Ionization Potentials of Seaborgium

E. Johnson*

Environmental Sciences Institute, Florida Agricultural and Mechanical University,
Tallahassee, Florida 32307-6600

V. Pershina

Gesellschaft fuer Schwerionenforschung, D-64291 Darmstadt, Germany

B. Fricke

Fachbereich Physik, Universitaet Kassel, D-34109 Kassel, Germany

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Multiconfiguration relativistic Dirac−Fock values were calculated for the first six ionization potentials of seaborgium and of the other group 6 elements. No experimental ionization potentials are available for seaborgium. Accurate experimental values are not available for all of the other ionization potentials. Ionic radii for the 4+ through 6+ ions of seaborgium are also presented. The ionization potentials and ionic radii obtained will be used to predict some physicochemical properties of seaborgium and its compounds.

I. Introduction

The knowledge of the electronic energy structure of an atom with a given number of electrons is an indispensable ingredient for the understanding of its physical and chemical behavior. Of course it is clear that atomic structure calculations alone are not sufficient in this respect, but they are a most important and very helpful starting point for any kind of chemical interpretation.

Most elements were discovered in the past century or earlier, so there was no opportunity to make quantum mechanical predictions during the investigation of their basic chemical properties. This was also true for the actinides in the 40s and 50s of this century. But it is not true for all of the elements above element 103, lawrencium. Good information about the chemical behavior of all elements up to element 173 was obtained from quantum mechanical atomic calculations.[1] The situation changed during the past 20 years for the first elements of the transactinides, the 6d elements, which start with element 104, rutherfordium. A large amount of chemical information has been accumulated since for elements 104 and 105, because isotopes have been found with half-lives of 65 and 34 s, respectively.[2] For these two elements, very accurate atomic structure calculations on the multiconfiguration Dirac−Fock[3,4] (MCDF) and the couple-cluster single and double excitation[5] (CCSD) levels as well as relatively good Dirac−Fock−Slater (DFS) calculations for a few chemical compounds were available.[6−8] These results were an excellent guide in this very complicated "one atom at a time" chemistry. The whole field with the results and comparisons for the transactinide elements has been reviewed by Pershina[9] and Pershina and Fricke.[10]

Now that chemical experiments for element 106, seaborgium, are under way, it is absolutely necessary to continue the same type of study for element 106 which has been the basis for the predictions of chemical properties of elements 104 and 105. What are still missing up to now for seaborgium are accurate atomic structure calculations. In this article, we present extensive results of such a study on the level of the relativistic MCDF method. We used the computational method that was developed by Desclaux.[11]

The most important numbers with respect to chemical studies are the values for the ionization potentials and radii in the various ionization states. To get values that are as accurate as possible, our predictions are based on the relative trend of theoretical and experimental values that is given by the differences between MCDF and experimental values for homologous elements. The ionization potentials and ionic radii presented here will be used to make predictions about the chemistry of element 106. Initial experimental studies of the oxychloride and oxide compounds of element 106 have already been performed.[12]

The first six ionization potentials of seaborgium are presented here. Values for these have not been published elsewhere. Values for the second through sixth ionization potentials of tungsten are also given. Only the first ionization potential of tungsten has been accurately determined by experiments. It appears that the empirical value given here for the fourth ionization potential of molybdenum is more accurate than the experimental value. Radii for the +4, +5, and +6 charged ions of element 106 are also obtained.

In section II, the method used to obtain ionization potentials and ionic radii is summarized. Results are given in section III. Some conclusions are presented in section IV.

II. Method

The general theory of the MCDF method which we use here is presented elsewhere.[13,14] We use an updated version of the MCDF computer program that was written by Desclaux,[11] which today is more or less standard but which is not trivial and is very complicated in the handling of the actual calculations. What we need to know here is the fact that this method solves the

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* To whom correspondence should be addressed.

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TABLE 1: Configurations Used in MCDF Calculations for Positive Parity States[a] (Nonrelativistic Nomenclature)

configurations for charge (q) + [core[b]]					
(0)	(+1)	(+2)	(+3)	(+4)	(+5)
md^{4}ns^2	md^{3}ns^2	md^{2}ns^2	md^{1}ns^2	ns^2	ns^1
md^{5}ns^1	md^{4}ns^1	md^{3}ns^1	md^{2}ns^1	md^{1}ns^1	md^1
md^6	md^5	md^4	md^3	md^2	
md^{4}np^2	md^{1}ns^{2}np^2	ns^{2}np^2	ns^{1}np^2	np^2	
md^{3}ns^{1}np^2	md^{2}ns^{1}np^2	md^{1}ns^{1}np^2	md^{1}np^2		
md^{2}ns^{2}np^2	md^{3}np^2	md^{2}np^2			
md^{2}np^4	ns^{1}np^4	np^4			
md^{1}ns^{1}np^4	md^{1}np^4				
ns^{2}np^4					
np^6					
$J = 0;105^{c,d}$	$J = 1/2;88$	$J = 0;29$	$J = 1/2;13$	$J = 0;6$	$J = 1/2;1$
$J = 1;213$	$J = 3/2;142$	$J = 1;45$	$J = 3/2;21$	$J = 1;3$	$J = 3/2;1$
$J = 2;314$	$J = 5/2;157$	$J = 2;70$	$J = 5/2;20$	$J = 2;7$	$J = 5/2;1$
$J = 3;283$	$J = 7/2;125$	$J = 3;50$	$J = 7/2;11$	$J = 3;2$	
$J = 4;238$	$J = 9/2;85$	$J = 4;41$	$J = 9/2;7$	$J = 4;2$	
$J = 5;136$	$J = 11/2;40$	$J = 5;16$	$J = 11/2;1$		

[a] n is the principal quantum number (4, 5, 6, and 7 for Cr, Mo, W, and Sg, respectively). Here $m = n - 1$. [b] Core = Ar for Cr; Kr for Mo; Xe(4f)^{14} for W; and Rn(4f)^{14} for Sg. [c] The number of configurations included in the calculation follows the associated J value. [d] For the +6 charge state $J = 0$ and the number of configurations is equal to 1.

TABLE 2: Configurations Used in MCDF Calculations for Negative Parity States[a] (Nonrelativistic Nomenclature)

configurations for charge (q) + [core[b]]					
(0)	(+1)	(+2)	(+3)	(+4)	(+5)
md^{3}ns^{2}np^1	md^{2}ns^{2}np^1	md^{1}ns^{2}np^1	ns^{2}np^1	ns^{1}np^1	np^1
md^{4}ns^{1}np^1	md^{3}ns^{1}np^1	md^{2}ns^{1}np^1	md^{1}ns^{1}np^1	md^{1}np^1	
md^{5}np^1	md^{4}np^1	md^{3}np^1	md^{2}np^1		
md^{1}ns^{2}np^3	ns^{2}np^3	ns^{1}np^3	np^3		
md^{2}ns^{1}np^3	md^{1}ns^{1}np^3	md^{1}np^3			
md^{3}np^3	md^{2}np^3				
ns^{1}np^5	np^5				
md^{1}np^5					
$J = 0;86^{c,d}$	$J = 1/2;88$	$J = 0;20$	$J = 1/2;13$	$J = 0;2$	$J = 1/2;1$
$J = 1;228$	$J = 3/2;145$	$J = 1;53$	$J = 3/2;22$	$J = 1;5$	$J = 3/2;1$
$J = 2;298$	$J = 5/2;153$	$J = 2;65$	$J = 5/2;19$	$J = 2;5$	
$J = 3;294$	$J = 7/2;129$	$J = 3;57$	$J = 7/2;13$	$J = 3;3$	
$J = 4;227$	$J = 9/2;83$	$J = 4;38$	$J = 9/2;6$	$J = 4;1$	
$J = 5;140$	$J = 11/2;43$	$J = 5;19$	$J = 11/2;2$		

[a] n is the principal quantum number (4, 5, 6, and 7 for Cr, Mo, W, and Sg, respectively). Here $m = n - 1$. [b] Core = Ar for Cr; Kr for Mo; Xe(4f)^{14} for W; and Rn(4f)^{14} for Sg. [c] The number of configurations included in the calculation follows the associated J value. [d] For the +6 charge state $J = 0$, the number of configurations is equal to 1 and the parity is even.

exact many-particle Dirac equation

$$H\Psi = E\Psi$$

with the following two approximations. First, the Hamiltonian operator H is approximated by the relativistic kinetic operator $c\vec{\alpha}\cdot\vec{p}$, the $1/r$ interaction of the electrons with the nucleus, and the $1/r$ interactions between the electrons. The additional Breit interaction is taken into account only as a perturbation, and the effect of the extended nucleus is treated by assuming that the nucleus has a uniform charge distribution with radius given by Johnson and Soff.[15] No quantum electrodynamic contributions were included. The second approximation is the ansatz used for the wave function, Ψ. In the MCDF method, this wave function is written as a linear combination of Slater determinants that are constructed with the open shell single particle wave functions. Since in an atom the total angular momentum as well as the projection of the z-component are good quantum numbers, one has to construct the Slater determinants as eigenfunctions to these angular momentum operators. Due to the limited computational capacities, we have to restrict valence electrons to the single particle wave functions ns, np$_{1/2}$, np$_{3/2}$, (n-1)d$_{3/2}$, (n-1)d$_{5/2}$ where $n = 7$ for seaborgium, 6 for tungsten, 5 for molybdenum, and 4 for chromium. The number of possible configuration state functions which can be constructed for a certain total angular momentum and parity is listed in Table 1 for the positive parity states and in Table 2 for the negative parity states.

Table 1 lists six of the seven possibilities explored for positive parity states for the neutral atoms to 6+ ions. Column I lists all combinations of the single particle wave functions in the nonrelativistic nomenclature for the MCDF calculations on the neutral group 6 elements where six electrons are distributed in the valence orbitals; column II lists the single ionized species with five active electrons; et cetera. For all of the configurations used, the only orbitals that were not fully occupied with electrons are the outer d, s, and p orbitals. This condition seems to cause the MCDF excitation energies to be too small.[5] To improve the MCDF excitation energies for Sg, an extrapolation procedure was used. This extrapolation is based on the experimental and MCDF values for the other three group 6 elements. This procedure is described in ref 3 and the values which result are given in Table 5.

The electronic energies were found for the four group 6 elements. This was done to predict the quality of the MCDF results for seaborgium by comparing the MCDF results for chromium, molybdenum, and tungsten with experimental results for these elements.[16] It was found that these differences are similar in value. The difference for seaborgium was then approximated as the average of the differences for chromium, molybdenum, and tungsten. This procedure for finding electronic energies is a constant first difference extrapolation.

In some cases experimental values were not available for all three of these elements, so the average of available first difference values was used. For example, for the 3+ charge state, only the first difference for chromium is available, so finding higher differences for this charge state is not possible now. For the +1 to +5 ionization states, no ionization potentials are available for tungsten, so the differences for chromium and molybdenum were used to compute the average, except for the +3 oxidation state where only the chromium difference was used. The experimental ionization potential of +3 molybdenum seems to be very inaccurate. This ionization potential was obtained by extrapolation of ionization potentials of an isoelectronic series.[17,18] Table 5 of ref 17 seems to indicate that the irregular doublet law[19] on which this extrapolation is based is not well followed for the [Kr](4d)^3 electronic configuration of Mo(3+). The unavailability of certain ionization potentials for Mo and W increases the uncertainty of the associated empirical values.

Effective radii for the neutral and +1 ions of chromium, molybdenum, and tungsten are not available.[20] Also, ionic radii have not been determined for the +2 and +3 ions of tungsten. The extrapolation procedure used to determine both ionization potentials and ionic radii is based on standard finite difference methods of numerical analysis.[21] For ionization potentials, a constant first difference assumption was used. For the ionic radii, a constant third difference assumption was used. The first difference for the radii is the value of $R_{\max}$ minus the corresponding effective radius given in ref 20. Let the first difference for Cr, Mo, and W be denoted by (ΔCr, ΔMo, ΔW)

TABLE 3: Calculated Electronic Ground States for Cr, Mo, W, and Sg in the Charge States 0 to +6[a]

element	I	II	III	IV (%)	V (eV)
Cr	283	3+	[Ar](3d)^5(4s)^1	99.6	−28551.534
Cr(1+)	157	5/2+	[Ar](3d)^5	99.1	−28545.519
Cr(2+)	29	0+	[Ar](3d)^4	99.9	−28530.372
Cr(3+)	21	3/2+	[Ar](3d)^3	99.3	−28500.611
Cr(4+)	7	2+	[Ar](3d)^2	100.0	−28452.574
Cr(5+)	1	3/2+	[Ar](3d)^1	100.0	−28383.991
Cr(6+)	1	0+	[Ar]	100.0	−28294.401
Mo	283	3+	[Kr](4d)^5(5s)^1	99.3	−110027.750
Mo(1+)	157	5/2+	[Kr](4d)^5	99.0	−110021.489
Mo(2+)	29	0+	[Kr](4d)^4	99.9	−110006.421
Mo(3+)	21	3/2+	[Kr](4d)^3	99.2	−109980.344
Mo(4+)	7	2+	[Kr](4d)^2	100.0	−109941.175
Mo(5+)	1	3/2+	[Kr](4d)^1	100.0	−109887.740
Mo(6+)	1	0+	[Kr]	100.0	−109820.045
W	105	0+	[Xe](4f)^{14}(5d)^4(6s)^2	88.7	−438887.943
W(1+)	88	1/2+	[Xe](4f)^{14}(5d)^4(6s)^1	97.7	−438880.972
W(2+)	29	0+	[Xe](4f)^{14}(5d)^4	97.3	−438866.158
W(3+)	21	3/2+	[Xe](4f)^{14}(5d)^3	98.1	−438841.430
W(4+)	7	2+	[Xe](4f)^{14}(5d)^2	99.9	−438804.560
W(5+)	1	3/2+	[Xe](4f)^{14}(5d)^1	100.0	−438754.257
W(6+)	1	0+	[Xe](4f)^{14}	100.0	−438690.669
Sg	105	0+	[Rn](5f)^{14}(6d)^4(7s)^2	86.5	−1105324.629
Sg(1+)	142	3/2+	[Rn](5f)^{14}(6d)^3(7s)^2	87.6	−1105317.600
Sg(2+)	45	1+	[Rn](5f)^{14}(6d)^3(7s)^1	96.7	−1105301.747
Sg(3+)	21	3/2+	[Rn](5f)^{14}(6d)^3	77.0	−1105277.134
			[Rn](5f)^{14}(6d)^2(7s)^1	17.7	
			[Rn](5f)^{14}(6d)^1(7s)^2	3.6	
Sg(4+)	7	2+	[Rn](5f)^{14}(6d)^2	98.5	−1105242.850
Sg(5+)	1	3/2+	[Rn](5f)^{14}(6d)^1	100.0	−1105196.540
Sg(6+)	1	0+	[Rn](5f)^{14}	100.0	−1105138.387

[a] Column I: number of configurations used in the calculation. Column II: angular momentum and parity of the ground state. Column III: dominant configurations found. Column IV: configuration weights in percent. Column V: total energy of the ground state in eV.

where, for example, ΔCr = ($R_{\max}$ for Cr − effective radius for Cr). The second differences are (ΔΔMo, ΔΔW) where ΔΔMo = (ΔCr − ΔMo). There is only one third difference for the set Cr, Mo, and W which is ΔΔΔW = (ΔΔMo − ΔΔW). For the 4+ charge state, for example, ΔΔΔW for the ionic radius is equal to 0.0112 nanometers. The constant third difference assumption implies that ΔΔΔSg is equal to 0.0112 nm also. Knowledge of the third difference for Sg allows the second and first differences to be determined. For the 4+ charge state, ΔΔSg and ΔSg are 0.0052 and 0.0037 nm, respectively. The values of $R_{\max}$ for Sg and ΔSg imply that the effective ionic radius of Sg^{4+} is 0.083 nm. This value of the effective radius is called empirical, because it was determined by extrapolation.

III. Results

For each atom and charge state in Table 3, the number of configurations in the calculation, the angular momentum eigenvalue, parity, dominant configurations and corresponding weights, and energy are given for the lowest electronic state obtained by MCDF calculations using the basis sets given in Tables 1 and 2. The ground-state configurations and total angular momenta presented in Table 3 are in agreement with experimental results.[22] The MCDF ground states for seaborgium differ from two of the other elements in group 6, chromium and molbydenum. Seaborgium and tungsten ground states have more s-character. This change results from relativistic effects.[23,24] This effect is clearly seen for the Sg(1+), Sg(2+), and Sg(3+) ions.

TABLE 4: Some Calculated Electronic Excited States for Cr, Mo, W, and Sg in the Charge States 0 to +5[a]

element	I	II	III	IV (%)	V (eV)
Cr	213	1+	[Ar](3d)^4(4s)^2	92.1	0.188
Cr(1+)	88	1/2+	[Ar](3d)^4(4s)^1	99.9	0.889
Cr(2+)	45	1+	[Ar](3d)^4	99.9	0.008
	70	2+	[Ar](3d)^4	98.4	0.022
Cr(3+)	20	5/2+	[Ar](3d)^3	100.0	0.028
	11	7/2+	[Ar](3d)^3	100.0	0.068
Cr(4+)	2	3+	[Ar](3d)^2	100.0	0.060
	2	4+	[Ar](3d)^2	100.0	0.139
Cr(5+)	1	5/2+	[Ar](3d)^1	100.0	0.113
Mo	105	0+	[Kr](4d)^4(5s)^2	89.5	1.313
Mo(1+)	88	1/2+	[Kr](4d)^4(5s)^1	99.8	1.422
Mo(2+)	45	1+	[Kr](4d)^4	99.9	0.026
	70	2+	[Kr](4d)^4	98.4	0.074
Mo(3+)	20	5/2+	[Kr](4d)^3	100.0	0.089
	11	7/2+	[Kr](4d)^3	100.0	0.204
Mo(4+)	2	3+	[Kr](4d)^2	100.0	0.183
	2	4+	[Kr](4d)^2	100.0	0.394
Mo(5+)	1	5/2+	[Kr](4d)^1	100.0	0.306
W	213	1+	[Xe](4f)^{14}(5d)^4(6s)^2	88.6	0.144
	314	2+	[Xe](4f)^{14}(5d)^4(6s)^2	87.5	0.320
W(1+)	142	3/2+	[Xe](4f)^{14}(5d)^4(6s)^1	97.8	0.139
	157	5/2+	[Xe](4f)^{14}(5d)^4(6s)^1	98.0	0.308
W(2+)	45	1+	[Xe](4f)^{14}(5d)^4	98.6	0.208
	70	2+	[Xe](4f)^{14}(5d)^4	98.3	0.436
W(3+)	20	5/2+	[Xe](4f)^{14}(5d)^3	99.9	0.377
	11	7/2+	[Xe](4f)^{14}(5d)^3	99.5	0.754
W(4+)	2	3+	[Xe](4f)^{14}(5d)^2	100.0	0.699
	2	4+	[Xe](4f)^{14}(5d)^2	100.0	1.333
W(5+)	1	5/2+	[Xe](4f)^{14}(5d)^1	100.0	1.003
Sg	213	1+	[Rn](5f)^{14}(6d)^4(7s)^2	88.0	0.519
	314	2+	[Rn](5f)^{14}(6d)^4(7s)^2	85.5	0.894
Sg(1+)	157	5/2+	[Rn](5f)^{14}(6d)^3(7s)^2	87.8	0.720
	88	1/2+	[Rn](5f)^{14}(6d)^4(7s)^1	66.0	0.738
			[Rn](5f)^{14}(6d)^3(7s)^2	27.0	
Sg(2+)	70	2+	[Rn](5f)^{14}(6d)^2(7s)^2	72.4	0.180
			[Rn](5f)^{14}(6d)^3(7s)^1	19.8	
	29	0+	[Rn](5f)^{14}(6d)^2(7s)^2	33.3	
			[Rn](5f)^{14}(6d)^4	32.8	0.348
			[Rn](5f)^{14}(6d)^3(7s)^1	32.1	
Sg(3+)	20	5/2+	[Rn](5f)^{14}(6d)^2(7s)^1	90.3	
			[Rn](5f)^{14}(6d)^3	8.0	0.777
			[Rn](5f)^{14}(6d)^1(7s)^2	1.6	
	13	1/2+	[Rn](5f)^{14}(6d)^3	70.0	1.512
			[Rn](5f)^{14}(6d)^2(7s)^1	29.9	
Sg(4+)	2	3+	[Rn](5f)^{14}(6d)^2	100.0	1.429
	5	0+	[Rn](5f)^{14}(6d)^2	98.8	1.790
Sg(5+)	1	5/2+	[Rn](5f)^{14}(6d)^1	100.0	1.825

[a] Column I: number of configurations used in the calculation. Column II: angular momentum and parity of the state. Column III: dominant configurations found. Column IV: configuration weights in percent. Column V: energy of the state above the ground state of the corresponding neutral atom or ion in eV.

Some MCDF excited-state energies are presented in Table 4. The trend in the values of MCDF excitation energies is in good agreement with experimental values. The accuracy of the calculations can be seen from the following examples. For the +2 charge state of molybdenum, the experimental first and second excitation energies are 0.0301 and 0.08302 eV.[22] The MCDF first and second excitation energies for molybdenum are 0.026 and 0.073 eV. For neutral tungsten, the experimental first and second excitation energies are 0.207090 and 0.412313 eV.[22] The corresponding MCDF first and second excitation energies are 0.14 and 0.32 eV. MCDF, experimental, and empirical ionization potentials for the group 6 elements are presented in Table 5. The uncertainty of the empirical ionization potentials seems to be about ±0.5 eV.

Empirical, MCDF, and effective ionic radii for the group 6 elements are presented in Table 6. Values for the ionic radii of seaborgium presented here were obtained by using the location of the maximum of the charge density,[25,26] $R_{\max}$, in outer occupied orbitals of chromium, molybdenum, tungsten, and

TABLE 5: Ionization Potentials in eV for Group 6 Elements[a]

I	II	III	IV (eV, MCDF)	V (eV, exptl)	VI (eV, ext)
(0)→(1+)	Cr(0)	$(3d)^5(4s)^1(J = 3+) \rightarrow (3d)^5(J = 5/2+)$	6.02	6.76664	6.84
	Mo(0)	$(3d)^5(4s)^1(J = 3+) \rightarrow (4d)^5(J = 5/2+)$	6.26	7.09243	7.08
	W(0)	$(5d)^4(6s)^2(J = 0+) \rightarrow (5d)^4(6s)^1(J = 1/2+)$	6.97	7.8640	7.79
	Sg(0)	$(6d)^4(7s)^2(J = 0+) \rightarrow (6d)^3(7s)^2(J = 3/2+)$	7.03		7.85
(1+)→(2+)	Cr(1+)	$(3d)^5(J = 5/2+) \rightarrow (3d)^4(J = 0+)$	15.15	16.4857	16.36
	Mo(1+)	$(4d)^5(J = 5/2+) \rightarrow (4d)^4(J = 0+)$	15.07	16.16	16.28
	W(1+)	$(5d)^4(6s)^1(J = 1/2+) \rightarrow (5d)^4(J = 0+)$	14.81		16.02
	Sg(1+)	$(6d)^3(7s)^2(J = 3/2+) \rightarrow (6d)^3(7s)^1(J = 1+)$	15.85		17.06
(2+)→(3+)	Cr(2+)	$(3d)^4(J = 0+) \rightarrow (3d)^3(J = 3/2+)$	29.76	30.96	30.89
	Mo(2+)	$(4d)^4(J = 0+) \rightarrow (4d)^3(J = 3/2+)$	26.08	27.13	27.21
	W(2+)	$(5d)^4(J = 0+) \rightarrow (5d)^3(J = 3/2+)$	24.73		25.86
	Sg(2+)	$(6d)^3(7s)^1(J = 1+) \rightarrow (6d)^3(J = 3/2+)$	24.61		25.74
(3+)→(4+)	Cr(3+)	$(3d)^3(J = 3/2+) \rightarrow (3d)^2(J = 2+)$	48.04	49.16	49.16
	Mo(3+)	$(4d)^3(J = 3/2+) \rightarrow (4d)^2(J = 2+)$	39.17	46.4	40.29
	W(3+)	$(5d)^3(J = 3/2+) \rightarrow (5d)^2(J = 2+)$	36.87		37.99
	Sg(3+)	$(6d)^3(J = 3/2+) \rightarrow (6d)^2(J = 2+)$	34.28		35.40
(4+)→(5+)	Cr(4+)	$(3d)^2(J = 2+) \rightarrow (3d)^1(J = 3/2+)$	68.58	69.46	69.55
	Mo(4+)	$(4d)^2(J = 2+) \rightarrow (4d)^1(J = 3/2+)$	53.44	54.49	54.41
	W(4+)	$(5d)^2(J = 2+) \rightarrow (5d)^1(J = 3/2+)$	50.30		51.27
	Sg(4+)	$(6d)^2(J = 2+) \rightarrow (6d)^1(J = 3/2+)$	46.31		47.28
(5+)→(6+)	Cr(5+)	$(3d)^1(J = 3/2+) \rightarrow [\mathrm{core}](J = 0+)$	89.59	90.6349	90.68
	Mo(5+)	$(4d)^1(J = 3/2+) \rightarrow [\mathrm{core}](J = 0+)$	67.70	68.8276	68.79
	W(5+)	$(5d)^1(J = 3/2+) \rightarrow [\mathrm{core}](J = 0+)$	63.59		64.68
	Sg(5+)	$(6d)^1(J = 3/2+) \rightarrow [\mathrm{core}](J = 0+)$	58.15		59.24

[a] Column I: change in charge state. Column II: element. Column III: transition between configurations (see Table 3). Column IV: MCDF ionization potentials. Column V: experimental ionization potentials. Column VI: extrapolated ionization potentials.[3]

TABLE 6: Empirical Ionic Radii in Nanometers of the +4 through +6 Charged Ions of Seaborgium that Were Determined by Extrapolation of the Radii of Maximum Charge Density, R_{max}, of the Orbitals Specified

element	charge	orbital	R_{max} (nm)	effective radius from ref 20 (nm)	empirical radius (nm)
Cr	0	4s	0.1537		
Mo	0	5s	0.1600		
W	0	6s	0.1473		
Sg	0	7s	0.1391		
Cr	+1	$3d_{5/2}$	0.0456		
Mo	+1	$4d_{5/2}$	0.0737		
W	+1	$5d_{5/2}$	0.0801		
Sg	+1	$6d_{5/2}$	0.0946		
Cr	+2	$3d_{5/2}$	0.0441	0.080	
Mo	+2	$4d_{5/2}$	0.0717		
W	+2	$5d_{5/2}$	0.0788		
Sg	+2	$6d_{5/2}$	0.0917		
Cr	+3	$3d_{5/2}$	0.0424	0.0615	
Mo	+3	$4d_{5/2}$	0.0697	0.069	
W	+3	$5d_{5/2}$	0.0768		
Sg	+3	$6d_{5/2}$	0.0887		
Cr	+4	$3d_{5/2}$	0.0407	0.055	
Mo	+4	$4d_{5/2}$	0.0679	0.0650	
W	+4	$5d_{5/2}$	0.0749	0.066	
Sg	+4	$6d_{5/2}$	0.0870		0.083
Cr	+5	$3d_{3/2}$	0.0392	0.049	
Mo	+5	$4d_{3/2}$	0.0659	0.061	
W	+5	$5d_{3/2}$	0.0718	0.062	
Sg	+5	$6d_{3/2}$	0.0822		0.077
Cr	+6	$3p_{3/2}$	0.0406	0.044	
Mo	+6	$4p_{3/2}$	0.0556	0.059	
W	+6	$5p_{3/2}$	0.0583	0.060	
Sg	+6	$6p_{3/2}$	0.0665		0.065

seaborgium, and an empirical procedure.[21] The quantity R_{max} is the location of the maximum in $r^2R(r)^2$ where $R(r)$ is the radial part of the wave function probability density for the outer orbital and r is the distance from the origin.

The empirical procedure used to determine ionic radii is described in the previous section. The values of the ionic radii for Sg for the +4 through +6 charge state are given in Table 6. The uncertainty of these radii is ±0.005 nanometers. The value of ±0.005 nanometers is the largest of the first differences associated with Table 6.

IV. Conclusions

The electronic states, electronic transition energies between them, including ionization potentials and R_{max} of the "outermost valence orbitals", have been calculated for Cr, Mo, W, and Sg from the MCDF method. Using extrapolation procedures, "empirical" values for ionization potentials and ionic radii were obtained for Sg.

The relativistic MCDF total angular momentum eigenvalues and dominant configurations calculated for the lowest energy states agree with experimental results. There is also good agreement between the excitation energies calculated and corresponding experimental values. The empirical ionization potentials obtained have an accuracy of 0.5 eV in comparison with experimental values, and the ionic radii have an accuracy of 0.005 nm. Better results could be obtained by using a larger set of basis functions;[5] in particular, the basis set should allow excitations of nonvalence electrons. The use of a larger basis set with the MCDF method is, unfortunately, not practical for the group 6 elements, because the computational requirements are more than can be conveniently met today. The accuracy of the results shows that the MCDF method is quite adequate for describing the ionization potentials and ionic radii given.

The information obtained on ionization potentials and ionic radii is very valuable, since even for the lighter homologues of Sg, only a small amount of experimental data is available. Knowledge about the electronic states of Sg as well as the ionic radii and ionization potentials will be used to predict important physicochemical properties of this element and its compounds in comparison with the lighter homologues. This will contribute to answering fundamental questions about the analogy between the transactinides and the 4d and 5d elements. These properties are the stability of oxidation states and redox potentials, the heats of hydration and sublimation, and the extraction of various complexes of Sg from aqueous solutions by organic solvents. We plan to do further work on some of these topics.

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