Outline: Super Heavy Elements

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web-page: <u>https://web-docs.gsi.de/~wolle/</u> and click on



- 1. history
- 2. cold and hot fusion
- 3. nuclear structure of SHE
- 4. chemistry of SHE



Super Heavy Elements





The Chart of Nuclides the "playground" for Nuclear Physics





Periodic table of the elements

Dmitri Mendeleev (1869)

Internet Contents Recences wall & constantingto un arranner the as gadenty -, De Mencureto. Ji=st He=90 ?= 180. U=51 Nb=94 Ja=182. $\begin{array}{c} \mathcal{K} = \mathcal{S} \\ \mathcal{K} = \mathcal{G}_{n} \mathcal{S}_{n} \mathcal{$? G= 5%? da= 94 ? 9t= 60? Si=95 ? Sa= 75 [?] Sh= 118? Essai d'une des les de ments d'après leurs poils atomiques et d'ancage forchions chiniques fore d'aller elle for preter de de de l'ancage 18 15 69. J8 II 69. I yracy bedauto reages Cononersion verque de писания, по чискачеро, modesteke usino. andre undy, & Toursation I bab separa by Sales and the



Search for transuranium elements (1934)

$${}^{238}_{92}U + n \rightarrow {}^{239}_{92}U^* \rightarrow {}^{239}_{93}Np + e^- + \bar{\nu}$$



Otto Hahn and Lise Meitner

Hans-Jürgen Wollersheim - 2022



Discovery of nuclear fission (1938)



Liquid drop model: G. Gamow; Proc. Roy. Soc. London A123, 373 (1929) N. Bohr & J.A. Wheeler; Phys. Rev. 56, 426 (1939)



Transuranium elements (1940)



60-inch cyclotron (Berkeley, 1939)

 H_2^+ , ²H & ⁴He beams (Q/A = ¹/₂)

$${}^{238}_{92}U + {}^{1}_{0}n \rightarrow {}^{239}_{92}U^* \xrightarrow{\beta^-}_{23\ min} {}^{239}_{93}Np \xrightarrow{\beta^-}_{2.355\ days} {}^{239}_{94}Pu$$



Neptunium sphere with Ni clad in U shells



Edwin M. McMillan



Philip H. Abelson

Hans-Jürgen Wollersheim - 2022



Making new elements by simple reactions

$${}^{238}_{92}U + {}^{2}_{1}H \rightarrow {}^{238}_{93}Np + 2{}^{1}_{0}n$$

$${}^{238}_{93}Np \frac{\beta^{-}}{t_{1/2}=2.12 \text{ days}} {}^{238}_{94}Pu(t_{1/2} = 87.7 \text{ years})$$





Joseph W. Kennedy 1940



Arthur C. Wahl and Glenn T. Seaborg (1966)





Making new elements by simple reactions - the role of chemistry

The discovery of elements 95 (Am) and 96 (Cm)



Glenn T. Seaborg

$${}^{239}_{94}Pu + {}^{1}_{0}n \rightarrow {}^{240}_{94}Pu + \gamma$$

$${}^{240}_{94}Pu + {}^{1}_{0}n \rightarrow {}^{241}_{94}Pu + \gamma$$

$${}^{241}_{94}Pu \frac{\beta^{-}}{t_{1/2}=14.4 \text{ years}} {}^{241}_{95}Am(t_{1/2} = 432.7 \text{ years})$$

$${}^{241}_{95}Am + {}^{1}_{0}n \rightarrow {}^{242}_{95}Am + \gamma$$

$${}^{242}_{95}Am \frac{\beta^{-}}{t_{1/2}=16.0 \text{ h}} {}^{242}_{96}Cm$$



Making new elements with nuclear weapons

✤ The discovery of elements 99 (Md) and 100 (Fm)



TABLE 6.1 Neutron Addition Paths to 7	Fransuranium Synthesis (Cra 74)
---------------------------------------	---------------------------------

Neutron Addition Process	Neutron Flux (n/cm ² s ¹)	Reaction Time	Neutron Exposure (n/cm ²)	Average Neutron Energy (keV)
High flux reactor	$\approx 5 \times 10^{15}$	0.5 years	≈10 ²³	2.5×10^{-5}
Stellar s process	≈10 ¹⁶	$\approx 10^3$ years	$\approx 10^{26}$	≈10
Stellar r process	≥10 ²⁷	1-100 s	>10 ²⁷	≈100
Nuclear explosion	>10 ³¹	$< 10^{-6}$ s	$\approx 10^{25}$	≈20

MIKE



Figure 2.9 Closeup view of Mike device with its associated cryogenic equipment.

MIKE



MIKE-2



Samples of the bomb debris were collected on filter papers by aircraft flying through the mushroom cloud





Albert Ghiorso



Glenn Seaborg



Synthesis of elements 101 - 106

- Making elements one atom at a time



VOLUME OF ELUANT



Figure 2.20 The ionization recording chart showing the first four events of the disintegration of mendelevium. The ordinate is the event time while the abscissa is the intensity of the ionization. The four pulses occurred at 1:15 a.m., 1:37 a.m., 2:40 a.m., and 10:35 a.m. on February 19, 1955. At 11:56 a.m., Ghiorso and Harvey made a note directly in the chart: "This experiment conclusively proves the chemical identification of element 101."



Hot fusion (1961-1974) successful up to element 106 (Seaborgium)

Coulomb barrier V_C between projectile and target nucleus has to be exceeded

$$V_{C} = \frac{Z_{p} \cdot Z_{t} \cdot e^{2}}{R_{int}} = 126.2 \, MeV \quad ({}^{26}Mg + {}^{248}Cm)$$

 $\succ \quad \text{reaction: } a + A \rightarrow C^* \rightarrow B + b$

$$\Delta m = m_a + m_A - m_{CN}$$

$$\Delta m = (25.983 + 248.072 - 274.143) * 931.478 \text{ MeV/c}^2$$

$$= -82.153 \text{ MeV/c}^2$$

- ► excitation energy of compound nucleus $E^* = E_{kin} + \Delta m \cdot c^2 = 126.2 \text{ MeV} - 82.2 \text{ MeV} = 44.0 \text{ MeV}$
- > approximate 4 neutrons will be evaporated to avoid fission





http://nuclear.lu.se/database/masses/

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The problem



Figure 13

The half-lives of the longest-lived isotope of each element versus atomic number *Z*, *circa* 1970.

element	name	longest-lived isotope	half-life [s]
95	Americium	²⁴³ Am	$2.3 \cdot 10^{11}$
96	Curium	²⁴⁷ Cm	5.0·10 ¹⁴
97	Berkelium	²⁴⁷ Bk	$3.2 \cdot 10^{10}$
98	Californium	²⁵¹ Cf	$2.8 \cdot 10^{10}$
99	Einsteinium	²⁵² Es	4.1·10 ⁷
100	Fermium	²⁵⁷ Fm	8.7·10 ⁶
101	Mendelevium	²⁵⁸ Md	4.4·10 ⁶
102	Nobelium	²⁵⁹ No	3.5·10 ³
103	Lawrencium	²⁶⁶ Lr	3.6.104
104	Rutherfordium	²⁶⁷ Rf	4.7·10 ³
105	Dubnium	²⁶⁸ Db	1.1·10 ⁵
106	Seaborgium	²⁶⁹ Sg	1.8·10 ²
107	Bohrium	²⁷⁰ Bh	6.0·10 ¹
108	Hassium	²⁷⁷ Hs	3.0·10 ¹
109	Meitnerium	²⁷⁸ Mt	$4.0 \cdot 10^{0}$
110	Darmstadtium	²⁸¹ Ds	$1.4 \cdot 10^{1}$
111	Roentgenium	²⁸² Rg	$1.2 \cdot 10^2$
112	Copernicium	²⁸⁵ Cn	3.0·10 ¹
113	Nihonium	²⁸⁶ Nh	$8.0 \cdot 10^{0}$
114	Flerovium	²⁸⁹ Fl	$2.0 \cdot 10^{0}$
115	Moscovium	²⁹⁰ Mc	8.0·10 ⁻¹
116	Livermorium	²⁹³ Lv	6.0·10 ⁻²
117	Tennessine	²⁹⁴ Ts	5.0.10-2
118	Organesson	²⁹⁴ Og	7.0.10-4



The solution – The Darmstadt Area

- "Cold fusion" reactions
- Bombarding Pb or Bi with heavy ions the resulting species are borne "cold"
 with low excitation energies they survive better



Peter Armbruster



Gottfried Münzenberg



Sigurd Hofmann



Cold fusion (1981-1996)

Coulomb barrier V_C between projectile and target nucleus has to be exceeded

$$V_{C} = \frac{Z_{p} \cdot Z_{t} \cdot e^{2}}{R_{int}} = 223.3 \, MeV \quad ({}^{58}Fe + {}^{208}Pb)$$

$$\succ \quad \text{reaction: } a + A \rightarrow C^* \rightarrow B + b$$

$$\Delta m = m_a + m_A - m_{CN}$$

$$\Delta m = (57.933 + 207.977 - 266.130) * 931.478 \text{ MeV/c}^2$$

$$= -205.045 \text{ MeV/c}^2$$

excitation energy of compound nucleus

$$E^* = E_{kin} + \Delta m \cdot c^2 = 223.3 \text{ MeV} - 205.0 \text{ MeV} = 18.2 \text{ MeV}$$

> approximate 1-2 neutrons will be evaporated to avoid fission

reaction	Q _{gg} (MeV)	$V_{C}(R_{int}) (MeV)$	E* (MeV)
${}^{48}_{20}Ca + {}^{208}_{82}Pb \rightarrow {}^{256}_{102}No$	-153.796	175.05	21.25
${}^{54}_{24}Cr + {}^{209}_{83}Bi \rightarrow {}^{263}_{107}Bh$	-189.911	210.00	20.09
${}^{58}_{26}Fe + {}^{208}_{82}Pb \rightarrow {}^{266}_{108}Hs$	-205.045	223.31	18.27
${}^{58}_{26}Fe + {}^{209}_{83}Bi \rightarrow {}^{267}_{109}Mt$	-208.526	225.86	17.33
${}^{62}_{28}Ni + {}^{208}_{82}Pb \rightarrow {}^{270}_{110}Ds$	-223.225	238.84	15.62
${}^{64}_{28}Ni + {}^{209}_{83}Bi \rightarrow {}^{273}_{111}Rg$	-228.52	240.78	12.26
${}^{70}_{30}Zn + {}^{208}_{82}Pb \rightarrow {}^{278}_{112}Cn$	-244.38	252.67	8.29



http://nuclear.lu.se/database/masses/ G. Audi et al. Nucl. Phys. A729 (2003) 337



Excitation functions

G. Münzenberg / Nuclear Physics A 693 (2001) 207-218

209



Fig. 1. Excitation functions for the production of elements 104, 108, 110, and 112 plotted versus the excitation energy of the compound system (left-hand side) and versus the excitation energy corrected by subtraction of the neutron binding energy [6] (right-hand side).

Synthesis of heavy elements





Fusion / fission competition





Fusion / fission competition





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Fusion and evaporation



Both decay processes are determined by the level density, either from the residual nucleus or at the saddle point.

level density: $\rho(E^*) = const \cdot \exp(E^*/T)$

$$\frac{\Gamma_n}{\Gamma_f} = \frac{2 \cdot T \cdot A_{CN}^{2/3}}{K_0} \cdot \exp\left[\left(B_f - B_n\right)/T\right]$$

$$K_0 = \hbar^2 / 2 \cdot m \cdot r_0^2 \approx 11.4 \, MeV \qquad T = \sqrt{8 \cdot E^* / A_0}$$



Separator for Heavy Ion Products (SHIP)



Separator for Heavy Ion Products (SHIP)

Fusion products are slower than scattered or transfer particles

$$v_{CN} = \left[m_p / \left(m_p + m_t \right) \right] \cdot v_p$$

 $e.\,q.\,v_p\approx 10.3\% \ \ \rightarrow \ \ v_{CN}\approx 2.2\%$

E- and B-field are perpendicular to each other

$$B \cdot \rho = \frac{m \cdot v}{e \cdot q}$$
$$E \cdot \rho = \frac{m \cdot v^2}{e \cdot q}$$

$$F_{mag} = F_{el} \Rightarrow F_{tot} = 0$$



electric deflectors: ±330 kV dipole magnets: 0.7 T max



Separator for Heavy Ion Products (SHIP)

The choice of E and B determines the transmitted velocity

$$v = \frac{E}{B}$$

The rejected beam will be stopped on a cooled Cu plate



SHIP – stop detector



 \succ

position sensitive Silicon detector determines the position an energy of SHE and α , β , ...

area: 27*87mm², thickness: 0.3mm, 16 strips energy resolution $\Delta E=18-20 \text{ keV} @ E_{\alpha} > 6 \text{MeV}$ (cooling 260K) position resolution $\Delta x=0.3 \text{mm}$ (FWHM)



SHE will be measured in a pixel

Wait for the emission of an α -particle (or β -particle) **correlation method: implantation and decay event in the same pixel**



Synthesis and identification of heavy elements with SHIP





Synthesis and identification of heavy elements with SHIP





 $^{208}\text{Pb} + {}^{64}\text{Ni} \rightarrow {}^{272}\text{Ds}^*$



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The average decay properties of even mass decay chains match the Geiger-Nuttall relationship



Coulomb barrier



Y. Oganessian; J. Phys. G: Nucl. Part. Phys. 34 (2007) E165

Increase of Q_{α} values for the isotopes with Z = 112-118





The end of the "cold fusion" path?







"Hot fusion" - The Dubna Era



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✤ ⁴⁸Ca projectiles produced by U400 heavy ion accelerator

energy: 235 -250 MeV beam intensity: $1.0 - 1.5 \text{ p}\mu\text{A}$ consumption: 0.5 - 0.8 mg/hbeam dose: $(0.3 - 3.0) \cdot 10^{19}$



year	element	reaction	number of atoms
2000	114	$^{48}Ca \rightarrow ^{244}Pu$	50
2004	113	decay product of Z=115	8
2004	115	$^{48}Ca \rightarrow ^{243}Am$	30
2005	116	$^{48}Ca \rightarrow ^{248}Cm$	30
2006	118	$^{48}Ca \rightarrow ^{249}Cf$	3 - 4
2010	117	${}^{48}\text{Ca} \rightarrow {}^{249}\text{Bk}$	6

prices per 1 mg
$^{197}Au \approx 0.03$ \$
239 Pu \approx 4 \$
$^{48}\text{Ca} \approx 80$ \$
$^{249}Cf \approx 60\ 000\$



✤ ⁴⁸Ca projectiles produced by U400 heavy ion accelerator

energy: 235 -250 MeV beam intensity: $1.0 - 1.5 \text{ p}\mu\text{A}$ consumption: 0.5 - 0.8 mg/hbeam dose: $(0.3 - 3.0) \cdot 10^{19}$



reaction	Q _{gg} (MeV)	$V_{\rm C}({\rm R}_{\rm int})~({\rm MeV})$	E* (MeV)
${}^{48}_{20}Ca + {}^{244}_{94}Pu \rightarrow {}^{292}_{114}Fl$	-160.5	197.3	36.8
${}^{48}_{20}Ca + {}^{243}_{95}Am \rightarrow {}^{291}_{115}Mc$	-170.6	199.7	29.1
${}^{48}_{20}Ca + {}^{248}_{96}Cm \rightarrow {}^{296}_{116}Lv$	-166.6	201.1	34.5
${}^{48}_{20}Ca + {}^{249}_{97}Bk \rightarrow {}^{297}_{117}Ts$	-170.1	203.2	33.1
$\frac{{}^{48}_{20}Ca}{{}^{249}_{20}Cf} \rightarrow {}^{297}_{118}Og$	-174.3	205.4	31.1

 Q_{gg} and $V_{C}(Bass)$ from <u>http://nrv.jinr.ru/nrv/webnrv/qcalc/</u>



Irradiation of targets at HFIR reactor (Oak Ridge)

$${}^{238}_{92}U + {}^{1}_{0}n \longrightarrow {}^{239}_{92}U \xrightarrow{\beta^{-}}_{23.5 \ min} {}^{239}_{93}Np \xrightarrow{\beta^{-}}_{2.357 \ d} {}^{239}_{94}Pu$$

$$\overset{239}{_{94}}Pu \xrightarrow{(n,\gamma)} \overset{240}{_{94}}Pu \xrightarrow{(n,\gamma)} \overset{241}{_{94}}Pu \xrightarrow{\beta^{-}} \overset{241}{_{14.35\,a}} Mm \left(\frac{\alpha}{_{432.2\,a}} \overset{237}{_{93}}Np \right)$$

- ✤ Irradiation in the HFIR flux trap (18 month)
 - thermal-neutron flux of
 - $2.5 \cdot 10^{15}$ neutrons/(s · cm²)
 - 31 target positions
 - (10-13 targets typically irradiated)
 - produces ~35 mg ²⁵²Cf per target (smaller quantities of Bk, Es, Fm)






22 mg of $^{249}Bk \approx 1$ M\$, 250 day irradiation in HIFR (ORNL)



 $Bk(NO_3)_3$ product

The two year experimental campaign began with a 250 day irradiation in HFIR, producing 22 milligram of ²⁴⁹Bk, which has a 320 day halflife. The irradiation was followed by 90 days of processing at radiochemical Engineering Development Center (REDC) to separate and purify the Berkelium. The ²⁴⁹Bk target was prepared at Dimitrovgrad and then bombarded for 150 days at the Dubna facility.



22 mg of $^{249}Bk \approx 1$ MS, 250 day irradiation in HIFR (ORNL)















Dubna gas filled recoil separator (DGFRS)







Cross sections - fission barriers



Y. Oganessian; J. Phys. G: Nucl. Part. Phys. 34 (2007) E165



Spontaneous fission half-lives of actinides



Y. Oganessian; J. Phys. G: Nucl. Part. Phys. 34 (2007) E165



Chart of nuclides: the domain of heavy and super heavy elements







Chart of nuclides: the domain of heavy and superheavy elements



What is the structure of SHE?





Influence of shell effects on fission barrier



macroscopic barrier: disappears at Z ~ 104!



Influence of shell effects on fission barrier



macroscopic barrier: disappears at Z ~ 104!

- with shell structure:

spherical \leftrightarrow deformed ground state

fission barrier is also > 0 for $Z \ge 104$

some fission barriers have complicated shapes, multi-humped structure

elements exist only due to shell effects:

superheavy elements







tagging instrumentation at JYFL (Jyväskylä) JUROGAM, RITU, GREAT



Spinning the heaviest elements



S. Eeckhaupt et al.; EPJA 26 (2005), 227



Rotational Bands





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Single particle orbitals

R. Chasman et al. Rev. Mod. Phys. 49 (1977), 833



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Stability of heavy elements - Nilsson level energy gap





Shiptrap: Probing the strength of shell effects



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Isomeric states in even-even nuclei

Why K-isomers occur?

- deformed nuclei
- breaking of particle pair at Fermi surface
- Selection rule for electromagnetic transitions λ ≥ ΔK is not fulfilled
- excitation energy of quasi-particle: $E = \sqrt{(\varepsilon - \lambda)^2 + \Delta^2}$

What we can learn?

- information about Nilsson level energy gaps
- influence on stability of superheavy elements
- pairing interaction







Isomeric states in even-even nuclei

Why K-isomers occur?

- deformed nuclei
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What we can learn?

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K-isomers in ²⁵²No



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Neutron single particle states in ²⁵²No

7/2⁺[624] Nilsson configuration $i_{11/2}$

9/2⁻[734] Nilsson configuration $j_{15/2}$

$$g(j) = \begin{cases} \frac{2\ell \cdot g_{\ell} + g_s}{2\ell + 1} & \text{for } j = \ell + 1/2\\ \frac{2(\ell + 1) \cdot g_{\ell} - g_s}{2\ell + 1} & \text{for } j = \ell - 1/2 \end{cases}$$

 $\begin{array}{ll} \mbox{proton:} & g_{\ell} = 1 & g_{s} = 5.59 \\ \mbox{neutron:} & g_{\ell} = 0 & g_{s} = -3.83 \end{array}$

 $g(\mathbf{i}_{11/2}) = +0.295 \qquad g(\mathbf{j}_{15/2}) = -0.255$ $g(j_1 \times j_1; J) = \frac{1}{2} \cdot (g_1 + g_2) + \frac{j_1(j_1 + 1) - j_2(j_2 + 1)}{2J(J + 1)} \cdot (g_1 - g_2)$

 $g(i_{11/2} \ge j_{15/2}; 8) = 0.09$

$$B(M1; I \to I - 1) = \frac{3}{4\pi} [g_K - g_R]^2 \cdot K^2 |\langle IK10|(I - 1)K \rangle|^2$$

$$B(E2; I \to I - 2) = \frac{5}{16\pi} Q_0^2 |\langle IK20|(I - 2)K \rangle|^2$$

$$g_R = Z/A = 0.40$$

$$g_k \pi \pi (\text{th} I) = 0.001$$

Branching ratio

$$R_{\rm exp} = I_{\gamma}(J \rightarrow J - 1) / I_{\gamma}(J \rightarrow J - 2)$$



The isomer K=8⁻ is based on 2-qn excitation



K-isomeric states



Level scheme of ²⁵³No (151 neutrons)





R. Chasman et al.; Rev. Mod. Phys. 49 (1977) 833



Level scheme of ²⁵³No (151 neutrons)





Alpha decay of ²⁵³No



In general, α -decay in even-even parents lead to the ground state of the daughter nucleus so that the emitted particle carries away as much energy as possible and as little angular momentum as possible. *a-decays* of *odd-A* heavy nuclei populate predominantly low-lying excited states that *match the spin of the parent* so that the orbital angular momentum of the α -particle can be zero.

Spectroscopy of element 115



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Spectroscopy of element 115





Spectroscopy of element 115

Highly efficient multi-coincidence spectroscopy set-up for TASCA's very compact focal plane image

1 Implantation DSSSD (1024 pixels) 4 box-DSSSDs (1024 pixels) → ~ 80% α-detection efficiency

4 Ge Clover (4.4 crystals) 1 Ge Cluster (7 crystals) $\rightarrow \sim 40\% \gamma$ -detection eff. at 150 keV



L.-L. Andersson et al.; NIM A622, 164 (2010) L. G. Sarmiento et al.; NIM A667, 26 (2011)



TAsca Small Image mode SPECtroscopy



GSI

Characteristic X-rays







2 3 10 13 15 $Group \rightarrow 1$ 4 5 7 8 9 11 12 14 16 17 18 6 ↓Period 2 1 1 He Н 3 10 4 5 6 7 8 9 2 С Li В Ν 0 F Be Ne 11 12 13 15 16 17 18 14 3 Si S Ρ CI Na Mg AI Ar 21 31 19 20 22 23 24 25 26 27 28 29 30 32 33 34 35 36 4 Sc Ti V Co Ca Cr Mn Fe Ni Cu Zn Ga Ge As Se Br Kr Κ 39 37 38 40 41 42 43 44 45 47 49 50 51 52 53 54 46 48 5 Υ Rb Sr Zr Nb Rh Pd Cd Sn Sb Xe Мо Tc Ru Ag In Te Ι 55 57 56 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 * 6 Cs Ba La Hf Та W Re Os Ir Pt Au Hg TI Pb Bi Po At Rn 89 87 88 104 105 106 107 108 109 110 111 112 113 114 115 116 118 117 7 * Fr Ra Ac Rf Db Bh Mt Nh FI Sq Hs Ds Rq Cn Mc Ts Og Lv 64 71 58 59 60 61 62 63 65 66 67 68 69 70 * Ce Pr Nd Pm Sm Eu Gd Tb Dv Ho Er Tm Yb Lu * 90 91 92 93 94 95 96 97 98 99 100 101 102 103 Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Chemistry of superheavy elements

Are the new elements in the same period?

Does e.g. Lv show the same chemical properties as O, S, Se, Te and Po?



Chemistry of superheavy elements

relativistic effect: important for large Z

 $E = mc^2$



- ✤ High atomic number: strong Coulomb attraction causes electrons to move faster.
- ★ Causes relativistic mass increase $m = m_0(1 \beta^2)^{-1/2}$, with β = v/c; and as a consequence, *contraction of spherical orbitals* (ns, np_{1/2})
- The s and $p_{1/2}$ atomic orbitals contract relativistically.
- * The shrinking of the inner shells results in an increased screening of the nuclear charge, and this gives rise to an expansion of the $p_{3/2}$ and of higher angular momentum orbitals.
- Strong spin-orbit splitting

Bohr model: $E = -(2\pi^2 e^4/n^2 h^2) \cdot m \cdot Z^2$ $r = Ze^2/m \cdot v^2$ $v = (2\pi e^2/n \cdot h) \cdot Z$

for hydrogen, $m/m_0 = 1.000027$, for element Z=114 , $m/m_0 = 1.79$, for element Z=118, $m/m_0 = 1.95$



Chemistry of superheavy elements

relativistic effect: important for large Z

$$E = mc^2$$





Solution of the Dirac equation (relativistic quantum mechanics) for a hydrogen-like atom:

$$E_{1s} = mc^2 \sqrt{1 - (Z\alpha)^2} \sim mc^2 \cdot \left(1 - \frac{(Z\alpha)^2}{2} - \frac{(Z\alpha)^4}{8} + \cdots\right)$$

relativistic effect



Famous example of relativistic effects: the color of gold





Gold looked like silver if there was no relativistic effect!



Famous example of relativistic effects: the color of gold





Famous example of relativistic effects: the color of gold






Group→1 Period		2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 0	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc		22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y		40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	*	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
				*	58	59	60	61	62	63	64	65	66	67	68	69	70	71	
					Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Но	Er	Tm	Yb	Lu	
				* *	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

Chemistry of superheavy elements

✤ Gold is smaller than Silver

Roentgenium is of the same size as Copper



2 3 10 13 15 $Group \rightarrow 1$ 4 5 7 8 9 11 12 14 16 17 18 6 ↓Period 2 1 1 He Н 3 10 4 5 6 7 8 9 2 С Li В Ν 0 F Be Ne 11 12 13 15 16 17 18 14 3 Si S Ρ CI Na Mg AI Ar 21 31 32 19 20 22 23 24 25 26 27 28 29 30 33 34 35 36 4 Sc Ti V Co Ca Cr Mn Fe Ni Cu Zn Ga Ge As Se Br Kr K 39 37 38 40 41 42 43 44 45 47 49 50 51 52 53 54 46 48 5 Υ Rb Sr Zr Nb Ru Rh Pd Cd In Sn Sb Te Xe Мо Tc Ag Ι 55 57 56 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 * 6 Cs Ba La Hf Та W Re Os Ir Pt Au Hg TI Pb Bi Po At Rn 89 87 88 * 104 105 106 107 108 109 110 111 112 113 114 115 116 118 117 7 * Fr Ra Ac Rf Db Bh Mt Nh FI Sq Hs Ds Rq Cn Mc Ts Og Lv 71 58 59 60 61 62 63 64 65 66 67 68 69 70 * Ce Pr Nd Pm Sm Eu Gd Tb Dv Ho Er Tm Yb Lu * 90 91 92 93 94 95 96 97 98 99 100 101 102 103 Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Chemistry of superheavy elements

How do the relativistic effects alter the periodic table for SHE? \rightarrow a big open question

Chemistry of superheavy elements

Group→1 ↓Period		2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 0	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc		22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y		40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	*	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
				*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
				*	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

- Dubnium does not behave like Tantalum (1993)
- Sg (1997) Bh (2000) and Hs (2001) confirmed relativistic calculations predicting the expected behavior in the periodic table.
- ✤ Hassium, for instance, forms a gaseous oxide similar to Osmium.

The atomic orbitals $s_{1/2}$ and $p_{1/2}$ are contracted relativistically. The shrinking of the inner shells results in an increased *screening of the nuclear charge*, and this gives rise to an expansion of the $p_{3/2}$ and of higher angular momentum orbitals. Another relativistic effect is a *change in the spin-orbit coupling*. Both can produce drastic rearrangements of orbital levels. That is what is predicted to happen for Cn. Recent calculations indicate that the 7s orbital should be shifted below the $6d_{5/2}$ orbital due to relativistic effects. It is the large relativistic stabilization of its valence 7s orbital, combined with its closed shell electron configuration, that has led to the prediction that element 112 is chemically inert (not very reactive).

Chemistry of the superheavy elements with Z > 118 is believed to show relativistic effects that are so large that comparison with lighter elements or nonrelativistic results is meaningless.



The limits of the periodic table

✤ Can this go forever? NO!!!

The relativistic Dirac equation gives the ground state energy as

where m_0 is the rest mass of the electron. For Z > 137, the wave function of the Dirac ground state is oscillatory, rather than bound.

More accurate calculations taking into account the effects of the finite size of the nucleus indicate that the binding energy first exceeds $2mc^2$ for Z > 173.

✤ The end of chemistry

- Does the periodic table has limits? Yes!!!
- At some point $(Z \sim 122)$ all the electron energy levels of adjacent elements are similar so that there are no differences in their chemical behavior.

$$E = \frac{m_0 \cdot c^2}{\sqrt{1 + \frac{Z^2 \cdot \alpha^2}{n - (j + 1/2) + \sqrt{(j + 1/2)^2 - Z^2 \cdot \alpha^2}}}}$$



Chart of nuclides: the domain of heavy and superheavy elements



Calc.: A. Sobiczewski

