

Chemical and Physical Properties of Superheavy Elements

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A knowledge of the physical and chemical properties of superheavy elements is expected to be of great value for the detection of these elements, owing to the need for chemical separation in their isolation and identification. The methods for predicting their electronic structures, expected trends in their chemical and physical properties and the results of such predictions for the individual superheavy elements are reviewed. The periodic table is extended up to element 172.

Introduction

The discovery of element 106 was recently announced in Dubna by Oganessian, Flerov, and coworkers [1] and in Berkeley by Ghiorso and coworkers [2], thus indicating the addition of a new element to the periodic table. The significance of these announcements can be appreciated when one realizes that until 1940 the heaviest known element was uranium (atomic number 92) and Seaborg's actinide concept [3] was no more than a hypothesis. Seen in relation to the periodic table and compared to the progress which has been made since, element 106 is probably only one more step toward an even longer system of the elements.

The upper limit which can be reached for the production of still heavier elements by bombarding atoms of high Z with atoms of small Z is expected to occur at about element 108 or 109. The alternative to this approach is to bombard a very heavy element with another very heavy element, a method which under favorable conditions could lead to the direct production of superheavy elements and their simultaneous discovery. This method which is in its preparatory stages at a number of laboratories, i.e. Dubna in the USSR, Berkeley in the USA, Orsay in France, and Darmstadt in Germany will probably overlap at its lower end with the first method. In support of these experiments, there is general agreement that theoretic predictions of nuclear stability define a range of superheavy elements with sufficiently long half-lives to allow their study. Whether or not nuclear reactions exist which would synthesize these elements in quantities sufficient to permit their detection on the earth is not known.

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From the point of view of nuclear physics, one may define the end of the transuranium elements and the beginning of the superheavy elements as the element with which the nuclear stability of the longest lived isotope begins again to increase, with increasing Z .

From the point of view of chemistry, all of these elements are well defined according to their location in the periodic table. Several articles dealing mainly with the chemical behavior of superheavy elements [4], the search for such elements in nature [5] and the electronic structures of these elements have been published.

This paper deals with the chemical and physical properties of superheavy elements. While this knowledge is interesting in its own right, it is also expected to be of considerable importance, because methods of chemical separation will play an important role in the detection of superheavy elements.

Basis for the Predictions

Electronic Structure

The first step toward predicting chemical and physical properties for the superheavy elements is to predict their electronic structures. A good review of the connection between the two by Jørgensen [6] provides insight into this, in some cases, rather complicated problem, as regards the superheavy elements. An excellent review of this subject will also be published by J.B. Mann [7] in the near future. In general, the prediction of the properties entails extrapolation according to the periodic table, *ab-initio* atomic calculations or a combination of the two.

Continuation of the Periodic Table: As early as 1926, Madelung [8] was able to state the empirical rules for the filling of electron shells in the ground-state

Table 1. Atomic ground-state configurations for neutral elements 103–172 and 184 according to the self-consistent Hartree-Fock calculations of Mann [7] and Fricke and Waber [20, 35]

Element	Rn core + 5f ¹⁴ +	Element	Z = 120 core +	Element	Z = 120 core + + 8p _{1,2} ² +	Element	Z = 120 core + + 8p _{1,2} ² 5g ¹⁸ 6f ¹⁴ +
103	7s ² 7p	121	8p	139	5g ¹³ 6f ² 7d ²	157	7d ³
104	7s ² 6d ²	122	8p 7d	140	5g ¹⁴ 6f ³ 7d ¹	158	7d ⁴
105	7s ² 6d ³	123	8p 7d 6f	141	5g ¹⁵ 6f ² 7d ²	159	7d ⁴ 9s ¹
106	7s ² 6d ⁴	124	8p 6f ³	142	5g ¹⁶ 6f ² 7d ²	160	7d ⁵ 9s ¹
107	7s ² 6d ⁵	125	8p 6f ³ 5g	143	5g ¹⁷ 6f ² 7d ²	161	7d ⁶ 9s ¹
108	7s ₂ 6d ⁶	126	8p 7d 6f ² 5g ²	144	5g ¹⁸ 6f ¹ 7d ³	162	7d ⁸
109	7s ² 6d ⁷	127	8p ² 6f ² 5g ³	145	5g ¹⁸ 6f ³ 7d ²	163	7d ⁹
110	7s ² 6d ⁸	128	8p ² 6f ² 5g ⁴	146	6f ⁴ 7d ²	164	7d ¹⁰
111	7s ² 6d ⁹	129	8p ² 6f ² 5g ⁵	147	6f ⁵ 7d ²	165	7d ¹⁰ 9s ¹
112	7s ² 6d ¹⁰	130	8p ² 6f ² 5g ⁶	148	6f ⁶ 7d ²	166	7d ¹⁰ 9s ²
113	7s ² 6d ¹⁰ 7p	131	8p ² 6f ² 5g ⁷	149	6f ⁶ 7d ³	167	7d ¹⁰ 9s ² 9p _{1,2} ²
114	7s ² 6d ¹⁰ 7p ²	132	8p ² 6f ² 5g ⁸	150	6f ⁶ 7d ⁴	168	7d ¹⁰ 9s ² 9p _{1,2} ²
115	7s ² 6d ¹⁰ 7p ³	133	8p ² 6f ³ 5g ⁸	151	6f ⁸ 7d ³	169	7d ¹⁰ 9s ² 9p _{1,2} ² 8p _{3,2} ¹
116	7s ² 6d ¹⁰ 7p ⁴	134	8p ² 6f ⁴ 5g ⁸	152	6f ⁹ 7d ³	170	7d ¹⁰ 9s ² 9p _{1,2} ² 8p _{3,2} ²
117	7s ² 6d ¹⁰ 7p ⁵	135	8p ² 6f ⁴ 5g ⁹	153	6f ¹¹ 7d ²	171	7d ¹⁰ 9s ² 9p _{1,2} ² 8p _{3,2} ³
118	7s ² 6d ¹⁰ 7p ⁶	136	8p ² 6f ⁴ 5g ¹⁰	154	6f ¹² 7d ²	172	7d ¹⁰ 9s ² 9p _{1,2} ² 8p _{3,2} ⁴
119	7s ² 6d ¹⁰ 7p ⁶ 8s	137	8p ² 6f ³ 7d 5g ¹¹	155	6f ¹³ 7d ²		Z = 172 core +
120	7s ² 6d ¹⁰ 7p ⁶ 8s ²	138	8p ² 6f ³ 7d 5g ¹²	156	6f ¹⁴ 7d ²	184	6g ⁵ 7f ⁴ 8d ³

configurations of neutral atoms, which can be formulated as follows:

1. Electron shells are filled in order of increasing value of the sum ($n+l$), where n is the principal quantum number and l the orbital quantum number.
2. For a given value of $n+l$, shells fill in order of increasing n .

These systematics provide a correct explanation for almost all neutral atomic configurations in the region of known elements. Apart from small discrepancies, there seems to be general agreement that the unfinished 8th row of the periodic table will involve the completion of the 6d series of elements at 112 and the 7p elements at 118.

Speaking cautiously, it can be expected that any extrapolation into the region beginning with element 121 will be very speculative. Nevertheless, one should be able to rely on the positions of elements in the periodic table.

Ab-initio Atomic Calculations: The reliability of predictions for the electronic configurations of the superheavy elements was greatly increased with the introduction of *ab-initio* atomic calculations of sufficient accuracy for application to these elements. All of these calculations use a set of usually coupled differential equations, the so-called Hartree-Fock equations which depend on the ansatz for ψ , the electronic wave function, and H the Hamiltonian.

The result of the non-relativistic approximations give rise to increasing errors with increasing nuclear charge so that only relativistic calculations lead to reasonable results in the region of very heavy elements.

A number of papers calculating the ground-state configurations of superheavy atoms by this so-called relativistic Hartree-Fock or Dirac-Fock (DF) method have been published since 1969 [9–10] and the subject is discussed in detail by J.B. Mann [7]. An approximation to this method introduced by Slater [11] leads

to much simpler but almost as good calculations which are called relativistic Hartree-Fock-Slater or Dirac-Fock-Slater (DFS) [12–13] methods and have been used by several authors [14–16] for the superheavy elements. The results for the ground-state configurations of all superheavy elements up to 172 and also for element 184 are given in Table 1 [7, 20, 35]. Only in a very few cases are the results of the two best methods, DF and DFS, different, but these very small differences are such that the configuration cannot be unambiguously defined.

Trends Expected in the Chemical and Physical Properties

Trends Emerging from the Calculations: While we are not able to calculate the properties of superheavy molecules at present, the atomic calculations provide more than just the electronic structures of the neutral elements. One has to bear in mind that two elements from the same chemical group, which often have the same outer electronic structure, will be chemically and physically slightly different. To some extent this can be explained as the effect of their somewhat different sizes and ionization potentials and the different energies and radial distributions of the wave functions between analogous shells.

There is considerable agreement that the ionization potentials have to be calculated in the adiabatic approximation, in which it is assumed that during the removal of an electron sufficient time elapses for the other electrons to rearrange themselves, so that the ionization potential is given by the difference in total energy of the two calculations with m and $m-1$ electrons. The other method of using the calculated energy eigenvalues [21] can only be taken as an approximation to this physical quantity.

In the first part of the periodic table it is relatively

easy to relate these quantities to chemical behavior, because of the few shells involved and the large separations between them. Proceeding to the heavy elements at the end of the periodic table, the number of shells increases, the binding energies of the last electrons decrease and there is competition between shells; hence the influence of the inner electrons becomes more significant.

This rather complex behavior becomes further complicated by the fact that relativistic effects begin to be important and the coupling between the angular momenta of the electrons changes from LS to intermediate or j - j coupling. The main change due to relativistic effects is the splitting of all shells with $l > 0$ into two subshells with $j = l + 1/2$ and $j = l - 1/2$. This effect is of direct relevance for the chemical behavior of all elements in which these shells are the outer electron shells. This is, for example, the reason why in group IV elements the +2 valency becomes dominant for large Z , as is already the case for lead, and why element 115 (eka-bismuth) is expected to have a monovalent state. This spin-orbit stabilization also plays a dominant role in atomic lawrencium ($Z = 103$), which probably has [22] a $7s^2 7p_{1/2}^1$ ground state instead of the expected $7s^2 6d^1$, as well as in all the elements beyond 120.

Two more relativistic effects will influence the chemical behavior of the superheavy elements. The first is the so-called direct relativistic effect, which is the increase in the binding of the $s_{1/2}$ and $p_{1/2}$ levels relative to nonrelativistic calculations. Even for large principal quantum numbers, these levels have nonzero wave functions in the vicinity of the nucleus, where the potential is large and the relativistic effects increase faster than Z . This explains why the $7s$ electrons are so strongly bound toward the end of the $6d$ transition series, so that the two $7s$ electrons remain bound in elements 110 and 111 and possibly also in the ionized states of element 112, which would drastically change their chemical behavior from the behavior predicted by simple continuation of the periodic table. This effect also explains why the trend toward decreased binding energy of the s electrons in the alkaline and alkaline earth metals stops with Fr and Ra and in the next members in these groups the s electrons should again be more tightly bound. Along with this result, Fig. 1 shows the calculated radii of these elements, taken from [23]. Agreement with experiment is seen to be excellent. From these calculations it can be concluded that Cs is the largest atom in the entire periodic system, at least up to element 172.

The so-called indirect relativistic effect describes the increased shielding and therefore the decreased bonding of the electrons with large angular momentum; the electrons with low angular momentum are drawn as a result of the direct relativistic effect into the atom so that the shielding of the outer electrons increases. This effect is expected to affect the chemistry at the end of the series of $7p$ elements near element

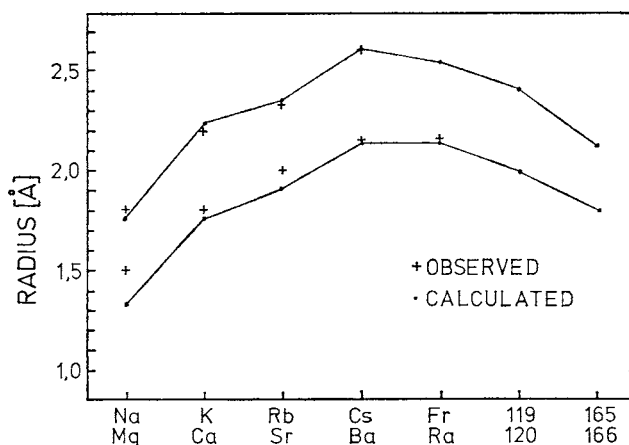
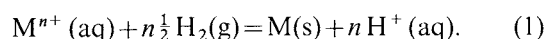


Fig. 1. Comparison of experimental and calculated atomic radii of alkali and alkaline earth elements from DFS calculations [23]

118, where, instead of a noble gas element, a very reactive element with an easily obtainable +4 state is to be expected due to the loosely bound last four $7p_{3/2}$ electrons. The calculated quantities can only be regarded as relative, and the results have to be scaled to fit experimental knowledge in the known part of the periodic table. Therefore all the predictions of all quantities can only be made by a combination of continuing the physical and chemical properties of a particular chemical group into the region of unknown elements and the results of the calculations, if this is possible. But although the calculations do not always yield absolutely correct values, they are necessary in an unknown region, where the chemical behavior becomes changed owing to the relativistic effects.

Empirical and Semi-Empirical Methods: The extrapolation of properties within either rows or groups of elements in the periodic table was and still is the best way of predicting the properties of unknown elements. There are quite a number of empirical and semi-empirical laws which have proved successful, including the valence-bond theory [6], which must be used with caution, the Born-Haber cycle [24, 25], Jørgensen's ingenious variation of this [26–28] and other much more complicated extrapolations. The DF and DFS computer programs allow calculations of electronic energy levels, ionization potentials, and atomic and ionic radii from hydrogen into the superheavy region. In order to arrive at the most probable oxidation states for the superheavy elements and the relative stabilities of these states, the above properties must be related to calculable electronic properties. The relationship between reduction potentials and the Born-Haber cycle offers an effective approach to the solution of this problem [24, 25].

Electrode potentials are usually related to the standard H^+/H_2 couple, whose potential is set equal to zero. We therefore consider the change in state for reduction of the aqueous metallic cation, M^{n+} (aq) to the metal, $M(s)$:



The change in Gibbs free energy is related to the reduction potential and to the enthalpy and entropy by the equation

$$-\Delta G = nE = -\Delta T + T\Delta S. \quad (2)$$

By considering all components in their standard states of unit activity or fugacity, we can obtain the standard electrode potential of the $M^{n+}/M(s)$ couple, as defined according to the IUPAC convention, from these equations.

ΔS must be considered in each case. In most considerations relating to the superheavy region, it has either been chosen small or shown to be small [29]. For simplicity, then only H^0 , which can be obtained through the Born-Haber cycle, needs to be considered. First the heat of sublimation, S_M , must be obtained by extrapolation, preferably against the row of the periodic table. Secondly the approximate ionization energy, I_n , has to be calculated using *ab-initio* calculations. This value must then be corrected as discussed in the preceding paragraph. The difference between the calculated and experimental values in the region of known elements has to be extrapolated and then added to the calculated value.

The next part of the Born-Haber cycle is most conveniently taken to be the single-ion hydration energy, $H_{M^{n+}}$, although this quantity cannot be defined from a thermodynamic point of view. $H_{M^{n+}}$ can be obtained by simple extrapolation or by calculation, using various empirical modifications of the Born equation. Since we are not considering the entropy, we have for the change in state (1)

$$-\frac{1}{n}\Delta H^0 = E^0 \\ = \frac{1}{n}[(I_n + S_M + H_{M^{n+}}) - n(\frac{1}{2}D_{H_2} + I_H + H_{H^+})] \quad (3)$$

where $\frac{1}{2} D_{H_2}$, half the energy of dissociation of the hydrogen molecule, is 2.26 eV; I_H , the ionization energy of the hydrogen atom, is 13.59 eV, and we take the single-ion hydration energy of the proton as -11.3 eV [30]. This yields a value of 4.5 eV for the energy released when one gram equivalent of hydrogen ions is combined with electrons.

Eq. (3) can be used to calculate the standard electrode potentials. Calculations based on the Born-Haber cycle to obtain the relative stabilities of oxidation states are known as "Oxidation State Diagrams" and have been found useful in clarifying inorganic chemical behavior [24], even though their accuracy is sometimes low. Using this equation (3) Jørgensen [26–28] has formulated an ingenious approach for predicting the stabilities of oxidation states for which we cite the references above.

Another helpful scheme is the classification of ions with hard and soft Lewis acids by Ahrlund [31] and Pearson [32]. These general principles can be used to predict a little more about the compounds or complex ions expected for the superheavy elements. It also had been used to rationalize the difference in the chemistry of the light and heavy actinides. These

considerations are especially helpful in the region of the superactinides ($Z=121-154$), because the deeply buried but loosely bound 5g electrons have no analogs in the known part of the periodic table but their behavior may be inferred by analogy to the behavior of the 5f electrons.

Predictions of Properties for the Individual Superheavy Elements

The 6d Transition Elements ($Z=104$ to 112)

Although elements 104, 105, (and very recently also 106) are known, their chemical behavior has not yet been studied in any detail. Zvára and coworkers [33] believe they have shown element 104 to be tetravalent, although no independent confirmation from other groups has been reported. Zvára has also given a preliminary discussion of the chemical separation of element 105 [34].

With certain exceptions in the 4th and 5th periods, the electronic configurations of the outer electrons of almost all the d-transition elements are given by the expression $(n-1)d^m ns^2$, where n is the number of the period and m ranges from 1 to 10. The exceptions to this configuration are found when the increasing binding energy of the d electrons and the greater shielding of the s electrons with higher Z , along with the stabilizing effect of the half-filled and filled d shell, lead to greater stability for the configuration in which one of the "s electrons" returns to the d shell.

The main difference between the elements of the 4th and 5th periods and those of the 6th period is due to the fourteen 4f electrons filled in between filling of the 6s² and 5d electrons. The filling of the 4f shell shields the less penetrating 5d orbitals more effectively than the 6s orbitals, because the d electrons are more effectively kept away from the inner parts of the atom by the centrifugal force $l(l+1)/r^2$, so that the stability of the $d^m s^2$ configuration is increased in the 6th period (except for Pt and Au). This effect will be even greater for the 6d elements, because the 7s electrons should drop relatively deeply into the atom and thus feel the very strong potential near the nucleus, whereas the 6d electrons are expected to be shielded more strongly by the 5f electrons. Fig. 2 shows the energy eigenvalues [16, 35] from DFS calculations of the outer s and d transition elements of the 6th, 7th, and 8th periods. The s electrons are seen to be more strongly bound in the higher periods, the d shell becomes split more and more into its subshells and there should be no deviations from the $6d^m 7s^2$ configuration for the transition elements of the 7th period. In the 6d elements the ionization of one 6d electron will always lead to the most stable ion. The relatively low ionization energy at the beginning of the 6d series is an indication that the maximum oxidation states for these elements will be higher than or at least as high as those of the 5d elements.

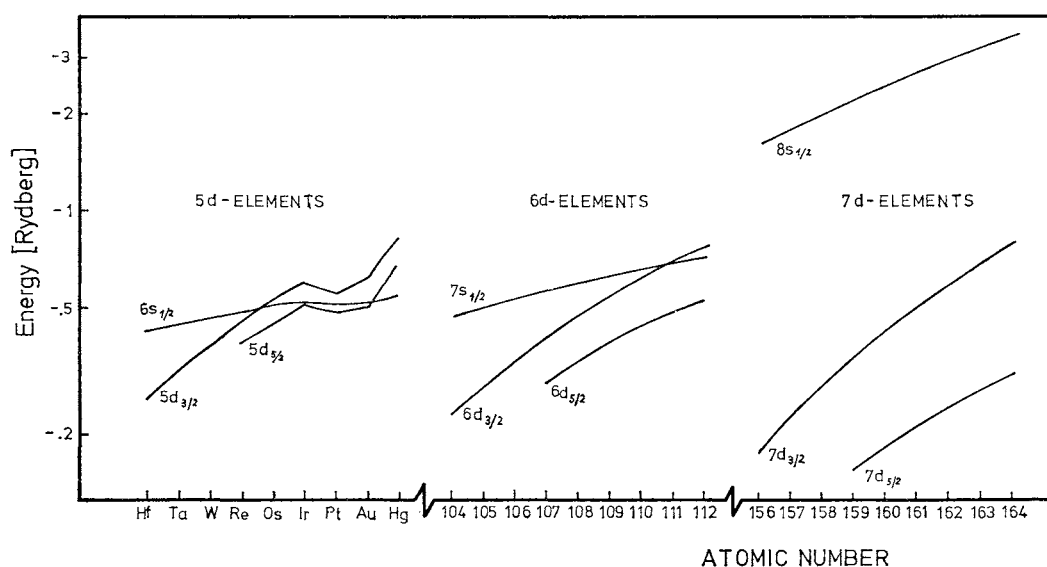


Fig. 2. Dirac-Slater (DFS) energy eigenvalues of outer electrons for the 5d, 6d, and 7d elements. Note strong increase in binding of last s shell and increase in splitting of d subshells due to relativistic effects [35]

Table 2. Summary of predictions for elements 104–112

Element	104	105	106	107	108	109	110	111	112
Chemical group	IV B	V B	VI B	VII B	VIII	VIII	VIII	I B	II B
Stable oxidation states	4, 3	5, 4, 3	6, 4	5, 7, 3	3, 4, 6, 8	3, 6, 1	4, 2, 6, 0	3	2
First ionization energy [eV]									
calc. (DF)	5.1	6.6	7.6	6.9	7.8	8.7	9.6	10.5	11.4
best expec. value				5.9	6.9	8.3	9.9	10.7	11.4
Second IP [eV] (DFS) extr.				18.7	17.6	18.9	19.6	21.5	21.1
Third IP [eV] (DFS) extr.				27.9	29.2	30.1	31.4	31.9	32.8
Fourth IP [eV] (DFS) extr.				37	38	40	41	42	44
Fifth IP [eV] (DFS) extr.				49	52	51	53	55	57
Atomic radius [Å]	1.49	1.42	1.36	1.31	1.26	1.22	1.18	1.14	1.10
								1.2	
Ionic radius [Å]	(+4) 0.71	(+5) 0.68	(+4) 0.86	(+5) 0.83	(+4) 0.80	(+3) 0.83	(+2) 0.80	(+3) 0.76	
	0.78								
Metallic radius [Å]	1.66	1.53	1.47	1.45	1.43	1.44	1.46	1.52	1.60
	1.50	1.39	1.32	1.28	1.26	1.28	1.32	1.38	1.47
Density [g/cm ³]	17	21.6	23.2	27.2	28.6	28.2	27.4	24.4	16.8
	23.2	29.3	35.0	37.1	40.7	37.4	34.8	28.7	23.7
Heat of sublimation [kcal/mol]				220	201	180	210	125	small
Standard electrode potential [V]	0 → +4								
	< 1.7								
Melting point [°C]	2,100								
Boiling point [°C]	5,500								
									Electron affinity [eV] ~ 1.6

The properties predicted for the 6d transition elements, i.e. elements 104–112 are summarized in Table 2. A detailed review of these predictions is given in [4].

The 7p and 8s Elements ($Z=113-120$)

Since the predicted lifetimes of the elements near $Z=114$ are in the order of years or even longer, the chemistry of these elements is of particular interest. The 7p electrons will be filled in with the elements

113–118, and the 8s electrons with the elements 119 and 120, as Table 1 shows. There is a great similarity in the occupation patterns of these valence electrons and those of the 6p elements Tl to Ra. However, the s electrons in the 7p elements are bound more strongly and the splitting of the 7p shell is greater than that in the 6p shell. The oxidation states of the elements 113–118 are expected to follow the known systematics of the group III to group VIII elements, so that the lower oxidation states will be preferred with increasing Z . Among the later members of this series, only the $7p_{3/2}$ electrons can

Table 3. Summary of the predictions for elements 113–120

Element	113	114	115	116	117	118	119	120
Chemical group	III A	IV A	V A	VI A	halogen	noble gas	alkali	alkaline earth
Stable oxidation states	1,3	2	1,3	2,4	3,1,5,−1	4,2,6	1, others	2, others
Ionization potentials [eV]								
I best value	7.4	8.5	5.5	7.5				
I DF calculation	8.0	8.9	5.5	6.6	7.7	8.7	4.8	6.0
II (DFS)	23.2	16.6	18.2	13.8		16.2	17.6	
III (DFS)	33.2	34.9	27.5	29.5				
IV (DFS)	45.1	45.6	48.5	39.5				
V (DFS)	59	60.6	59.3	63				
Standard electrode potential [eV]	(0→1) +0.6	(0→2) +0.9	(0→1) +1.5		(−1→0) +0.25 −0.5		(0→1) 2.9	(0→2) 2.9
Atomic radius [Å]			2.0				2.4	2.0
Ionic radius [Å]	(+1) 1.4	(+2) 1.2	(+1) 1.5 (+3) 1.0				(+1) 1.8	(+2) 1.6
Metallic radius [Å]	1.7 1.62	1.8 1.68	1.87 1.67	1.83 1.69			2.4	2.0
Density [g/cm ³]	16	14	13.5	12.9			3	7
Melting point [°C]	430	67	400		350 550	−15	0 30	680
Boiling point [°C]	1130	147 ~1000 2840			610	−10	630	1700
Heat of vaporization [kcal/g-atom]	31	9	33	10				
Heat of sublimation [kcal/g-atom]	34	10	34	47			10	33
Standard enthalpie [kcal/g-atom]	26±2	17±4	36±3	20±4	19±2			
Entropy [cal deg ^{−1} (g-atom) ^{−1}]	17	20	16					

be expected to remain chemically active, since (at least in j - j coupling) the $7p_{1/2}$ electrons form a spherical shell.

Apparently due to possible pronounced hybridization effects in the compounds of these elements, the most reliable predictions of atomic and ionic radii are based on a continuation of known trends in the periodic system, as done by Grosse [36], Keller *et al.* [29], and Cunningham [37]. Fricke, Greiner, and Waber [16] have also given predictions for the metallic radii of these elements.

The properties predicted for these elements are summarized in Table 3. A detailed review of the predictions is given in [4].

The 6f and 5g Elements ($Z=121$ to 154)

These elements belong to a very long transition series characterized by the simultaneous filling of the 6f and 5g electronic shells and for which there is no analogous series in the known region of the periodic table. Seaborg [38] has called these elements the superactinides. Unfortunately, although their chemistry would without a doubt be very interesting, nuclear stability calculations indicate that these elements will be very unstable and will thus have only very short half-lives.

At the beginning of the series, not merely two (as in the lanthanides and actinides) but four electron shells, namely the $8p_{1/2}$, $7p_{3/2}$, $6f_{5/2}$, and $5g_{7/2}$, are expected to compete for the electrons and determine

the chemical behavior of these elements. The results of self-consistent Hartree-Fock calculations for their ground-state configurations are given in Table 1.

Beginning with element 121, the $7p_{1/2}$ electrons will be filled in, and at least one of these electrons remains in all subsequent elements. This is a direct relativistic effect, which can only be understood as a consequence of the large spin-orbit splitting. During the filling of the electronic shells in these elements, some other electrons in addition to the 5g and 6f electrons will always remain in the ground-state configuration, in contrast to the behavior observed for the lanthanides and the actinides. The effective binding of an electron with large values of angular momentum will be accompanied by the radial collapse of the orbital, the centrifugal term $l(l+1)/r^2$ keeping it extended. Mann [7, 10] has calculated that this collapse will occur as late as element 125 as a consequence of the indirect relativistic effect.

The very low binding energies of all electrons in the $8s_{1/2}$, $8p_{1/2}$, $7d_{3/2}$, $6f_{5/2}$, and $5g_{7/2}$ shells suggest that most of these electrons can be oxidized, so that very high oxidation states might be possible in complex compounds. Hybridizations of unknown complex character should be possible, because these shells are extended far enough radially and are thus available for hybridization with different angular momenta where the energy remains approximately the same. The divalent ions can be expected to act as soft Lewis acids and possibly form complex ions readily. Crystal or ligand fields will influence the nature of hybridiza-

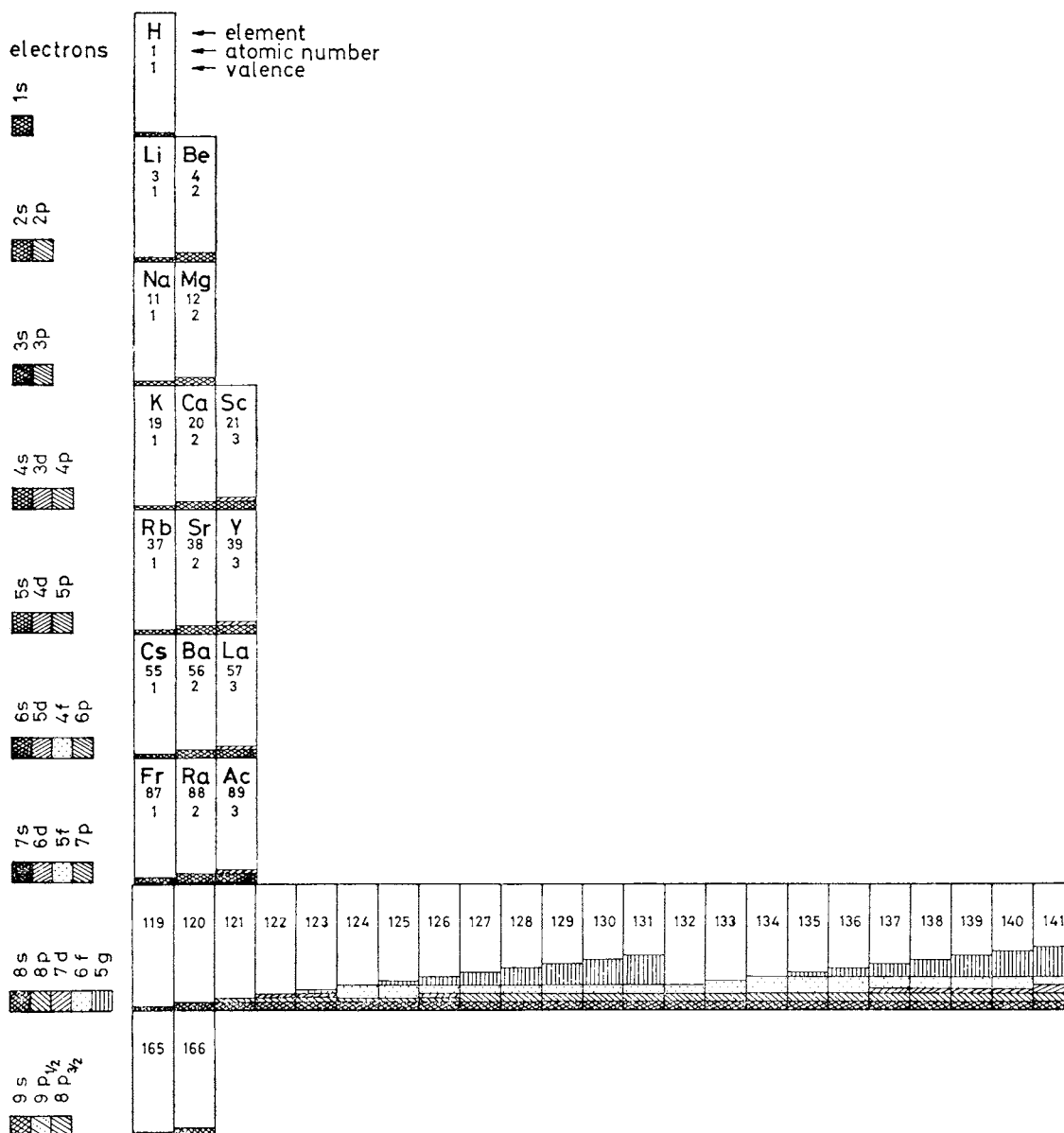


Fig. 3. Periodic system of elements continued up to element 172. Chemical symbols, atomic numbers, and oxidation states are also given. Outer electrons are drawn schematically [16]

tion. From a comparison of the energy eigenvalues for the different shells, one may conclude that oxidation states may well be very high at or near element 128 for complex compounds, but that the principal oxidation state of these elements in ionic compounds will be 4.

The expected contraction, analogous to the lanthanide and actinide contractions, is expected to be a very large effect owing to filling deep within the 5g and 6f shells, and should be about 0.02 Å per element.

The chemical behavior at the beginning of the series, where high oxidation states should be reached easily, should be very different from that at the end of the series, where stronger binding of the outer electrons will lead to a relatively noble character with normally low oxidation states. A detailed review of the predictions is given in [4].

The Elements $Z=155-172$ and $Z=184$

Since the remote possibility remains that some elements near the predicted magic proton number 164 may have half-lives long enough to permit their chemical study, a discussion of their chemistry is more than purely academic.

The calculations [7, 16] show that the elements 155–164 are formally the d transition elements of the 8th period. The relativistic enhancement of the subshells with $j=1/2$ will be so large in the elements 165–168 that the 9s and 9p_{1/2} states will be occupied instead of the 8p_{3/2} states, and the 8p_{3/2} electrons will not be filled in until the elements 169–172. The 9th period will therefore be quite analogous to the 2nd or 3rd period of the periodic system. A more detailed prediction for these elements is given in [4].

In a rather speculative study [20] of element 184 its

																		He 2 0														
																		B 5 3	C 6 4,2,-4	N 7 -3,2,5	O 8 -2	F 9 -1	Ne 10 0									
																		Al 13 3	Si 14 4	P 15 5,3,-3	S 16 6,4,-2	Cl 17 -1,5	Ar 18 0									
																		Ti 22 4,3	V 23 5,4,2	Cr 24 3,6,2	Mn 25 2,3,4,6,7	Fe 26 3,2	Co 27 2,3	Ni 28 2,3	Cu 29 2,1	Zn 30 2	Ga 31 3	Ge 32 4	As 33 3,-3,5	Se 34 4,6,-2	Br 35 -1,5	Kr 36 0
																		Zr 40 4	Nb 41 5,3	Mo 42 6,5,3	Tc 43 7	Ru 44 3,4,6,8	Rh 45 3,4	Pd 46 2,4	Ag 47 1	Cd 48 2	In 49 3	Sn 50 4,2	Sb 51 3,5	Te 52 4,6,-2	J 53 -1,5,7	Xe 54 0
Ce 58 3,4	Pr 59 3	Nd 60 3	Pm 61 3	Sm 62 3	Eu 63 3,2	Gd 64 3	Tb 65 3	Dy 66 3	Ho 67 3	Er 68 3	Tm 69 3	Yb 70 3,2	Lu 71 3	Hf 72 4	Ta 73 5	W 74 6	Re 75 7,4,-1	Os 76 4,6,8	Jr 77 3,4,6	Pt 78 4,2	Au 79 3,1	Hg 80 2,1	Tl 81 1,3	Pb 82 2,4	Bi 83 3,5	Po 84 2,4	At 85	Rn 86 0				
Th 90 4	Pa 91 5,4	U 92 6,5,4,3	Np 93 5,6,4,3	Pu 94 4,6,5,3	Am 95 3,4,5,6	Cm 96 3	Bk 97 3,4	Cf 98 3	Es 99 3	Fm 100 3,2	Md 101 2,3	No 102 2	Lw 103 3	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118				
142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164										
																							167	168	169	170	171	172				

chemical behavior has been found to be even simpler than for the first members of the superactinides. The most interesting overall question for the superheavy elements is of course their location in the periodic table. We therefore show in Fig. 3 the continuation of the periodic system up to $Z=172$ as taken from [16]. Up to element 121 everything looks very normal. The 8th period contains the superactinide series and it ends with element 164 below element 112. The elements 165 and 166 are alkaline and alkaline earth elements and from 167 to 172 we have relatively normal p elements, so that the 9th period will be very short again.

Conclusion

While the predictions presented here can be viewed as only the starting point for studying the chemical behavior of the superheavy elements, it seems very

reasonable that they will be quite realistic, at least up to $Z=120$. These elements are still close enough to the known part of the periodic system, so that neither relativistic effects nor other uncertainties will give rise to totally unexpected and new behavior. For the elements beyond 120, one must contend with the unknown chemical behavior of five rather loosely bound shells and with the totally unknown chemical behavior of g electrons. Conclusions can be drawn only by analogy and even the chemical classification of these elements can no longer be straightforward. The predictions of chemical behavior near the second quasistable island are supported only by the Hartree-Fock calculations. But these calculations are expected to be so accurate that minor changes in the results [20] will not change the chemical behavior significantly.

After many years of apparently fruitless and inconclusive searches for evidence of superheavy elements in

nature, the attempt to detect these elements has now shifted in the direction of heavy ion studies. Flerov, Oganessian, and coworkers [39] at Dubna have made chemical separations following the bombardment of uranium with xenon ions, as have Kratz, Liljenzin, and Seaborg [40] for the bombardment of uranium with argon and krypton ions. Both attempts had negative results. At the present time, a concentrated research effort is also underway at the heavy-ion accelerator laboratory (GSI) in Darmstadt, Germany. The hope persists that the use of very heavy ions, even up to uranium in connection with greater beam intensities will make the synthesis and identification of superheavy elements possible and thus may lead to a totally new realm of physics.

Work supported in part by GSI.

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Received September 12, 1975