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The Continuation of the Periodic Table up to $Z = 172$. The Chemistry of Superheavy Elements*

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The chemical elements up to $Z = 172$ are calculated with a relativistic Hartree-Fock-Slater program taking into account the effect of the extended nucleus. Predictions of the binding energies, the X-ray spectra and the number of electrons inside the nuclei are given for the inner electron shells. The predicted chemical behaviour will be discussed for all elements between $Z = 104$—120 and compared with previous known extrapolations. For the elements $Z = 121$—172 predictions of their chemistry and a proposal for the continuation of the Periodic Table are given. The eighth chemical period ends with $Z = 164$ located below Mercury. The ninth period starts with an alkaline and alkaline earth metal and ends immediately similarly to the second and third period with a noble gas at $Z = 172$.

Mit einem relativistischen Hartree-Fock-Slater Rechenprogramm werden die chemischen Elemente bis zur Ordnungszahl 172 berechnet, wobei der Einfluß des ausgedehnten Kernes berücksichtigt wurde. Für die innersten Elektronenschalen werden Voraussagen über deren Bindungsenergie, das Röntgenspektrum und die Zahl der Elektronen im Kern gemacht. Die voraussichtliche Chemie der Elemente zwischen $Z = 104$ und 120 wird diskutiert und mit bereits vorhandenen Extrapolationen verglichen. Für die Elemente $Z = 121$—172 wird eine Voraussage über das chemische Verhalten gegeben, sowie ein Vorschlag für die Fortsetzung des Periodensystems gemacht. Die achte chemische Periode endet mit dem Element 164 im Periodensystem unter Quecksilber gelegen. Die neunte Periode beginnt mit einem Alkali- und Erdalkalimetall und endet sofort wieder wie in der zweiten und dritten Periode mit einem Edelgas bei $Z = 172$.

Les éléments chimiques jusqu'à $Z = 172$ sont calculés à l'aide d'un programme Hartree-Fock-Slater relativiste en tenant compte de l'extension du noyau. On fournit des prédictions quant aux énergies de liaison, aux spectres X et au nombre d'électrons dans les noyaux pour les couches électroniques internes. Le comportement chimique prévu est discuté pour tous les éléments entre $Z = 104$–120 et comparé aux extrapolations connues auparavant. Pour les éléments $Z = 121$–172 on effectue des prévisions de propriétés chimiques et l'on propose un prolongement du Tableau Périodique. La huitième période chimique se termine à $Z = 164$ sous le mercure. La neuvième période débute avec un métal alcalin et alcalino-terreux et se termine comme la seconde et la troisième période avec un gaz rare à $Z = 172$.

Introduction

Recent developments in the calculation of the stability of superheavy elements suggest that nuclei with large proton numbers will exist with halflives up to many years [1–3]. Two regions of relative stability are expected between $Z = 110$–120

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and $Z = 154$–170. The experimental proof of their existence will be given for very short lifetimes either by observing their decay products or in observing their X-ray spectrum. If they exist longer than milliseconds, mass spectroscopy, optical spectroscopy or even chemical methods will be possible to detect them. It may be possible to find superheavy elements in small amounts on earth so that the knowledge of their chemical properties is not only interesting but most important [4]. Another possibility to find them will be in supernovae or neutron stars so that the X-ray astronomy might be able to detect them. The spectra are important because they are the first experimental information from a region where $Z\alpha$ (the perturbation parameter of the electromagnetic interaction) is large so that the calculations of the quantum electrodynamical effects can not be done by perturbation theory [5].

Theoretical predictions of the chemistry of superheavy elements can be done in two ways. First the behaviour of the well known elements as function of their chemical group and period can be extrapolated into the unknown regions. Secondly eigenvalues, wavefunctions, most stable configurations etc. can be calculated theoretically so that on this basis the predictions of the chemistry can be done in a more accurate way. Self consistent calculations in the region near $Z = 100$ and beyond were done by several authors to get binding energies [6] and most stable electron configurations [7–12]. In the present paper self consistent relativistic Hartree-Fock-Slater calculations with a finite nucleus are extended to elements up to $Z = 172$.

In part 1 a short summary of the theory is given [13–15]. In part 2 the results for the inner electron shells will be investigated. In part 3 the chemistry of the elements $Z = 104$–112, $Z = 113$–120, $Z = 121$–155 and $Z = 156$–172 will be discussed separately.

1. Theory

The basis for the calculation of the atomic many body problem was established by Hartree and Fock [16]. The atomic wave-functions given by one or more Slater determinants are determined from a variation of the total energy of the system

$$E_T = \frac{1}{n!} \int \langle \Psi^* | \boldsymbol{H} | \Psi \rangle \, d\tau_1 \, d\tau_2 \ldots d\tau_n \tag{1}$$

so that E_T is a minimum. Here n is the number of electrons and H is the Hamiltonian of the atomic problem:

$$\begin{gathered} \boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{H}_{\text{int}} \\ \boldsymbol{H}_0 = \sum_i \boldsymbol{H}_0^{(i)} = \sum_i \boldsymbol{T}^{(i)} - \sum_i \frac{Ze^2}{\boldsymbol{r}_i}, \qquad H_{\text{int}} = \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} . \end{gathered} \tag{2}$$

With this Hamiltonian the Hartree-Fock equations can be written in the form

$$\begin{aligned} \boldsymbol{T}^{(i)} \Psi_i(\boldsymbol{r}) - \frac{Ze^2}{\boldsymbol{r}_i} \Psi_i(\boldsymbol{r}) + \left[\sum_{k=1}^{n} \int \Psi_k^*(\boldsymbol{r}') \, \Psi_k(\boldsymbol{r}') \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r}'|} d\tau' \right] \Psi_i(\boldsymbol{r}) \\ - \left[\sum_{k=1}^{n} \int \frac{\Psi_i^*(\boldsymbol{r}) \, \Psi_k^*(r') \, \Psi_k(r) \, \Psi_i(r')}{\Psi_i^*(\boldsymbol{r}) \, \Psi_i(\boldsymbol{r})} \cdot \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r}'|} d\tau' \right] \Psi_i(\boldsymbol{r}) = E_i \Psi_i(\boldsymbol{r}) \end{aligned} \tag{3}$$

and the total energy is given by

$$E_T = \sum_i \int \Psi_i^*(\boldsymbol{r})\, \boldsymbol{H}_0\, \Psi_i(\boldsymbol{r})\, d\tau + \frac{1}{2} \sum_{i,k} \iint d\tau\, d\tau'\, \Psi_i^*(\boldsymbol{r})\, \Psi_k^*(\boldsymbol{r}') \cdot \frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|} \cdot [\Psi_i(\boldsymbol{r})\, \Psi_k(\boldsymbol{r}') - \Psi_i(\boldsymbol{r}')\, \Psi_k(\boldsymbol{r})] . \tag{4}$$

The first term in Eq. (3) is the kinetic energy of the i^{th} electron while the second term represents the interaction of the electron with the nucleus; for an extended nucleus the integral over the nuclear charge density must be introduced instead of Z. The third term is the direct interaction of the i^{th} electron with all electrons including the i^{th} electron itself and the last term is the exchange energy, which substracts as well the self interaction of the i^{th} electron included in the third term.

For real calculations two approximations can be made. First the electron density is assumed to be spherical symmetric, so that the third term in Eq. (3) can be easily calculated in the following way

$$\begin{aligned} V_i &= \sum_{k=1}^{n} \int \Psi_k^*(\boldsymbol{r}')\, \Psi_k(\boldsymbol{r}') \frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\, d\tau' = \int \varrho(\boldsymbol{r}') \frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\, d\tau' \\ &= 4\pi e^2 \left\{ \frac{1}{r} \int_0^r r'^2\, \varrho(r')\, dr' + \int_r^\infty r'\, \varrho(r')\, dr' \right\} . \end{aligned} \tag{5}$$

This is an approximation which becomes better with higher Z. Since the non-locality of the exchange term would cause great difficulties in the calculation (nevertheless it is treated rigorously in many Hartree-Fock calculations [7, 12]) it is useful to follow Lindgren [17] who gave a modified ansatz of Slater's [18] exchange approximation which is an optimized local approximation for the non-local exchange term

$$V_{\text{exch}} = -\frac{C}{r} (81 r^n (4\pi r^2\, \varrho(r))^m / 32\pi^2)^{1/3} . \tag{6}$$

By minimizing the energy Rosén *et al.* [19] have shown that for large Z the parameter C is about 2/3 and n and m are nearly 1. These values are valid over large regions of the Periodic Table. We have, therefore, adopted them also for the calculation of the superheavy elements. For very large radii the approximation (6) will be unphysical because it becomes too large and the total potential (direct plus exchange term) changes sign. Latter [20] circumvented this difficulty by defining the potential equal $1/r$ when the total potential reaches this value.

With these approximations for the potential, the many particle Dirac equation which is the only equation of motion for electrons known to be approximately valid for large Z where relativistic effects are large can be solved and for which eigenvalues and wave functions can be obtained. This Hartree-Fock-Slater procedure is only a first approximation because of possible strong quantum electrodynamical effects as well as some other effects which are not included in the single particle Dirac equation[1].

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[1] The discussion of the validity of this approximation with respect to the approximations of the potential will be given in part 2.

It is of the form

$$[c\boldsymbol{\alpha p} + (\boldsymbol{\beta} - 1) m_0 c^2 + V(r)]\, \Psi_i = \varepsilon_i \Psi_i \tag{7}$$

where $\boldsymbol{p}$ is the momentum operator, c the velocity of light, m_0 the rest mass of the electron, ε the total energy minus the rest energy and $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are the Dirac matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}. \tag{8}$$

$\boldsymbol{\sigma}$ represents the Pauli spin matrices and $\mathbf{1}$ is a 2×2 unit matrix.

The large and small components $f(r) = F(r)/r$ and $g(r) = G(r)/r$ are given by the coupled differential equations

$$\frac{d}{dr}\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = \begin{pmatrix} -\kappa/r & \alpha(\varepsilon - V(r)) \\ -\alpha(\varepsilon - V(r)) + \dfrac{2}{\alpha} & \kappa/r \end{pmatrix} \cdot \begin{pmatrix} F(r) \\ G(r) \end{pmatrix} \tag{9}$$

where α is the fine structure constant, $\kappa = -(l-j)(2j+1)$, j the total angular momentum and the energies are measured in Hartree units. The wave function is given by

$$\Psi_{n\kappa m}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} G_{n\kappa}(r)\, \Omega_{-\kappa m}(\hat{r}) \\ i F_{n\kappa}(r)\, \Omega_{\kappa m}(\hat{r}) \end{pmatrix} \tag{10}$$

with $\Omega_{\kappa m}$ being the angular momentum function. Eq. (9) has to be solved numerically. For an extended nucleus the wave function can be expanded around the origin

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = r^s \sum_{n=0}^{\infty} \begin{pmatrix} a_n \\ b_n \end{pmatrix} r^n \tag{11}$$

with

$$a_n = \frac{\alpha(\varepsilon - V(0))\, b_{n-1}}{s + \kappa + n}$$

and

$$b_n = \frac{\left(-\alpha(\varepsilon - V(0)) + \dfrac{2}{\alpha}\right) a_{n-1}}{s - \kappa + n}$$

and

$$s = |\kappa|, \qquad a_0 = (s-\kappa)^{1/2}, \qquad b_0 = (s+\kappa)^{1/2}.$$

The Hartree-Fock-Slater equations are solved by iteration: With a zero order electron density the potential and from that the wave functions and energy eigenvalues can be calculated which leads to a new electron density, etc. In order to assure stability of the solutions the electron density for the next iteration is given by [7, 14]

$$\varrho_{\text{new}} = \phi \varrho_{\text{calc}} + (1 - \phi)\, \varrho_{\text{old}} \tag{12}$$

where ϕ was most times set to be 0.2.

The iteration is continued until

$$\left|\frac{V_{\text{new}}(r)-V_{\text{old}}(r)}{V_{\text{old}}(r)}\right|<\delta \tag{13}$$

where $\delta \lesssim 10^{-5}$ measures the accuracy.

The nuclear density is given by a Fermi distribution

$$\varrho_K=\frac{\varrho_0}{1+\exp(4\ln 3(r-c)/t)} \tag{14}$$

with $c=1.2\,A^{1/3}$ and $t\approx 2.5\,fm$. For $Z>100$ the atomic weight A was taken [21] to be $A=0.00733\cdot Z^2+1.3\cdot Z+63.6$.

2. Results for the Inner Electron Shells

The energy eigenvalues for the hydrogen problem with a point nucleus resulting from the single particle Dirac equation are given by

$$E_n=mc^2\left[1+\left(\frac{Z\alpha}{n-(j+1/2)+\sqrt{(j+1/2)^2-(Z\alpha)^2}}\right)^2\right]^{-1/2}. \tag{15}$$

This implies that the energy eigenvalues for the 1*s* level are imaginary for $Z>137$. This formula is changed considerably for large Z if an extended nucleus is considered [14, 22, 23]. Nevertheless a physical limit is given by the binding energy of $-mc^2$ because at this value the level drops into the continuum of filled states of negative energy. This occurs approximately at $Z=Z_{\text{critical}}\approx 175$. It is not yet clear whether this really happens or – what is more likely – that quantum electrodynamical effects e.g. vacuum polarization and fluctuation, become so large that the single particle Dirac equation breaks down completely. One possibility is, that the levels do not drop into the negative continuum but they will asymptotically reach the lower continuum for very large Z which would mean that in nature a maximal field strength would exist [24].

Another possibility is that spontanous electron-positron production occurs at the critical Z-value. Theoretical considerations for the quantum electrodynamics of strong fields are given by Reinhardt [5] *et al.*, but practical calculations are still missing. Because of this uncertainty, eigenvalues and wave functions given by the Dirac equation are only a first approximation for the inner electron shells. It is, nevertheless assumed that the influence on the outer valence electrons will be small, so that the chemistry can be essentially predicted without the consideration of quantum electrodynamical effects. The results of calculations of the inner single particle energy eigenvalues (without these effects) are shown in Fig. 1 where the result of Pieper *et al.* [23] is drawn together with the eigenvalues for the Thomas-Fermi potential [25] and the HFS calculations. Uncertainties coming from the relativistic corrections for the exchange potential which are not included are expected to lower the eigenvalues. Quantum electrodynamical effects will probably have the opposite sign e.g. enlarge the single particle energies.

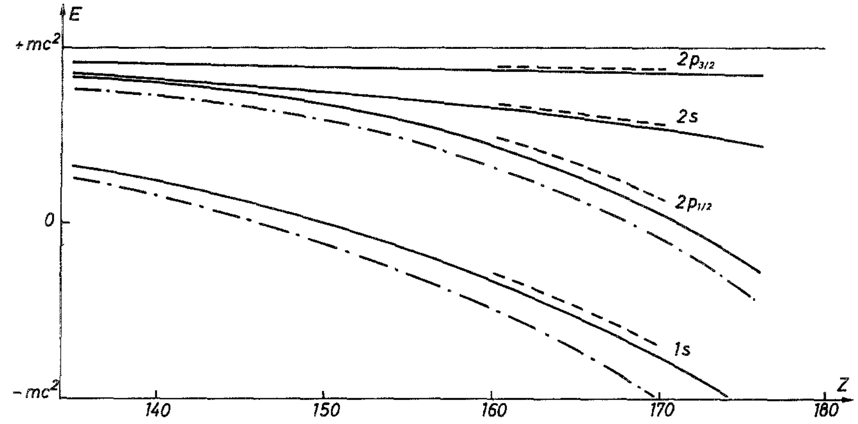


Fig. 1. The energy eigenvalues for the inner electron shells from the solution of the Dirac equation with an extended nucleus for the elements $Z = 135$—175 from Pieper *et al.* [23] (— · —), for the Thomas-Fermi potential [25] (——) and for $Z = 160$—170 with the selfconsistent potential (– – –)

Table 1. *The X-ray energies for some inner transitions for the elements* $Z = 156$, 160, 164 *and* 168. *These energies will be only a first approximation mainly because of the unknown quantum electrodynamical effects*

Transition	E (keV)			
	$Z = 156$	$Z = 160$	$Z = 164$	$Z = 168$
$2p_{1/2} - 1s_{1/2}$	381.8	402.2	420.1	434.9
$2p_{3/2} - 1s_{1/2}$	532.2	601.8	679.1	766.3
$3d_{3/2} - 2p_{1/2}$	192.5	242.6	305.7	367.7
$3d_{5/2} - 2p_{3/2}$	43.9	46.6	49.3	52.1

Therefore the absolute values of the binding energies as well as the observable transition energies in the X-ray spectrum as given in Table 1 for $Z = 156$, 160, 164 and 168 will be only approximately valid.

Table 2 shows, the influence of different parameters c and t of the Fermi type nuclear charge distribution on the energy eigenvalues for the elements $Z = 114$ and $Z = 164$. These results show that it is not easy to extract nuclear parameters of superheavy elements from their electronic X-ray spectrum, because several other uncertainties (see above) are of the same magnitude. Nevertheless the electron density and the number of electrons inside the nucleus can be calculated quite accurately. This magnitude is particular essential for the calculation of the electron capture which is an important decay process in the region of $Z = 164$ [26]. Differences of these quantities are measured as well in the isotope as in the isomer shift. The results are given in Table 3 for the elements Pb, U, $Z = 114$ and $Z = 164$. It is seen that even for $Z = 164$ only 5% of one electron are inside the nucleus, which means that the supposition that for large Z the inner electrons will be buried inside the nucleus is not quite correct. However, that this supposition contains some validity can be seen in Fig. 2 where the wave functions of some inner

Table 2. *Energy eigenvalues for the* 1*s and* $2p_{1/2}$ *levels for different parameters of the Fermi-type proton charge distribution for the elements* $Z = 114$ *and* $Z = 164$

	c (fm)	t (fm)	E_{1s} (keV)	$E_{2p_{1/2}}$ (keV)		c (fm)	t(fm)	E_{1s} (keV)	$E_{2p_{1/2}}$ (keV)
Z = 114	6.0	2.64	201.06	40.22	Z = 164	8.0	3.52	783.65	355.00
	7.0	3.08	200.74	40.20		9.0	3.95	753.99	331.73
	8.0	3.52	200.42	40.19		9.35	2.50	759.16	335.6o
	8.1	2.50	200.51	40.19		9.35	4.11	744.83	324.69
	8.1	3.56	200.39	40.19		10.0	4.39	729.18	312.81
	9.0	3.95	200.10	40.17		11.0	4.83	707.98	297.07

Table 3. *The number of electrons inside the nucleus for lead, uranium,* $Z = 114$ *and* $Z = 164$ *and their distribution to different shells*

Element	total	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$	$3s_{1/2}$	$3p_{1/2}$
Lead	$1.86\ 10^{-5}$	$7.66\ 10^{-6}$	$1.18\ 10^{-6}$	$9.47\ 10^{-8}$	$1.93\ 10^{-12}$	$2.73\ 10^{-7}$	$2.46\ 10^{-8}$
Uranium	$5.27\ 10^{-5}$	$2.11\ 10^{-5}$	$3.59\ 10^{-6}$	$3.98\ 10^{-7}$	$7.17\ 10^{-12}$	$8.54\ 10^{-7}$	$1.07\ 10^{-7}$
Z = 114	$4.21\ 10^{-4}$	$1.55\ 10^{-4}$	$3.40\ 10^{-5}$	$8.03\ 10^{-6}$	$6.52\ 10^{-11}$	$8.39\ 10^{-6}$	$2.20\ 10^{-6}$
Z = 164	$5.42\ 10^{-2}$	$1.24\ 10^{-2}$	$3.06\ 10^{-3}$	$9.23\ 10^{-3}$	$6.41\ 10^{-9}$	$7.04\ 10^{-4}$	$1.01\ 10^{-3}$

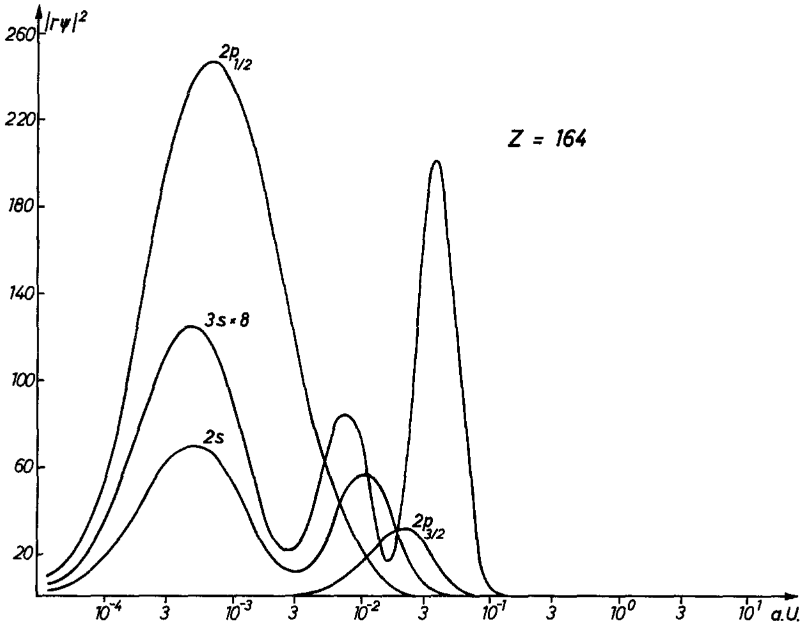


Fig. 2. The electron wave functions of some inner electrons for $Z = 164$

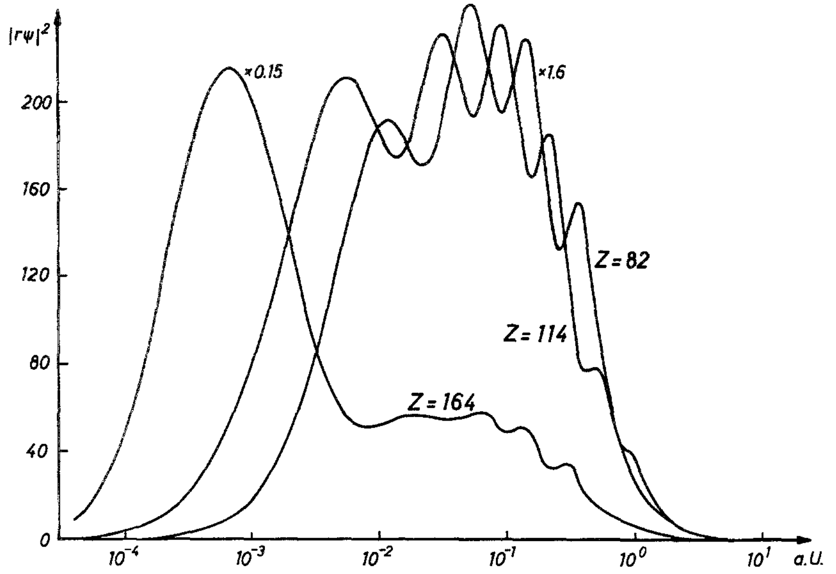


Fig. 3. The total electron densities of the elements Lead, $Z=114$ and $Z=164$. Most surprising is the first large maximum for $Z=164$

electrons of $Z=164$ are drawn. It is obvious that the first maxima are always very much enlarged. This is valid for all s and $p_{1/2}$ electrons whereas the maxima of the $p_{3/2}$ electrons are further away from the nuclear center. This behaviour leads to a total electron density of the form shown in Fig. 3, where the first peak near the nucleus for $Z=164$ is much larger than all the others.

3. The Chemistry of the Elements

a) The Elements $Z=104$–112

The experiments which prove that the element $Z=104$ is the chemical analog to Hafnium and Zirconium [27] and $Z=105$ behaves like Tantalum [28, 29] are the first indications for a normal continuation of the Periodic Table. This means that the elements $Z=104$–112 are the transition elements of the 7th period in which the 6d electrons determine the chemistry.

The predictions of the chemical and physical properties of these (and all other) superheavy elements has to be done in two ways: first the trends in the chemical groups and periods have to be extrapolated for high Z and, secondly, some results can be determined by use of HFS calculation. The validity of these calculations has to be shown in the known region of the Periodic Table.

The electron configuration of the outer electrons of the d transition elements is given by the rule $(n-1)\,d^m ns^2$ where n is the period and m goes from 1 to 10. This rule is not exactly valid in the 4th and 5th period in which in some elements the ns^2 electrons are removed and instead more d electrons are filled in. The principal difference between the elements of the 4th and 5th period to the 6th

Table 4. *The calculated total energies for different electron configurations of Ir, Pt and Au in comparison with the observed electron structure of the neutral atoms*

Element	electron configuration (plus Xe core)	$-E_T$ (Ry)	observed configuration
$_{77}$Ir	$5d^9\ 6s^0$	35672.783	
	$5d^8\ 6s^1$	35672.875	
	$5d^7\ 6s^2$	35672.910	$5d^7\ 6s^2$
$_{78}$Pt	$5d^{10}\ 6s^0$	36847.478	
	$5d^8\ 6s^2$	36847.522	
	$5d^9\ 6s^1$	36847.533	$5d^9\ 6s^1$
$_{79}$Au	$5d^9\ 6s^2$	38048.395	
	$5d^{10}\ 6s^1$	38048.451	$5d^{10}\ 6s^1$

period is caused by the 14 rare earth elements which come between the insertion of the $6s^2$ and the $5d$ electrons in the 6th period. This means that the $6s^2$ electrons are bound stronger than the analogous electrons of the 4th and 5th period. This effect becomes even larger for the high elements because the higher ns electrons drop deep into the atom so that they feel the very strong potential near the nucleus and thus their binding energy increases from period to period. Because of these two reasons the $6s^2$ shell is always filled in the 6th period except for the elements Pt and Au. The HFS calculation reproduces this behaviour exactly as it is seen in Table 4 where the total energies are given for different electron configurations.

Another test of the HFS calculations can be obtained in the region of the actinides. It is shown in Table 5 that even for these elements the most stable configurations for the atoms are reproduced. For Np it is experimentally not clear, because both the configurations $5f^5\,7s^2$ and $5f^4\,6d^1\,7s^2$ have been reported. The calculation for Cm gives the wrong answer. An explanation frequently suggested in the past is that the configuration $f^7\,ds^2$ is more stable because of a half-filled shell. However because of the large spin-orbit splitting, the configuration might better be represented as $(f_{5/2})^6\,(f_{7/2})^1\,(d_{3/2})^1\,s^2$. Possibly a better explanation is that the upper sub-shell actively competes with the $7d$ shell. With increasing Z the eigenvalue for $f_{7/2}$ falls more rapidly than that for $d_{3/2}$ and all successive actinide elements do not have an occupied d orbital in the ground state.

It is expected for the d elements of the 7th period ($Z = 104$–112) that the $7s$ electrons are bound even stronger than the analogous $6s$ electrons in the 6th period. Therefore the electron configuration of the transition elements in the 7th period will be given exactly by the rule $(n-1)d^m ns^2$ [9] as it is verified in the calculations shown in Table 6. Fig. 4 shows the calculated energy eigenvalues of the outer d and s electrons for the elements $Z = 104$–112, $Z = 156$–164 and $Z = 72$–80 for comparison. The trend is simple: the s electrons are bound stronger in the higher periods whereas the d electrons are lowered and, in addition, the shell is split more and more into the two subshells.

Fig. 5 shows the experimental first ionization energies of the transition elements for the 4th, 5th and 6th period as well as the calculated values for the 6th to the 8th period. Because the $6d$ shell is filled uniformly the ionization energy

Table 5. *The calculated total energies of the Actinides for different electron configurations and a comparison with the observed electron structure of the neutral atoms*

Element	electron configuration (plus Rn core)	$-E_T$ (Ry)	observed configuration
89^{Ac}	$5f^1\ 7s^2$	51497.447	
	$6d^1\ 7s^2$	51497.643	$6d^1\ 7s^2$
90^{Th}	$5f^2\ 7s^2$	52994.072	
	$5f^1\ 6d^1\ 7s^2$	52994.204	
	$6d^2\ 7s^2$	52994.247	$6d^2\ 7s^2$
91^{Pa}	$5f^3\ 7s^2$	54520.874	
	$5f^1\ 6d^2\ 7s^2$	54520.902	
	$5f^2\ 6d^1\ 7s^2$	54520.946	$5f^2\ 6d^1\ 7s^2$
92^{U}	$5f^2\ 6d^2\ 7s^2$	56077.247	
	$5f^4\ 7s^2$	56077.360	
	$5f^3\ 6d^1\ 7s^2$	56077.375	$5f^3\ 6d^1\ 7s^2$
93^{Np}	$5f^3\ 6d^2\ 7s^2$	57665.126	
	$5f^4\ 6d^1\ 7s^2$	57665.327	$5f^4\ 6d^1\ 7s^2$
	$5f^5\ 7s^2$	57665.369	
94^{Pu}	$5f^4\ 6d^2\ 7s^2$	59283.974	
	$5f^5\ 6d^1\ 7s^2$	59284.249	
	$5f^6\ 7s^2$	59284.352	$5f^6\ 7s^2$
95^{Am}	$5f^5\ 6d^2\ 7s^2$	60935.216	
	$5f^6\ 6d^1\ 7s^2$	60935.562	
	$5f^7\ 7s^2$	60935.641	$5f^7\ 7s^2$
96^{Cm}	$5f^6\ 6d^2\ 7s^2$	62617.762	
	$5f^7\ 6d^1\ 7s^2$	62618.078	$5f^7\ 6d^1\ 7s^2$
	$5f^8\ 7s^2$	62618.211	
97^{Bk}	$5f^7\ 6d^2\ 7s^2$	64334.602	
	$5f^8\ 6d^1\ 7s^2$	64334.981	
	$5f^9\ 7s^2$	64335.161	$5f^9\ 7s^2$
98^{Cf}	$5f^8\ 6d^2\ 7s^2$	66086.846	
	$5f^9\ 6d^1\ 7s^2$	66087.284	
	$5f^{10}\ 7s^2$	66087.517	$5f^{10}\ 7s^2$
99^{Es}	$5f^9\ 6d^2\ 7s^2$	67872.847	
	$5f^{10}\ 6d^1\ 7s^2$	67873.345	
	$5f^{11}\ 7s^2$	67873.621	$5f^{11}\ 7s^2$
100^{Fm}	$5f^{10}\ 6d^2\ 7s^2$	69694.149	
	$5f^{11}\ 6d^1\ 7s^2$	69694.704	
	$5f^{12}\ 7s^2$	69695.027	$5f^{12}\ 7s^2$
101^{Md}	$5f^{11}\ 6d^2\ 7s^2$	71551.283	
	$5f^{12}\ 6d^1\ 7s^2$	71551.896	
	$5f^{13}\ 7s^2$	71552.261	$5f^{13}\ 7s^2$
102^{No}	$5f^{12}\ 6d^2\ 7s^2$	73442.397	
	$5f^{13}\ 6d^1\ 7s^2$	73443.066	
	$5f^{14}\ 7s^2$	73443.480	$5f^{14}\ 7s^2$
103^{Lw}	$5f^{14}\ 6d^1\ 7s^2$	75374.726	$5f^{14}\ 6d^1\ 7s^2$

Table 6. *The calculated total energies for different electron configurations of the elements* $Z = 104$–112

Element	electron configuration (+Rn core + $5f^{14}$)	$-E_T$ (Ry)	expected configuration
Z = 104	$6d^3\ 7s^1$	77343.974	
	$6d^2\ 7s^2$	77344.221	$6d^2\ 7s^2$
Z = 105	$6d^4\ 7s^1$	79352.600	
	$6d^3\ 7s^2$	79352.827	$6d^3\ 7s^2$
Z = 106	$6d^5\ 7s^1$	81401.167	
	$6d^4\ 7s^2$	81401.455	$6d^4\ 7s^2$
Z = 107	$6d^6\ 7s^1$	83490.694	
	$6d^5\ 7s^2$	83490.975	$6d^5\ 7s^2$
Z = 108	$6d^7\ 7s^1$	85622.194	
	$6d^6\ 7s^2$	85622.465	$6d^6\ 7s^2$
Z = 109	$6d^9\ 7s^0$	87796.593	
	$6d^8\ 7s^1$	87796.858	
	$6d^7\ 7s^2$	87797.103	$6d^7\ 7s^2$
Z = 110	$6d^{10}\ 7s^0$	90015.309	
	$6d^8\ 7s^1\ 7p^1$	90015.552	
	$6d^9\ 7s^1$	90015.560	
	$6d^8\ 7s^2$	90015.788	$6d^8\ 7s^2$
Z = 111	$6d^8\ 7s^2\ 8s^1$	92279.281	
	$6d^8\ 7s^2\ 7p^1$	92279.532	
	$6d^{10}\ 7s^1$	92279.611	
	$6d^9\ 7s^2$	92279.821	$6d^9\ 7s^2$
Z = 112	$6d^9\ 7s^2\ 7p^1$	94590.086	
	$6d^{10}\ 7s^2$	94590.421	$6d^{10}\ 7s^2$

curve of these elements is expected to be more rectilinear than for the $3d$ and $4d$ elements where nearly no systematics can be seen. The interpretation for the 6th period instead is very lucid. The decrease from La to Hf results from the $(4f)^{14}$ elements in between. The break between W and Re comes from the spin-orbit coupling: after the $5d_{3/2}$ subshell the $5d_{5/2}$ subshell is filled in Re. The linear behaviour is not continued for Pt and Au where the $5d$ shell is going to be closed earlier at the cost of the $6s$ electrons. The calculated ionization energies for the 6th period fits very well to the experimental curve. The values for the 7th period are expected to be linear with only one break where the $6d_{5/2}$ shell begins to be filled. The calculated values in Fig. 5 show exactly this behaviour. The absolute values are enlarged by 0.2 eV which equals the difference between the experimental and the calculated values for the 6th period.

The metallic radii of the d elements for all periods are shown in Fig. 6 [30]. The large reduction at the beginning and the large increase at the end of the shell stems mainly from the fact that electrons are lost to the crystal at the beginning of the shell so that the d character of the metallic binding is very large (Pauling [30]). Hence the radius decreases. The opposite is true at the end of the d elements

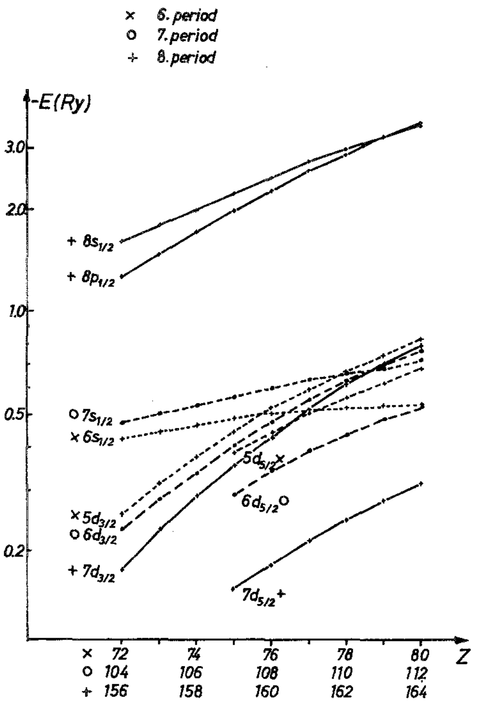


Fig. 4. The calculated energy eigenvalues of the outer electron shells for the elements $Z=72$—80, $Z=104$—112 and $Z=156$–164

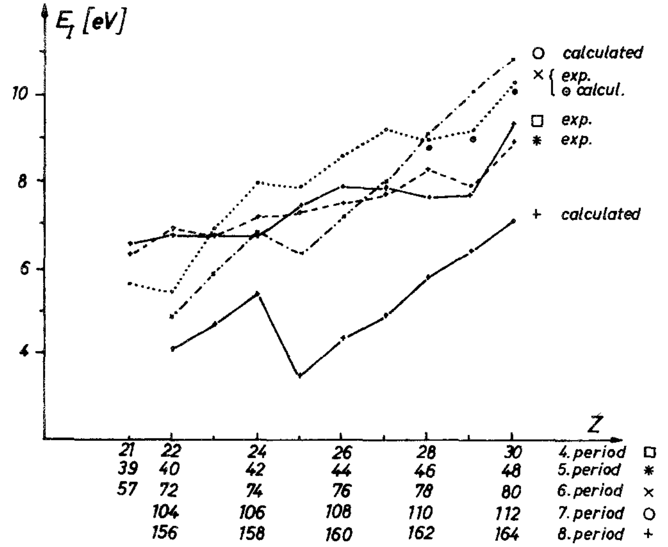


Fig. 5. The experimental first ionization energies of the transition elements from the 4th to the 6th period and the calculated values from the 6th to the 8th period

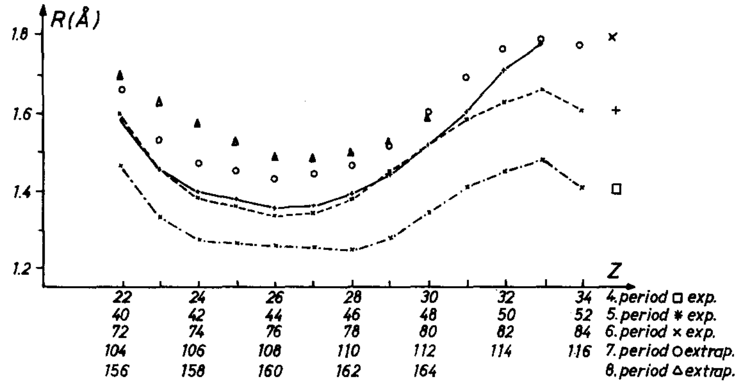


Fig. 6. The experimental metal radii of the transition elements from the 4th to the 6th period and the extrapolation for the 7th and 8th period. The values for the following *p* elements are also shown

so that the radius smoothly goes into the covalent radius at the beginning of the *p* elements which are also shown in Fig. 6. The metallic radius becomes larger from the 4th to the 5th period but stays rather constant in the 6th period. The normal expansion is nearly compensated by the lanthanide contraction since these elements are filled in between. The elements $Z = 104$–112 are totally analogous to the 5*d* elements in their position in the Periodic Table and because the actinide contraction is not as large as that of the lanthanides, the radius of these atoms will become larger again. From comparisons of the principal maxima of the outer electron shells in the 5th, 6th and 7th period it is expected that the metallic radii will increase by about 0.1 Å. This value will be smaller at the beginning and somewhat larger at the end of the 7th period. In contrast to that, the atomic radii of the 5*d* and 6*d* elements will be nearly the same because of the somewhat smaller radius of the 7*s* wave function compared to the analogous 6*s* wave function. The total electron density at the surface is in both cases quite similar.

The ionization energy (the difference between the total binding energy of the atom and the ion) is a valuable quantity for theoretical predictions of the valency of the elements. The free energy of hydration and of the crystal respectively has to be known additionally, since only the difference of both values gives the oxidation potential. This value is up to now, quantitatively not calculable. Nevertheless qualitatively there is a connection between the oxidation potential and ionization energy on one side and the size of the atom or ion and the radial distribution of the wave functions on the other side. Another point is that the ionization energy becomes larger if the wave function of a new additional electron is not screened by the other electrons with the same wave function. This altogether means that the ionization energy curve for the lanthanides is very flat and, therefore, the valency is always nearly the same. The curve becomes steeper for the actinides because the 5*f* electrons are not so buried in the atom as the 4*f* electrons in the lanthanides and thus the valency at the beginning is larger whereas it becomes smaller at the end. This is also true for the *d* elements, for which the ionization energy curves as shown in Fig. 5 become steeper for the higher period.

Since the elements of the 5th and 6th period have nearly the same radii their chemical behaviour will be very much the same as well as their possible oxidation states. The best example is the strong chemical relationship between Hafnium and Zirconium. The relative large ionization energy at the end of the 6th period confirms that their chemical behaviour is mainly inactive. Therefore the elements from Os to Hg are called noble metals. On the other hand when they are bound in chemical compounds they prefer the high oxidation states which mainly comes from the energetical separation of $d_{3/2}$ and $d_{5/2}$ subshell and the partial cancellation of the symmetry of the filled *d* shell. In addition the radius of the $d_{5/2}$ subshell becomes larger for the higher periods.

The conclusions from these considerations for the transition elements $Z=104$–112 are the following: Because of the probably larger metallic and covalent radii and the relative small ionization energy at the beginning of this group it is quite clear that these elements will reach their maximal oxidation states. The same argument is valid in the middle of these elements. The characteristic stability of the filled *d* shell will be even smaller because of the two separated subshells. Nevertheless the high ionization energies at the end shows that these elements will be good noble metals and their chemical dominant form will be the metallic one. This characteristic stems mainly from the fact that the 7*s* electrons have a larger ionization energy than in the periods before because of the larger relativistic effects and therefore this spherical symmetric 7*s* wave function at the surface of the atom prevents these elements from being too chemically active. If, however, the elements are bound in real chemical compositions and the 7*s* electrons are ionized then the *d* electrons will be ionized much easier than in the periods before so that they will reach more easily higher oxidation states.

In Table 7 the results for the elements $Z=104$–112 are summarized. Only those values are tabulated which can be determined directly or indirectly from the calculations. Quantities which can be determined only by extrapolation are deleted in this table. The chemistry of the elements $Z=104$ [31] and $Z=104$–112 has been also discussed by Cunningham [32] by pure extrapolations of the trends of the known elements.

Table 7. *The expected properties for the elements* $Z=104$–112 *which can be deduced directly or indirectly from the HFS calculations*

Element	104	105	106	107	108	109	110	111	112
Atomic weight	278	281	283	286	289	292	295	298	301
Chemical group	IV A	V A	VI A	VII A	VIII	VIII	VIII	I B	II B
Outer electrons	$7s^2\ 6d^2$	$7s^2\ 6d^3$	$7s^2\ 6d^4$	$7s^2\ 6d^5$	$7s^2\ 6d^6$	$7s^2\ 6d^7$	$7s^2\ 6d^8$	$7s^2\ 6d^9$	$7s^2\ 6d^{10}$
Most propable oxydation state	+ 4	+ 5	+ 6,4	+ 7,6,5	+ 8,6,4	+ 6,4	+ 4,6	+ 3,5	+ 2,4
Ionisation potential (eV)	5.1	6.2	7.1	6.5	7.4	8.2	9.4	10.3	11.1
Metalic radius (Å)	1.66	1.53	1.47	1.45	1.43	1.44	1.46	1.52	1.60
Density (g/cm^3)	17.0	21.6	23.2	27.2	28.6	28.2	27.4	24.4	16.8

b) The Elements $Z = 113$–120

The lifetimes of the elements near $Z = 114$ are expected to be years or even more [3]. Hence the knowledge of the chemistry of these elements is most important. This is especially true because it should be possible to find small amounts of these elements on earth [4].

As it is expected from a simple continuation of the Periodic Table the six $7p$ electrons will be filled between $Z = 113$ and $Z = 118$. The total energies for different configurations from the HFS-calculation are given in Table 8. The energy eigenvalues of the outer electrons of the p elements of the 6th and 7th period are drawn in Fig. 7. The great similarity in the structure of the valence electrons is noticed. However, two significant differences occur: The analogous s electrons are bound stronger for higher Z which results from the fact that they have a large probability density near the nucleus so that they feel the deep potential. This is especially true because the relativistic effects are fully included by use of the Dirac equation. The splitting of the $7p$ shell has increased compared to the $6p$ shell which is connected with a partial cancellation of the spherical symmetry from which an observable larger chemical activity results. This can be seen as well in Fig. 8 where the experimental ionization energies are drawn from the 2nd to the 6th period together with the calculated values for the 6th, 7th and 9th period. The ionization energy in each period raises linearly with only one break between the configuration p^3 and p^4. This behaviour is caused by the half filled shell where the 3 electrons occupy the three possible p orbitals with parallel spin. The pairing energy is negative so that the ionization energy is smaller for the 4th electron. This effect of the Russel-Saunders coupling is very significant in the first periods but becomes smaller for the higher periods because the $L - S$ coupling changes to the intermediate coupling and from there to the spin-orbit coupling.

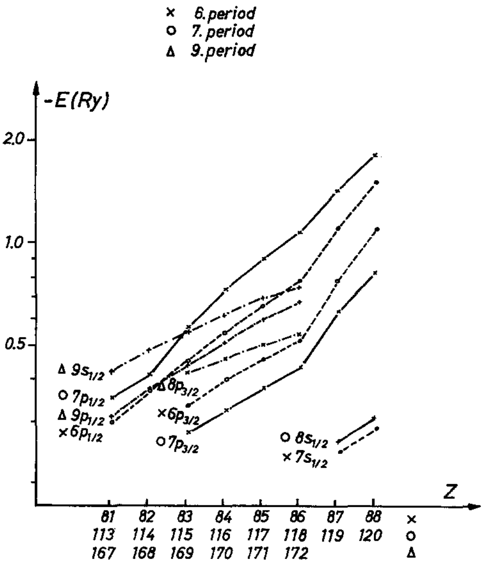


Fig. 7. The calculated energy eigenvalues of the outer electron shells of the elements $Z = 81$—88, $Z = 113$—120 and $Z = 167$—172

Table 8. *The calculated total energies for different electron configurations for the elements $Z = 113$–120*

Element	electron configuration (plus Rn core + $5f^{14}$ $6d^{10}$)				total energy	expected configuration
Z	$7s_{1/2}$	$7p_{1/2}$	$7p_{3/2}$	$8s_{1/2}$	$-E_T$ (Ry)	
113	2	-	-	1	96948.260	
	2	1	-	-	48.552	$7s^2$ $7p^1$
114	2	1	-	1	99355.408	
	2	1	1	-	55.516	
	2	2	-	-	55.771	$7s^2$ $7p^2$
115	2	2	-	1	101813.125	
	2	2	1	-	13.256	$7s^2$ $7p^3$
116	2	2	-	2	104322.218	
	2	2	1	1	22.487	
	2	2	2	-	22.678	$7s^2$ $7p^4$
117	2	2	1	2	106885.091	
	2	2	2	1	85.429	
	2	2	3	-	85.708	$7s^2$ $7p^5$
118	2	2	2	2	109503.051	
	2	2	3	1	03.447	
	2	2	4	-	03.757	$7s^2$ $7p^6$
119	2	2	3	2	112178.331	
	2	2	4	1	78.788	$7s^2$ $7p^6$ $8s^1$
120	2	2	4	2	114912.660	$7s^2$ $7p^6$ $8s^2$

In the 6th period the break between p^3 and p^4 has vanished but instead a break between p^2 and p^3 has begun as it is expected from the spin-orbit coupling in the $p_{1/2}$ and $p_{3/2}$ subshells. This break becomes even larger for the elements $Z = 113$–118, so that the ionization energy of the element $Z = 114$ is nearly as large as the same value for the "noble gas" at $Z = 118$. The experimental and the calculated curves for the 6th period are very parallel with a difference of 0.8 eV. (This difference may be interpreted as the influence of the $1/r$ approximation of the potential which acts mostly on the wave function at the surface of the atom.) Therefore the first ionization energies of the elements $Z = 113$–118 can be enlarged by 0.8 eV to get the possible realistic values. Keller *et al.* [33] obtained a correction factor of 0.72 eV for $Z = 114$ from an extrapolation of the correction factor as function of the period in one chemical group. It is not too effective to do this for each chemical group because the numerical error of the calculation is about 0.1 eV so that a correction factor of 0.8 eV for all elements will be sufficient.

The radii of the elements $Z = 113$–118 can be given only with large error bars as it was discussed for the d elements. The metallic character of the chemical bond becomes much weaker for the first p elements so that the valence electrons become more localized again and, therefore the radius will follow the normal contraction with increasing Z (see Fig. 6). The metallic and the covalent radii respectively have a maximum at the configuration p^3 where the metallic character has nearly totally vanished.

The oxidation states of the elements $Z = 113$–118 will follow the systematics for the chemical groups III to VIII where the elements with high Z prefer the lower oxidation states. This is the expression of the fact that the s electrons with their greater binding energy loose their chemical activity more and more so that

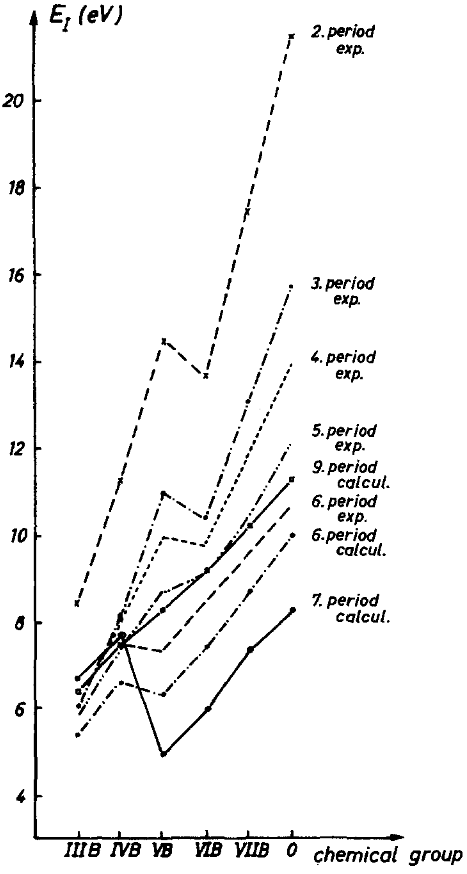


Fig. 8

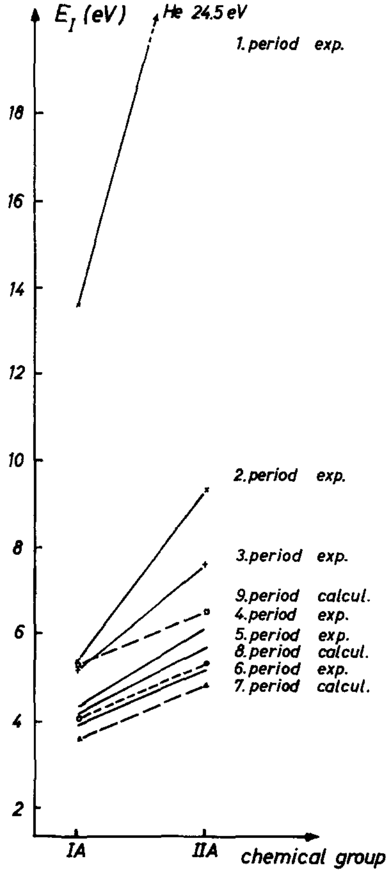


Fig. 9

Fig. 8. The experimental and calculated first ionization energies of the p elements from the 2nd to the 9th period

Fig. 9. The experimental and calculated first ionization energies of the alkali and alkaline earth elements from the 1st to the 9th period

the p electrons will be the only valence electrons. In the chemical group III the oxidation state is 3, only the valency of Tl is mostly 1 so that $Z = 113$ is expected to have only the oxidation state 1. From Si to Pb in the chemical group IV the oxidation state 4 decreases and 2 increases because of this reason. The valency of 4 especially in the chemical group IV is connected with a sp^3 hybridization. The energetical difference of the s and p electrons increases for the higher periods. Also the spin of the p electrons couples very strong to their own orbital angular momentum. Therefore a sp^3 hybridization is no more possible for $Z = 114$ which means that *the predominant oxidation state of* $Z = 114$ *is* 2. Keller *et al.* [31, 33] came to the same result. A larger spreading of the valence electrons in the 7th period may also lower the covalent bonding so that the lower oxidation states will be preferred as well [34]. But this effect may be not too large because the radius will

Table 9. *The expected properties for the elements Z = 113–120. The radii were deduced from a comparison of the maxima of the outer wavefunctions with the chemical analog elements*

Element	113	114	115	116	117	118	119	120
Atomic weight	304	307	310	313	316	319	322	325
Chemical group	III B	IV B	V B	VI B	VII B	0	I A	II A
Outer electrons	$7s^2\ 7p^1$	$7s^2\ 7p^2$	$7s^2\ 7p^3$	$7s^2\ 7p^4$	$7s^2\ 7p^5$	$7s^2\ 7p^6$	$8s^1$	$8s^2$
Most propable oxydation stat	+ 1	+ 2	+ 3,1	+ 2,4	+1,3,-1	0,4	+ 1	+ 2
Ionisation potential	7.5	8.5	5.9	6.8	8.2	9.0	4.1	5.3
Metalic radius (Å)	1.69	1.76	1.78	1.77			2.6	2.0
Covalent radius (Å)						2.2		
Density (g/cm^3)	14.7	15.1	14.7	13.6			4.6	7.2

not change much when going from the 6th to the 7th period because of the stronger binding and the smaller wave functions of the 7*s* electrons. However, strong oxidizers might form some compounds by some sort of *sd* hybridizations.

The $7p_{3/2}$ subshell begins at $Z = 115$ with a binding energy which is only half in magnitude compared to the $7p_{1/2}$ electrons so that the elements $Z = 115$, 116, and 117 will have 1, 2, and 3 as their normal oxidation states. The higher oxidation states will be possible only for strong oxidizers. The "noble gas" at $Z = 118$ will be a very weak noble gas in the sense of He and Ar but as well in comparison to Xe and Rn. The ionization energy is so small that normal covalent bondings are expected with oxidation states of 4 and 6. The extrapolation of Cunningham [35] expects a boiling point of −15° C so that it will be nearly a "noble fluid".

In the elements $Z = 119$ and 120 the 8*s* electrons will be filled in which are bound very tightly and therefore these two elements are expected to be chemically very similar to Cs and Ba or to Fr and Ra. Their main oxidation state will be 1 and 2 as it is normal for an alkali and alkaline earth metal. In Fig. 9 the first ionization potentials are shown for both these chemical groups. The absolute values as well as the steepness of the curves are smaller for higher *Z*. The absolute values decrease again for $Z = 119$ and 120 and even more for the 9th period, which mainly results from the effect of the strong field near the nucleus. In addition, the radius for the 8*s* wave function reduces (but the radii for some inner electron shells increases) in comparison to the analogous elements, so that the atomic radii will be the same as it was at Fr and Ra.

In Table 9 the chemical and physical properties for the elements $Z = 113$–120 are tabulated. Grosse [36] and Cunningham [35] extrapolate the properties of the elements $Z = 117$–120 only from the trend in the same chemical groups. Quite similar extrapolations to ours are those from Keller *et al.* [31].

c) *The Elements* $Z = 121$–155, *the Superactinide Series*

Some papers were published on the calculation of the most stable electron configurations of the elements near $Z = 126$ [10–12, 37] where some years ago – in analogy to the magic neutron number 126 – stable elements were expected.

Table 10. *The most stable electron configurations of the Superactinides* $Z = 121$–155 *from the calculations of Mann and Waber* [12]

Element	electron configuration from Mann and Waber(12) (plus Z = 118 core)						
Z	$8s_{1/2}$	$8p_{1/2}$	$5g_{7/2}$	$5g_{9/2}$	$6f_{5/2}$	$6f_{7/2}$	$7d_{3/2}$
121	2	1	-	-	-	-	-
122	2	1	-	-	-	-	1
123	2	1	-	-	1	-	1
124	2	1	-	-	3	-	-
125	2	1	1	-	3	-	-
126	2	2	2	-	2	-	-
127	2	2	3	-	2	-	-
128	2	2	4	-	2	-	-
130	2	2	6	-	2	-	-
132	2	2	8	-	2	-	-
134	2	2	8	-	4	-	-
136	2	2	8	2	4	-	-
138	2	2	8	4	3	-	1
140	2	2	8	6	3	-	1
141	2	2	8	7	2	-	2
142	2	2	8	8	2	-	2
144	2	2	8	10	1	-	3
145	2	2	8	10	3	-	2
146	2	2	8	10	4	-	2
149	2	2	8	10	6	-	3
150	2	2	8	10	6	-	4
152	2	2	8	10	6	3	3

Nowadays it is believed that this will be not true and that the magic proton number occurs instead at $Z = 114$. If this is correct, the lifetimes for nuclei around $Z = 126$ will be too small to detect them. Nevertheless the chemistry would be very interesting. Four electron shells, namely $7d_{3/2}$, $8p_{1/2}$, $6f_{5/2}$ and $5g_{7/2}$, are expected to be filled more or less simultaneously. The most stable configurations for the elements $Z = 121$–155 from the calculation of Mann and Waber [12] are given in Table 10. The chemical interpretation will be quite difficult because the chemistry with g electrons does not exist up to now. The very small binding energy of all electrons in these four shells plus the $8s$ shell makes it plausible that all electrons might be oxidized at the beginning, so that element $Z = 126$ could have 8 as the normal oxidation state. Hybridizations of unknown character will be possible because there are electrons with nearly the same energy but angular momenta between 0 and 4. Very high oxidation states for the following elements which are unknown up to now might be energetically possible.

When the $5g$ shell is filled at $Z = 144$ and the $6f$ shell at $Z = 154$ the $8p_{1/2}$ electrons are bound so strong that they are chemically totally inactive. This means that the superactinide series has $18 + 14 + 2$ members. The elements lanthanum and actinium are usually not counted as members of the lanthanides and actinides. Although element $Z = 121$ has the configuration s^2p^1 in the ground state the chemical behaviour will be similar to La and Ac. This means that the superactinide series starts with element $Z = 122$.

The main oxidation state will be reduced to 6 at $Z = 132$ and in the region of $Z = 144$ a valency of 3 or 4 will be normal. At the end the oxidation state will be maximally 2 (and possibly 0) because the $6f$ shell is buried deep inside the electron cloud and the $8p_{1/2}$ and $8s$ electrons are bound so strongly that they will be chemically inactive. Only the few electrons in the outer electron shells (see

Table 10) can be oxidized. The calculations show that in element 154 the f shell is filled and no d electron- or other wave functions are outside the $8s$ and $8p_{1/2}$ shell. This would mean that this element would be chemically very inactive with a behaviour of a noble gas. This is especially interesting because the newest calculations of the nuclear stability [3] show that the center of the island of stability lies a bit lower than 164.

The lanthanide contraction of about 0.044 Å per element is larger than the actinide contraction of about 0.03 Å per element [30], because the $4f$ wave function is more localized than the $5f$ wave function. An analogous contraction is expected in the superactinide series. The total effect will be very large because of the 32 electrons which will be filled in the deep $5g$ and $6f$ shell. From a comparison of the outer electron wave functions of the lanthanides of the actinides and of the superactinides a contraction of about 0.02 Å per element can be expected.

d) The Elements $Z = 156$–172

The latest very detailed calculations of Grumann *et al.* [3] make it plausible that a large island of stability will exist around the magic proton number $Z = 164$. Lifetimes of minutes and possibly years are expected between $Z = 152$ and $Z = 168$. Therefore the knowledge of the chemistry of these elements is very important.

In Table 11 the total energies of the most stable electron configurations are given. The differences are not large but nevertheless the trend of the calculated most stable electron configurations are very plausible so that – based on this systematics – the results are credible.

Formally these elements are the transition elements of the 8th period. The $8p_{1/2}$ shell is already filled up to $Z = 123$ and thus the filling of the $8p_{3/2}$ shell is expected for $Z = 165$. Table 11 shows instead the filling of the $9s$ and the $9p_{1/2}$ shell [37]. This surprising result makes it possible to give a formal continuation of the Periodic Table as it is shown in Fig. 10, because there are six p electrons from two different shells which are energetically very close, but they will nicely form a normal p shell so that the 9th period will be quite analogous to the 2nd and 3rd period.

The most important fact for the chemistry of the elements up to $Z = 164$ is that the $8s$ and the $8p_{1/2}$ shell are bound so strongly that they will not participate in the chemical binding. Normally all d and p elements are influenced in their valence and hybridization behaviour by the s electrons filled in at the beginning of the period. This difference can be seen easily in Fig. 4 where the energy eigenvalues of the outer electron shells of the 6th, 7th, and 8th period are shown. Therefore the normal oxidation state will be smaller by 2 for all transition elements of the 8th period. Because of systematical reasons $Z = 164$ is put below Hg in the Periodic Table of Fig. 10, whereas from chemical reasons alone this element should be located below Pt.

The noble metal character of the elements at the end of the $7d$ transition series will be important but not too dominant. The shielding of the outer s electrons as it is in the periods before is missing and the d shell is very much split into their

Table 11. *The calculated total energies for different electron configurations of the elements* $Z = 156$–172

Element	electron configuration (plus Z = 118 core + $8s^2\ 5g^{18}\ 6f^{14}$)						total energy	expected configuration
Z	$7d_{3/2}$	$7d_{5/2}$	$8p_{1/2}$	$8p_{3/2}$	$9s_{1/2}$	$9p_{1/2}$	$-E_T$ (Ry)	
156	2	-	2	-	-	-	284017.004	$7d^2$
157	4	-	1	-	-	-	291997.609	
	3	-	2	-	-	-	98.863	$7d^3$
158	4	1	1	-	-	-	300238.086	
	4	-	2	-	-	-	39.707	$7d^4$
159	4	2	1	-	-	-	308742.215	
	4	1	2	-	-	-	44.082	$7d^5$
160	4	-	2	-	2	-	317516.054	
	4	1	2	-	1	-	16.132	
	4	2	2	-	-	-	16.136	$7d^6$
161	4	1	2	-	2	-	326559.352	
	4	2	2	-	1	-	59.488	
	4	3	2	-	-	-	59.503	$7d^7$
162	4	3	2	1	-	-	335874.500	
	4	3	2	-	1	-	74.566	
	4	4	2	-	-	-	74.629	$7d^8$
163	4	4	2	1	-	-	345469.540	
	4	4	2	-	1	-	69.617	
	4	5	2	-	-	-	69.711	$7d^9$
164	4	5	2	1	-	-	355344.141	
	4	5	2	-	1	-	44.215	
	4	6	2	-	-	-	44.352	$7d^{10}$
165	4	5	2	-	2	-	365499.725	
	4	6	2	1	-	-	99.839	
	4	6	2	-	1	-	99.922	$9s^1$
166	4	6	2	2	2	-	375938.000	
	4	6	2	1	1	-	38.074	
	4	6	2	-	1	1	38.090	
	4	6	2	-	2	-	38.188	$9s^2$
167	4	6	2	3	-	-	386659.832	
	4	6	2	2	1	-	59.953	$9s^2\ 8p^1_{3/2}$
	4	6	2	1	2	-	60.080	oder
	4	6	2	-	2	1	60.082	$9s^2\ 9p^1_{1/2}$
168	4	6	2	4	-	-	397665.473	
	4	6	2	3	1	-	65.590	
	4	6	2	1	1	2	65.656	
	4	6	2	2	2	-	65.754	
	4	6	2	-	2	2	65.769	$9s^2\ 9p^2_{1/2}$
169	4	6	2	4	1	-	408955.508	
	4	6	2	3	2	-	55.680	
	4	6	2	2	2	1	55.710	
	4	6	2	1	2	2	55.750	$9s^2\ 9p^2_{1/2}\ 8p^1_{3/2}$
170	4	6	2	4	2	-	420529.949	
	4	6	2	3	2	1	30.019	
	4	6	2	2	2	2	30.090	$9s^2\ 9p^2_{1/2}\ 8p^2_{3/2}$
171	4	6	2	3	2	2	432388.285	$9s^2\ 9p^2_{1/2}\ 8p^3_{3/2}$
172	4	6	2	4	2	2	444529.128	$9s^2\ 9p^2_{1/2}\ 8p^4_{3/2}$

two subshells. Therefore, the first ionization energies shown in Fig. 5 are smaller than in the periods before. The principal maxima of the outer electron wave functions of the elements $Z = 82$, $Z = 114$, and $Z = 164$ which have formally the same electron configurations are shown in Fig. 11. However, the structure of the outer valence electrons of the element $Z = 164$ is related more to the noble gases where the lowest bound electrons are located in a closed shell with a relatively

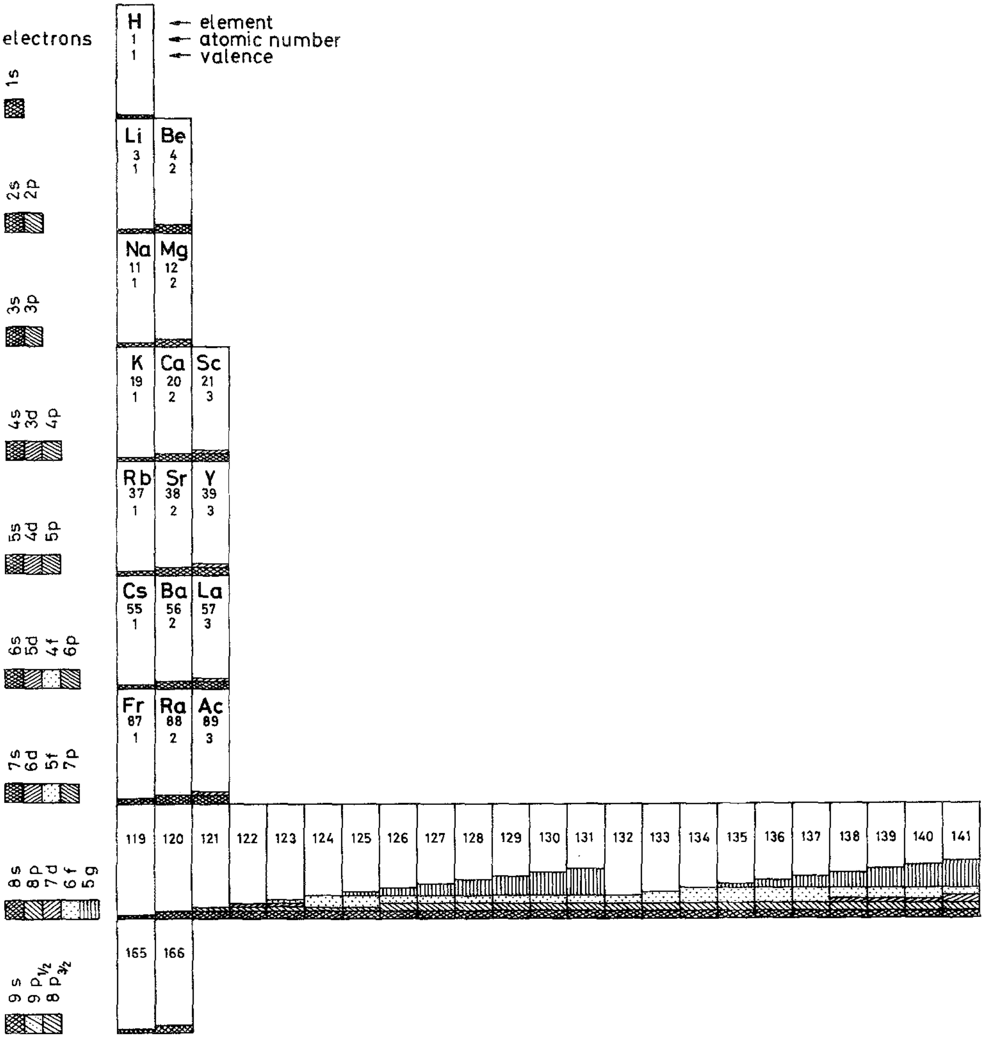
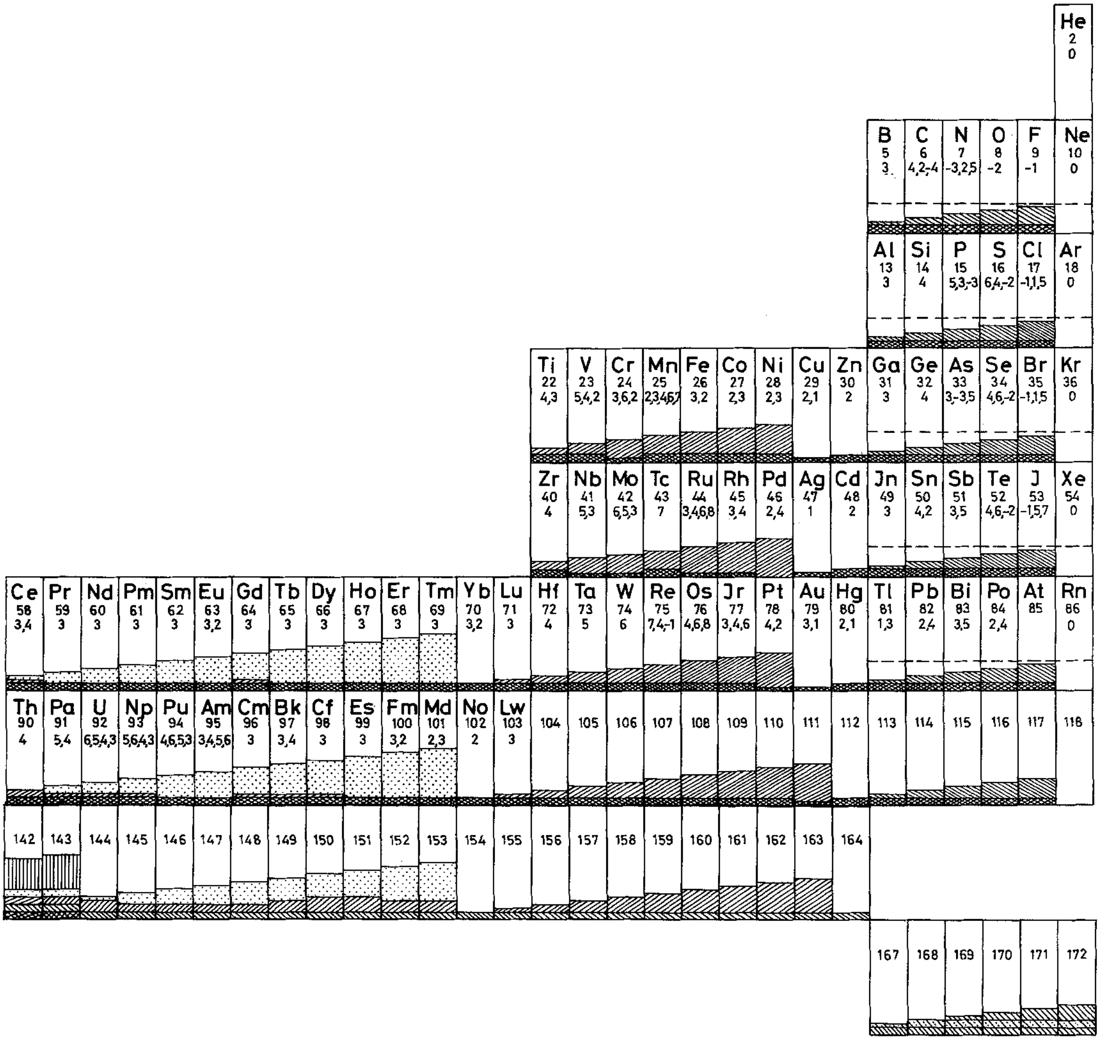


Fig. 10. The Periodic System in the continuation up to element $Z = 172$. The chemical symbols and the proton number are given as well as the outer electrons which are drawn schematically

large ionization energy at the surface of the atom [38]. The noble gas $Z = 118$ will be very similar to $Z = 164$; both elements have nearly the same electron structure and the same ionization energy. But we have seen that $Z = 118$ will be a very bad noble gas with possibly very high oxidation states and normal chemical compounds. Nevertheless we would expect that $Z = 164$ might be quite a good noble metal because the outer electrons are *d* electrons and Pauling [30] has shown that the binding length decreases very much when the *d* character is large. In contradiction to this is the fact that the radius of the element 164 can not become smaller than the 8*s* and $8p_{1/2}$ electron wave functions permit. Nevertheless the metal might lead to a larger crystal energy than nearly any other



composition would do. This would mean that $Z = 164$ might be a good noble metal with a quite high melting point. A prediction of the metallic radii are given in Fig. 6 and Table 12. A further detailed study of the chemistry of $Z = 164$ is given by Penneman *et al.* [39].

The 8th period ends with $Z = 164$ and this shows a further possibly general change in the Periodic Table: Helium forms a noble gas with a filled $1s^2$ shell. The next noble gases are formed by the filled outer *p* shells with decreasing ionization potentials. Here at $Z = 164$ the filled *d* shell finishes the period.

The 9th period begins as usual with elements of the chemical group I and II. The ionization energies of these 9*s* electrons reach nearly the values of the 3rd

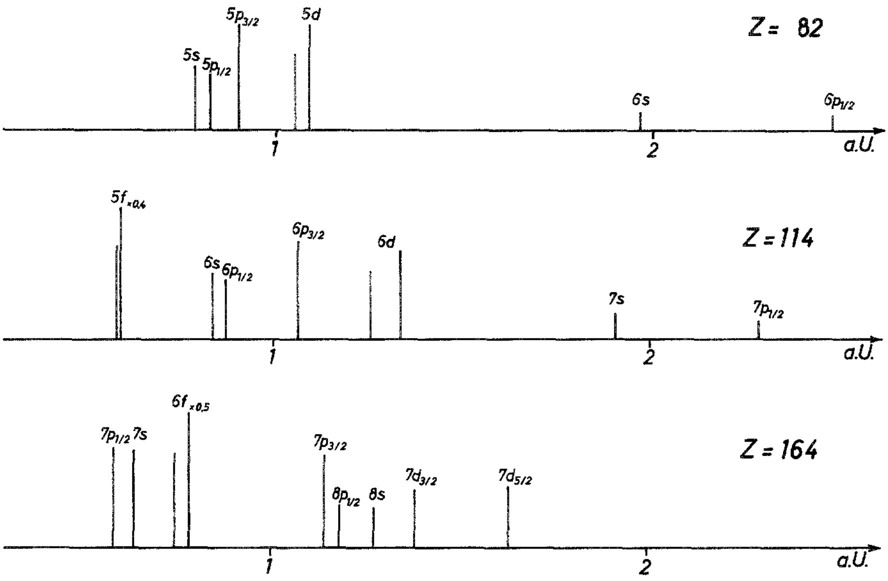


Fig. 11. The principal maxima of the outer electron shells for lead, $Z = 114$ and $Z = 164$

Table 12. *The chemical and physical properties of the elements $Z = 156$–172. The statements about the chemical most analog groups in this table do not coindice with the position in the Periodic Table (Fig. 10) because here the elements are ordered from a chemical, and in the Periodic Table from a systematical point of view. Uncertain are the values for the radii and the densities which are only first approximations*

Element	156	157	158	159	160	161	162	163	164	165	166
Atomic weight	445	448	452	456	459	463	466	470	474	477	481
Chemical most analog group		III A	IV A	V A	VI A	VII A	VIII	VIII	0,VIII	I A	II A
Outer electrons	$7d^2$	$7d^3$	$7d^4$	$7d^5$	$7d^6$	$7d^7$	$7d^8$	$7d^9$	$7d^{10}$	$9s^1$	$9s^2$
Most propable oxydation state	+ 2	+ 3	+ 4	+ 5,1	+ 6,2	+ 7,3	+ 4,8	+ 5	+ 6,0	+ 1	+ 2
Ionisation potential (eV)	4.1	4.7	5.4	3.5	4.4	4.9	5.8	6.4	7.1	5.4	6.5
Metalic radius (Å)	1.7	1.63	1.57	1.52	1.48	1.48	1.49	1.52	1.58	2.5	2.0
Density (g/cm^3)	26	28	30	33	36	40	45	47	46	7	11

Element	167	168	169	170	171	172
Atomic weight	485	489	493	496	500	504
Chemical most analog group	III B	IV B	V B	VI B	VII B	0
Outer electrons	$9s^2\ 9p^1_{1/2}$	$9s^2\ 9p^2_{1/2}$	$9s^2\ 9p^2_{1/2}\ 8p^1_{3/2}$	$9s^2\ 9p^2_{1/2}\ 8p^2_{3/2}$	$9s^2\ 9p^2_{1/2}\ 8p^3_{3/2}$	$9s^2\ 9p^2_{1/2}\ 8p^4_{3/2}$
Most propable oxydation state	+ 3	+ 4	+ 5	+ 6	+ 7,3	0,4,6,8
Ionisation potential (eV)	6.4	7.5	8.3	9.2	10.2	11.3
Metalic or covalent radius (Å)	1.9	1.8	1.75	1.7	1.65	2.2
Density (g/cm^3)	17	19	18	17	16	9

period as it can be seen in Fig. 9 which results from the strong relativistic effects in the binding of the 9*s* wave function. Element $Z=165$ will be a normal alkali and $Z=166$ a normal alkaline earth metal. Nevertheless it might be possible that in chemical compounds when the outer 9*s* electrons are ionized the oxidation state will become even higher because of the small ionisation energy of the 7*d* electrons. Between $Z=167$ and $Z=172$ the $9p_{1/2}$ and $8p_{3/2}$ electrons will be filled in and it is quite an accident that the energy eigenvalues are so close together that a *p* shell will result very analogous to the 2nd and 3rd period. The energy eigenvalues are compared with the *p* electrons of the 6th and 7th period in Fig. 7. This shows that the normal oxidation states of the elements $Z=167$–170 will be 3 to 6. $Z=171$ is expected to have many possible oxidation states between -1 and 7. Element $Z=172$ will be a very good noble gas with a closed *p* shell outside. The ionization energy of this element shown in Fig. 8, is very near to the value of Xe, so that it might be very similar to this element. The great difference Xe and $Z=172$ will only be that element $Z=172$ is expected to be fluid or even solid because of its large atomic weight.

In Table 12 the chemical and physical properties of the elements $Z=156$–172 are tabulated. The information about the radius and to an even larger extent on the density should only be considered as a first approximation.

The discussion of the chemistry of any higher element will be only of academic interest because it is very unlikely that any nucleus will be stable or even quasi stable for higher *Z*. On the other side it is not possible to calculate the atoms higher than 175 up to now because nobody knows what is happening when the 1*s* level drops into the negative continuum. In this region the quantum electrodynamical effects will be so strong that anything could happen and only the exact calculation of the atom plus the negative continuum can give the right answer.

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