the $d^{10} (J = 0^+)$ for the ground states of the lighter group 12 elements. In addition, with increasing ionization, the inversion of levels between $7s_{1/2}$ and $6d_{5/2}$ orbitals disappears in the monocation and dication, however, because the $7s$ and $6d$ orbitals are very close to each other the configuration interaction among the $6d^9, 6d^8 7s$ and $6d^7 7s^2$ is very strong for the ground state of Uub^{3+}.

3.1.2 Ionization potentials

The ionization potential (IP) reflects the relativistic effects on the atomic structure and is important in the analysis of some chemical properties. In theory, the ionization potentials of an atom (or ion) can be obtained by the differences of the ground state energies for two different charge states of the atom (or ion). Our results of single ionization potentials for elements Zn, Cd, Hg and Uub in the charge states 0 to 5+ are presented in Table 3. The terms and experimental ionization potentials for elements Zn, Cd, Hg as well as other results from references [13,24,25] for element Uub are also presented in this table. As can be seen from Table 3, for element Uub, the difference between our results for the ionization potentials and the values in reference [25], which are Dirac-Coulomb-Breit calculations, is large. In addition there exist very old results from reference [13], which are Dirac-Fock-Slater calculations. The same holds true for the modern coupled cluster results from reference [24] for the first IP.

The results which we have calculated here can be improved by extrapolation methods given in [30,31] where detailed studies of the first superheavy elements 104 to 108

Table 3. Ionization potentials (in eV) for Zn, Cd, Hg and Uub in the charge states 0 to 5+.

Elements	Transitions	Our calc.	Expt. [29]	Extrapolated	Other theory
Zn	$3d^{10}4s^2\ ^1\mathrm{S}_0 \rightarrow 3d^{10}4s\ ^2\mathrm{S}_{1/2}$	8.48	9.39		
Cd	$4d^{10}5s^2\ ^1\mathrm{S}_0 \rightarrow 4d^{10}5s\ ^2\mathrm{S}_{1/2}$	8.07	8.99		
Hg	$5d^{10}6s^2\ ^1\mathrm{S}_0 \rightarrow 5d^{10}6s\ ^2\mathrm{S}_{1/2}$	9.33	10.43		
	extended calc.	10.08			
Uub	$6d^{10}7s^2\ ^1\mathrm{S}_0 \rightarrow 6d^9 7s^2\ ^2\mathrm{D}_{5/2}$	10.75		11.73	11.97 [25]
	extended calc.	11.29			
					11.4 [13]
					11.5 [24]
Zn^{1+}	$3d^{10}4s\ ^2\mathrm{S}_{1/2} \rightarrow 3d^{10}\ ^1\mathrm{S}_0$	16.85	17.96		
Cd^{1+}	$4d^{10}5s\ ^2\mathrm{S}_{1/2} \rightarrow 4d^{10}\ ^1\mathrm{S}_0$	15.62	16.90		
Hg^{1+}	$5d^{10}6s\ ^2\mathrm{S}_{1/2} \rightarrow 5d^{10}\ ^1\mathrm{S}_0$	17.73	18.75		
Uub^{1+}	$6d^9 7s^2\ ^2\mathrm{D}_{5/2} \rightarrow 6d^8 7s^2\ ^3\mathrm{F}_4$	20.84		21.98	22.49 [25]
					21.1 [13]
Zn^{2+}	$3d^{10}\ ^1\mathrm{S}_0 \rightarrow 3d^9\ ^2\mathrm{D}_{5/2}$	37.46	39.70		
Cd^{2+}	$4d^{10}\ ^1\mathrm{S}_0 \rightarrow 4d^9\ ^2\mathrm{D}_{5/2}$	36.07	37.47		
Hg^{2+}	$5d^{10}\ ^1\mathrm{S}_0 \rightarrow 5d^9\ ^2\mathrm{D}_{5/2}$	32.56	34.20		
Uub^{2+}	$6d^8 7s^2\ ^3\mathrm{F}_4 \rightarrow 6d^9\ ^2\mathrm{D}_{5/2}$	30.86		32.62	32.8 [13]
Zn^{3+}	$3d^9\ ^2\mathrm{D}_{5/2} \rightarrow 3d^8\ ^3\mathrm{F}_4$	56.76			
Cd^{3+}	$4d^9\ ^2\mathrm{D}_{5/2} \rightarrow 4d^8\ ^3\mathrm{F}_4$	50.70			
Hg^{3+}	$5d^9\ ^2\mathrm{D}_{5/2} \rightarrow 5d^8\ ^3\mathrm{F}_4$	46.44			
Uub^{3+}	$6d^9\ ^2\mathrm{D}_{5/2} \rightarrow 6d^8\ ^3\mathrm{F}_4$	42.36			
Zn^{4+}	$3d^8\ ^3\mathrm{F}_4 \rightarrow 3d^7\ ^4\mathrm{F}_{9/2}$	81.10			
Cd^{4+}	$4d^8\ ^3\mathrm{F}_4 \rightarrow 4d^7\ ^4\mathrm{F}_{9/2}$	68.17			
Hg^{4+}	$5d^8\ ^3\mathrm{F}_4 \rightarrow 5d^7\ ^4\mathrm{F}_{9/2}$	61.64			
Uub^{4+}	$6d^8\ ^3\mathrm{F}_4 \rightarrow 6d^7\ ^4\mathrm{F}_{9/2}$	54.92			

have been published. We obtain more accurate ionization potentials for Uub, Uub^+ and Uub^{2+} which are 11.73 eV, 21.98 eV and 32.62 eV, respectively. These values are also included in Table 3. This extrapolation leads to ionization potentials for element Uub probably within an uncertainty of 0.5 eV. At the same time we find that the ionization potentials for Uub and Uub^+ are larger than for the lighter homologue elements, which indicates that in the group 12, element Uub is stronger chemically inert than e.g. Hg.

3.1.3 Resonance excitation energies and oscillator strengths

The excitation energies are helpful to analyze the chemical properties of the super-heavy elements [25,32], and are also needed in the atomic spectra measurement [12,23]. We calculated the resonance excitation energies and absorption oscillator strengths for Zn, Cd, Hg and Uub in all neutral and up to 5 times ionized species using Reos99 [33]. As can be seen from Table 4, our results are in agreement with experimental values for Zn, Cd and Hg, however, the difference increases with the charge state due to the same reasons like the results of ionization potentials. For the oscillator strengths, we present our results with length gauge and velocity gauge respectively, and the values in two gauges are consistent with each other. Moreover, the results for Cd and Hg are in good agreement with the experiments values given in references [34,35]. This further indicates that our wave functions for the calculation of the element Uub are appropriate.

3.2 Extended MCDF calculations

From above results we have found some peculiar properties for Uub, however, these results may not be precise enough for the prediction of the energy levels in an experiment. Moreover, as the super-heavy elements have to be produced on-line in nuclear collisions, the success of such experiments depends vitally on the quality of the theoretical predictions, from which the search for new lines starts. Therefore, we have calculated the five lowest resonance lines including virtual excitation within an increasing set of valence shells for Uub. Based on the SDTQ model, we also included the CSFs formed by single and double substitution from the three $6d^{10}7s^2$, $6d^{10}7s7p$ and $6d^9 7s^2 7p$ reference configurations to the active set $\{6d, 7s, 7p, 8s, 8p, 5g, 6f, 7d, 6g\}$. Similar computations have been performed for Hg with all the principle quantum numbers reduced by one. These results are presented in Tables 5 and 6.

As can be seen from Tables 5 and 6, we give more precise results for the low excitation energies and resonant oscillator strengths. For the values of the excitation energies, the uncertainty was improved to less than 0.25 eV for Hg and we hope that such calculations can reach the same uncertainty for Uub and the results are helpful for experimental investigation of atomic structure of the element Uub.

In addition, the first ionization potentials of Hg and Uub have been calculated using the extended MCDF

Table 4. Calculated resonance excitation energies (in eV) and oscillator strengths for Zn, Cd, Hg and Uub in the charge states 0 to 5+. (L: length gauge, V: velocity gauge).

		Transition energies		Oscillator strengths		
Elements	Transitions	Our calc.	Expt. [29]	L	V	Expt.
Zn	$3d^{10}4s^2\ ^1\mathrm{S}_0 \to 3d^{10}4s4p\ ^3\mathrm{P}_1$	4.05	4.03	1.84×10^{-4}	4.69×10^{-4}	
Cd	$4d^{10}5s^2\ ^1\mathrm{S}_0 \to 4d^{10}5s5p\ ^3\mathrm{P}_1$	3.67	3.80	1.20×10^{-3}	1.85×10^{-3}	$(2.00 \pm 0.003) \times 10^{-3a}$
Hg	$5d^{10}6s^2\ ^1\mathrm{S}_0 \to 5d^{10}6s6p\ ^3\mathrm{P}_1$	4.76	4.89	2.25×10^{-2}	1.59×10^{-2}	$(2.37 \pm 0.08) \times 10^{-2b}$
Uub	$6d^{10}7s^2\ ^1\mathrm{S}_0 \to 6d^{10}7s7p\ ^3\mathrm{P}_1$	6.57		9.24×10^{-2}	3.42×10^{-2}	
Zn^+	$3d^{10}4s\ ^2\mathrm{S}_{1/2} \to 3d^{10}4p\ ^2\mathrm{P}_{1/2}$	5.75	6.01	6.48×10^{-1}	5.88×10^{-1}	
Cd^+	$4d^{10}5s\ ^2\mathrm{S}_{1/2} \to 4d^{10}5p\ ^2\mathrm{P}_{1/2}$	5.16	5.47	6.64×10^{-1}	5.92×10^{-1}	
Hg^+	$5d^{10}6s\ ^2\mathrm{S}_{1/2} \to 5d^{10}6p\ ^2\mathrm{P}_{1/2}$	6.11	6.38	6.09×10^{-1}	5.21×10^{-1}	
Uub^+	$6d^97s^2\ ^2\mathrm{D}_{5/2} \to 6d^87s^27p\ ^2\mathrm{P}_{7/2}$	5.46		1.04×10^{-4}	5.94×10^{-3}	
Zn^{2+}	$3d^{10}\ ^1\mathrm{S}_0 \to 3d^94p\ ^3\mathrm{P}_1$	15.88	17.37	5.00×10^{-3}	6.80×10^{-3}	
Cd^{2+}	$4d^{10}\ ^1\mathrm{S}_0 \to 4d^95p\ ^3\mathrm{P}_1$	16.75	17.20	2.71×10^{-2}	2.98×10^{-2}	
Hg^{2+}	$5d^{10}\ ^1\mathrm{S}_0 \to 5d^96p\ ^3\mathrm{P}_1$	13.85	14.71	5.38×10^{-2}	6.65×10^{-2}	
Uub^{2+}	$6d^87s^2\ ^3\mathrm{F}_4 \to 6d^87s7p\ ^5\mathrm{D}_4$	6.36		8.22×10^{-2}	3.58×10^{-2}	
Zn^{3+}	$3d^9\ ^2\mathrm{D}_{5/2} \to 3d^84p\ ^4\mathrm{D}_{7/2}$	23.02		1.62×10^{-4}	1.15×10^{-3}	
Cd^{3+}	$4d^9\ ^2\mathrm{D}_{5/2} \to 4d^85p\ ^4\mathrm{D}_{7/2}$	20.53	21.37	4.26×10^{-4}	1.92×10^{-3}	
Hg^{3+}	$5d^9\ ^2\mathrm{D}_{5/2} \to 5d^86p\ ^4\mathrm{D}_{7/2}$	15.79		2.23×10^{-3}	4.88×10^{-3}	
Uub^{3+}	$6d^9\ ^2\mathrm{D}_{5/2} \to 6d^77s7p\ ^4\mathrm{P}_{3/2}$	8.73		7.85×10^{-2}	4.47×10^{-2}	
Zn^{4+}	$3d^8\ ^3\mathrm{F}_4 \to 3d^74p\ ^5\mathrm{F}_4$	34.23		2.48×10^{-2}	3.28×10^{-2}	
Cd^{4+}	$4d^8\ ^3\mathrm{F}_4 \to 4d^75p\ ^5\mathrm{F}_4$	26.77		8.44×10^{-2}	1.10×10^{-1}	
Hg^{4+}	$5d^8\ ^3\mathrm{F}_4 \to 5d^76p\ ^5\mathrm{F}_4$	20.09		7.06×10^{-2}	1.20×10^{-1}	
Uub^{4+}	$6d^8\ ^3\mathrm{F}_4 \to 6d^76p\ ^5\mathrm{F}_4$	10.97		7.53×10^{-3}	5.29×10^{-2}	
Zn^{5+}	$3d^7\ ^4\mathrm{F}_{9/2} \to 3d^64p\ ^6\mathrm{D}_{9/2}$	44.67		9.37×10^{-3}	1.03×10^{-2}	
Cd^{5+}	$4d^7\ ^4\mathrm{F}_{9/2} \to 4d^65p\ ^6\mathrm{D}_{7/2}$	32.80		1.53×10^{-2}	1.87×10^{-2}	
Hg^{5+}	$5d^7\ ^4\mathrm{F}_{9/2} \to 5d^66p\ ^6\mathrm{D}_{7/2}$	24.95		5.54×10^{-2}	6.95×10^{-2}	
Uub^{5+}	$6d^7\ ^4\mathrm{F}_{9/2} \to 6d^67p\ ^6\mathrm{D}_{7/2}$	14.33		8.01×10^{-2}	8.86×10^{-2}	

[a] Reference [34]; [b] Reference [35].

Table 5. Calculated low-lying resonances excitation energies (in eV) and oscillator strengths of Hg from its ground-state $5d^{10}6s^2\ ^1\mathrm{S}_0$ to a few excited states. (L: length gauge, V: velocity gauge).

		Transitions energies		Oscillator strengths	
Configurations	Terms	Our calc.	Expt. [29]	L	V
$5d^{10}6s6p$	$^3\mathrm{P}_1$	5.07	4.89	4.26×10^{-3}	1.34×10^{-2}
$5d^{10}6s6p$	$^1\mathrm{P}_1$	6.92	6.70	1.19	1.62
$5d^96s^26p$	$^1\mathrm{P}_1$	9.99	9.77	3.04×10^{-1}	3.49×10^{-1}
$5d^96s^26p$	$^3\mathrm{P}_1$	11.25	11.01	8.43×10^{-1}	9.49×10^{-1}
$5d^96s^26p$	$^3\mathrm{D}_1$	11.73	11.62	5.77×10^{-2}	6.20×10^{-2}

calculations, which are also included in Table 3. The results for both Hg and Uub are not only in reasonable agreement with the results from references [13,24,29] but also in good agreement with the extrapolated values. The discrepancies among the different calculations and experiment are less than 0.4 eV.

4 Summary

We have presented our results of the ionization potentials, excitation energies and oscillator strengths in the charge states 0 to 5+ of the element Uub and the homologue elements Zn, Cd and Hg. Due to the relativistic stabilization of the $7s_{1/2}$ orbital and the relativistic destabilization of the $6d_{5/2}$, the ground states of Uub are different from the lighter homologue elements Zn, Cd and Hg. Firstly, for the neutral element Uub, the energies of the $7s_{1/2}$ and $6d_{5/2}$ orbitals are reverse. Secondly, the ground states of Uub^+ and Uub^{2+}, which are $6d^97s^2(J = 5/2^+)$ and $6d^87s^2(J = 4^+)$, respectively, are different from the lighter homologues. Thirdly, for the ground state of Uub^{3+} there exists a strong configuration interaction among the $6d^9, 6d^87s$ and $6d^77s^2$ though the Uub^{3+}, Zn^{3+}, Cd^{3+} and Hg^{3+} have the same total angular momentum and parity. In addition, there are higher excitation energies expected for element Uub in the neutral state and much lower excitation energies for the charge states 2+ to 5+ compared with the homologue elements. We obtain the ionization potentials of element Uub derived from extended MCDF calculations and corrected via extrapolation schemes which allow an uncertainty of less than

Table 6. Calculated low-lying resonances excitation energies (in eV) and oscillator strengths of Uub from its ground-state $6d^{10}7s^2\ ^1\mathrm{S}_0$ to a few excited states. (L: length gauge, V: velocity gauge).

		Transitions energies	Oscillator strengths	
Configurations	Terms	Our calc.	L	V
$6d^{10}7s7p$	$^3\mathrm{P}_1$	6.66	8.88×10^{-2}	3.94×10^{-2}
$6d^{9}7s^{2}7p$	$^3\mathrm{P}_1$	9.21	1.68×10^{-1}	1.67×10^{-1}
$6d^{9}7s^{2}7p$	$^1\mathrm{P}_1$	9.75	1.62×10^{-1}	3.08×10^{-1}
$6d^{9}7s^{2}7p$	$^3\mathrm{D}_1$	12.01	5.64×10^{-3}	2.71×10^{-2}
$6d^{10}7s7p$	$^1\mathrm{P}_1$	12.59	5.22	3.98

0.5 eV, which are 11.73 eV for Uub, 21.98 eV for Uub^+ and 32.62 eV for Uub^{2+}, respectively. The high ionization potentials for Uub and Uub^{1+} indicate that element Uub is stronger chemically inert in the group 12. Further, we calculated the low-lying resonance excitation energies, absorption oscillator strengths and the first ionization potential for Hg and Uub using the sophisticated large-scale MCDF method, which improved the uncertainty of the excitation energies to less than 0.25 eV for Hg. We hope that with such calculations the same uncertainty can be obtained for Uub. Moreover, we hope that the results are helpful for the experimental investigation of the atomic structure of element Uub in the future, when either many atoms are present at the same time or when a single atom can be measured in a trap.

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