Ionization potentials of neutral and ionized species of elements 107 and 108 from extended MCDF calculations

T. Jacob[1], T. Inghoff[1], B. Fricke[1], S. Fritzsche[1], E. Johnson[2], V. Pershina[3]
[1]Fachbereich Physik, Universität Kassel, 34109 Kassel;
[2]Environmental Science Institute, Florida A&M University, Tallahassee, FL 32307, USA;
[3]GSI, Darmstadt

Theoretical predictions of the chemical behaviour of superheavy elements are very important for extensive and sophisticated "one-atom-at-a-time" chemical experiments. A number of experiments have been performed so far up to element 106 and recently a first experiment has been done for element 107. An important first step is the knowledge of the atomic data for each of these elements. (A review on this subject is given in Ref. [1] and [2])

Here we report on the very first large scale Multiconfiguration Dirac–Fock (MCDF) calculations on the elements 107 and 108 in neutral as well as ionized states up to 8+.

The actual calculations which we have performed here are extended relativistic Multiconfiguration Dirac–Fock calculations [3] using up to 650 configuration state functions. The method itself is best described by Grant [4] and Grant and Quiney [5].

Our calculations include all possible configurations which can be constructed from the relativistic ns, $np_{1/2}$, $np_{3/2}$, $(n-1)d_{3/2}$, and $(n-1)d_{5/2}$ single particle wavefunctions for a specific total angular momentum, parity, and charge state. Our assumption is that the core of each element is kept complete and the remaining electrons are distributed in all possible ways in the single particle wavefunctions given above.

Transition	Mn		Tc	
	MCDF	Exp.	MCDF	Exp.
0+→1+	6.84	7.43	6.33	7.28
0+→2+	21.7	23.1	20.6	22.54
0+→3+	54.2	56.8	49.3	52.08
0+→4+	104.4	108	90.9	
0+→5+	175.8	180	147.3	
0+→6+	270.5	275	219.5	
0+→7+	388.7	394	307.4	
Transition	Re		Bh	
	MCDF	Exp.	MCDF	Extrap.
0+→1+	6.84	7.46	6.82	7.5
0+→2+	22.4	25.53	23.4	25.5
0+→3+	48.9	56.58	49.0	53.4
0+→4+	87.9		85.3	89.0
0+→5+	140.4		133.3	137.5
0+→6+	207.6		194.5	199.0
0+→7+	289.1		268.4	273.7

Table 1: Multiple ionization potentials for group 7 elements in eV.

Due to some differences between the calculated (for the elements 104 to 106 see Ref. [6–8]) and experimental values of the ionization potentials, we have to "correct" the former for the elements 107 and 108 using an extrapolation procedure described in Ref. [6]. In this report we use in addition a double difference extrapolation scheme within the chemical rows 4 to 6 in order to get reliable values for the row 7 elements.

Our final results are summarized in the two Tables. For each element and all ionization states the theoretical MCDF results from these calculations are presented as well as the experimental values as far as they are known [9]. As can be seen easily the differences per ionization stage are in the order of 1 eV. This fact was used in the extrapolation schemes in the earlier publications of the analogue result for the elements 104 to 106. Using the extrapolation schemes which are discussed in Ref. [6] in detail we arrive at the values which are listed in both Tables for the elements Bh and Hs.

Transition	Fe		Ru	
	MCDF	Exp.	MCDF	Exp.
0+→1+	7.20	7.90	6.36	7.36
0+→2+	23.6	24.1	20.9	24.1
0+→3+	50.8	54.7	47.5	52.6
0+→4+	104.5	109.5	92.3	
0+→5+	178.7	184.5	151.6	
0+→6+	276.9	283.6	227.3	
0+→7+	401	409	320	
0+→8+			430	
Transition	Os		Hs	
	MCDF	Exp.	MCDF	Extrap.
0+→1+	7.45	8.43	6.69	7.7
0+→2+	23.2		23.3	26
0+→3+	48.7		50.4	54
0+→4+	89.7		87.0	92
0+→5+	144.5		137.4	142
0+→6+	214.2		200.5	206
0+→7+	300		278	
0+→8+	400		369	

Table 2: Multiple ionization potentials for group 8 elements in eV.

References

[1] V. Pershina and B. Fricke in Heavy Elements and Related New Phenomena, World Scientific 1999 (Ed. W. Greiner et al.) page 194
[2] J. V. Kratz, ibid., page 129
[3] J. P. Desclaux, Comp. Phys. Com., **9**, 31 (1975)
[4] I. P. Grant, Adv. Phys., **19**, 747 (1970)
[5] I. P. Grant and H. M. Quiney, Adv. Atom. Mol. Phys., **23**, 37 (1988)
[6] E. Johnson et al., J. Chem. Phys., **93**, 8041 (1990)
[7] B. Fricke et. al., Radiochim. Acta, **62**, 17 (1993)
[8] E. Johnson et al., J. Phys. Chem., **103**, 8458 (1999)
[9] CRC Handbook of Chem. and Phys. (Ed. David R. Lide), 78^{th} edition, New York (1997), page 10-214