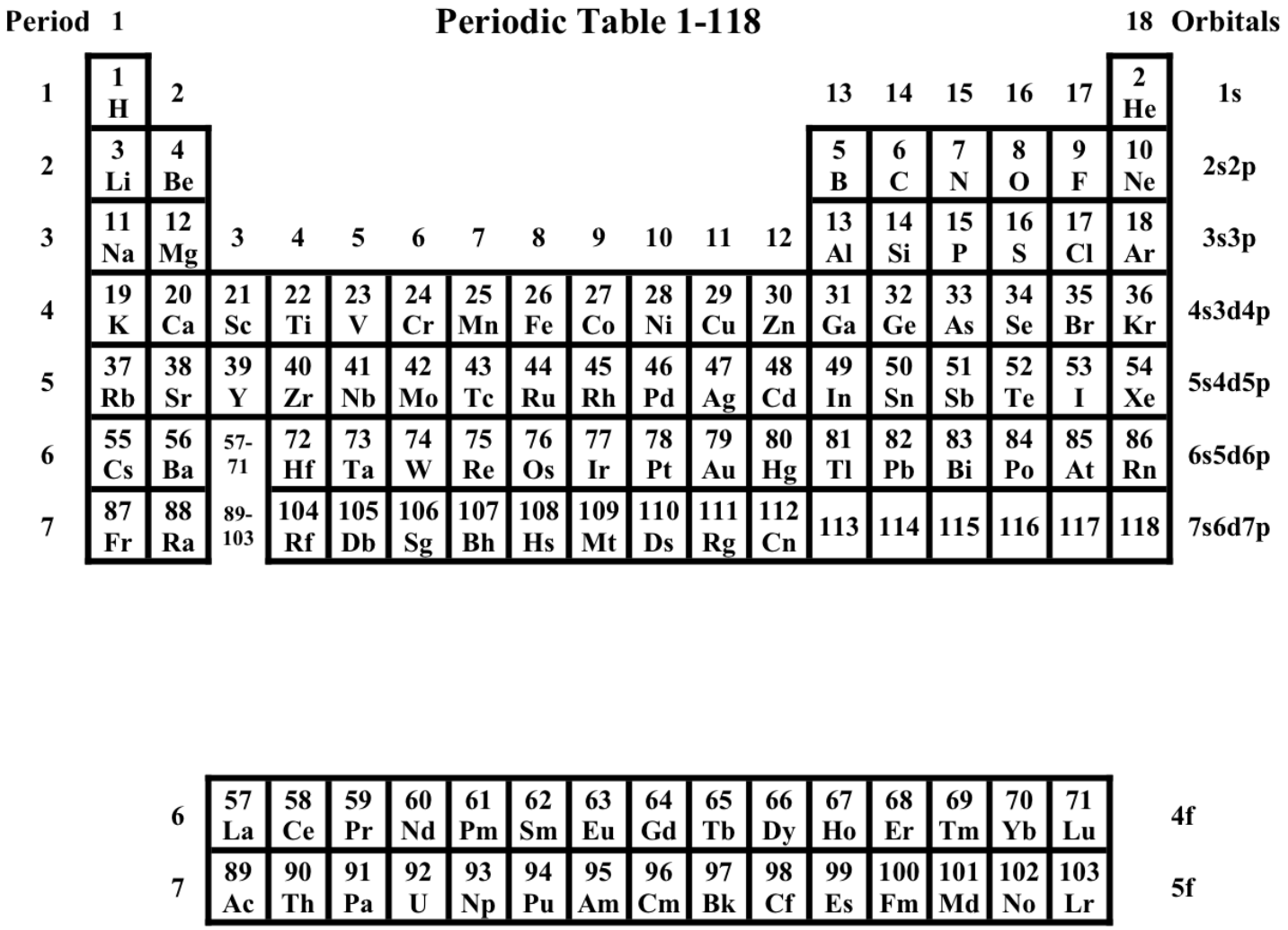
HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

THE PERIODIC SYSTEM CONTINUED TO Z=172

Pekka PYYKKÖ (Department of Chemistry, University of Helsinki, Finland)

Sotchi, Russia, September 7, 2011 (15')

THE PERIODIC SYSTEM 2010



Periodic Table 1-172

Period 1																	18	Orbitals
1	1 H	2										13	14	15	16	17	2 He	1s
2	3 Li	4 Be										5 B	6 C	7 N	8 O	9 F	10 Ne	2s2p
3	11 Na	12 Mg	3	4	5	6	7	8	9	10	11	12	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	3s3p
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	4s3d4p
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	5s4d5p
6	55 Cs	56 Ba	57-71	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	6s5d6p
7	87 Fr	88 Ra	89-103	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113	114	115	116	117	118	7s6d7p
8	119	120	121-	156	157	158	159	160	161	162	163	164	139	140	169	170	171	172	8s7d8p
9	165	166											167	168					9s9p

6	57 La	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	4f
7	89 Ac	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	5f
8	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	6f

8	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	5g

FRICKE, GREINER, WABER, TCA 21 (1971) 235.

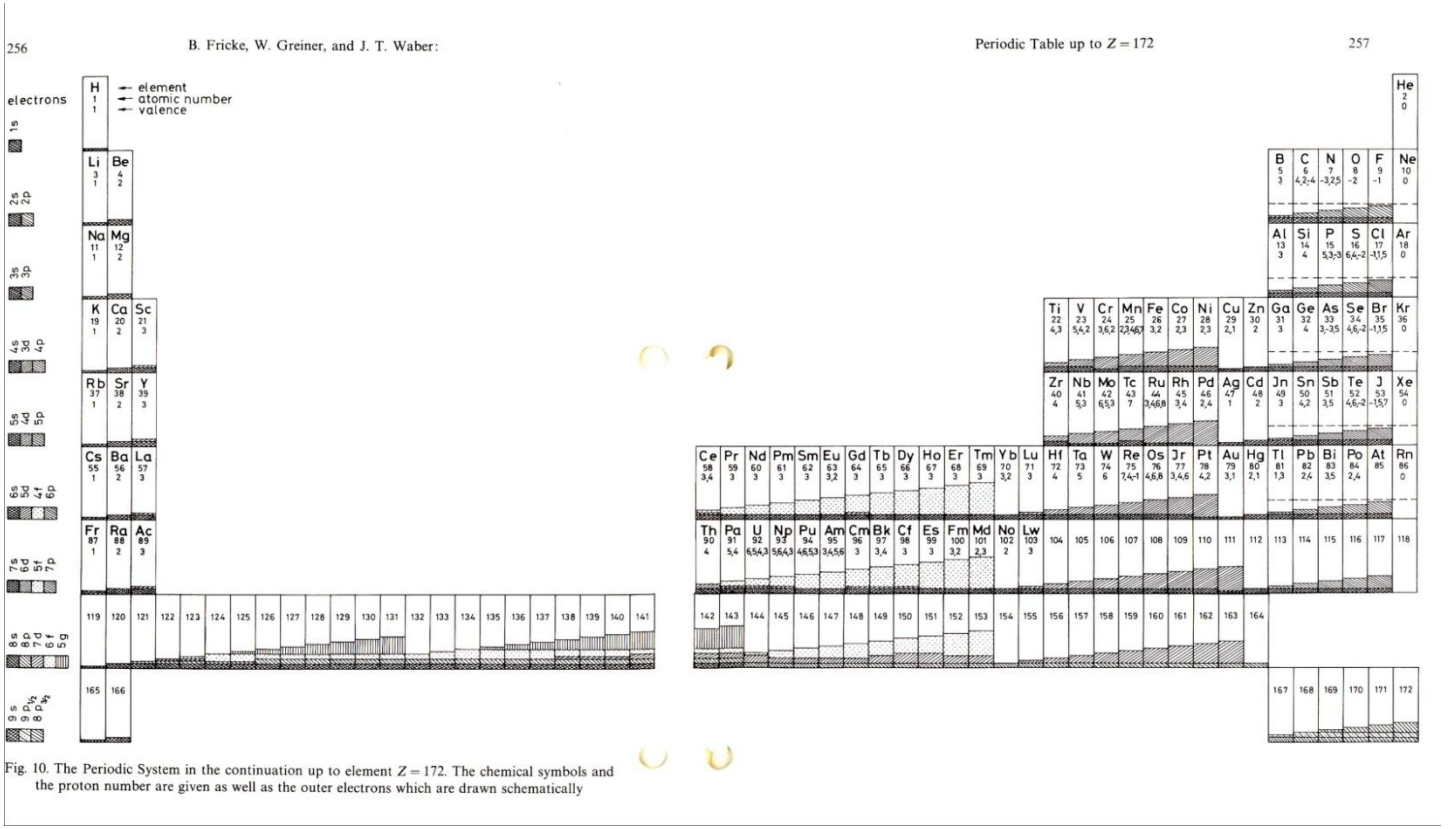
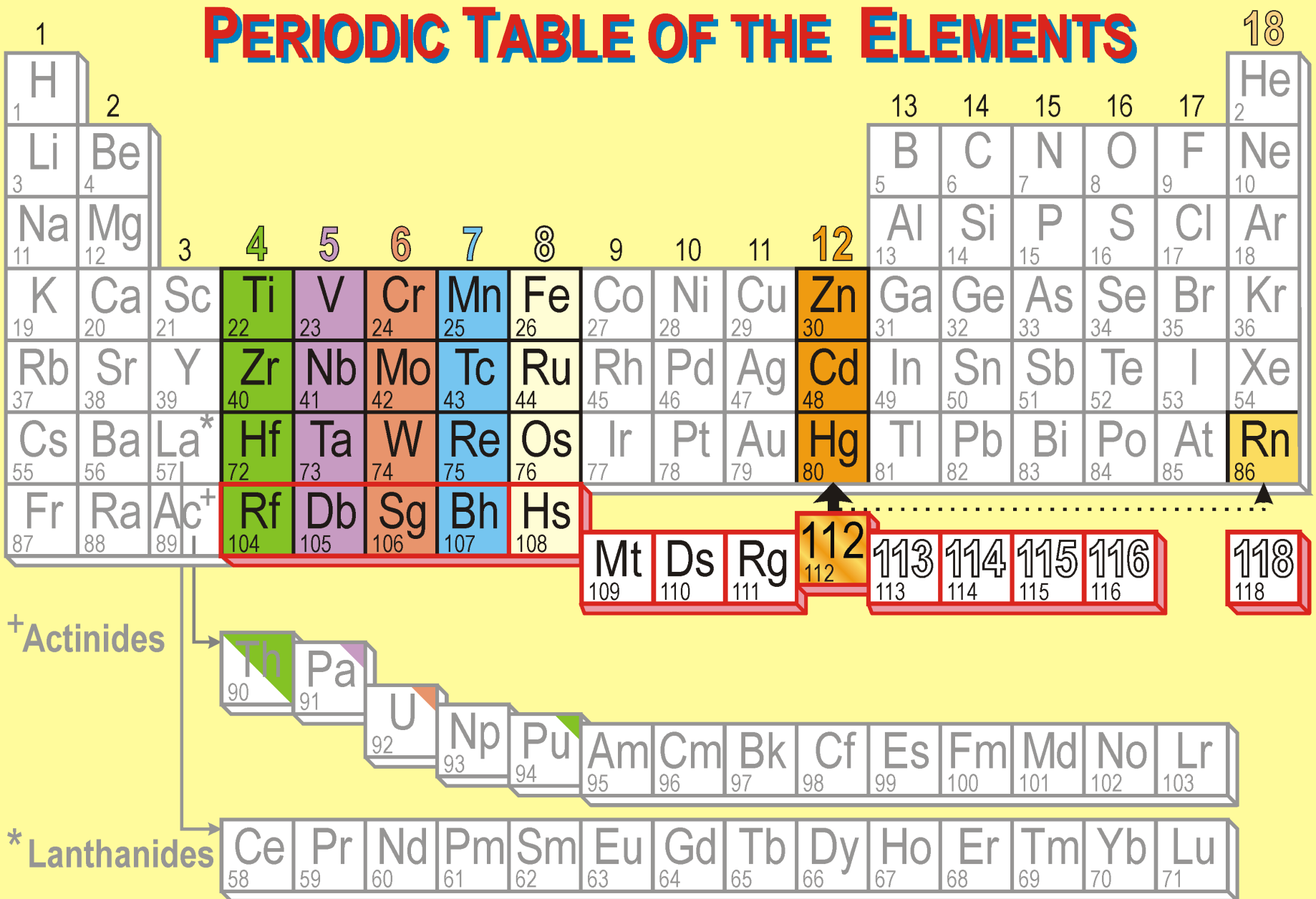
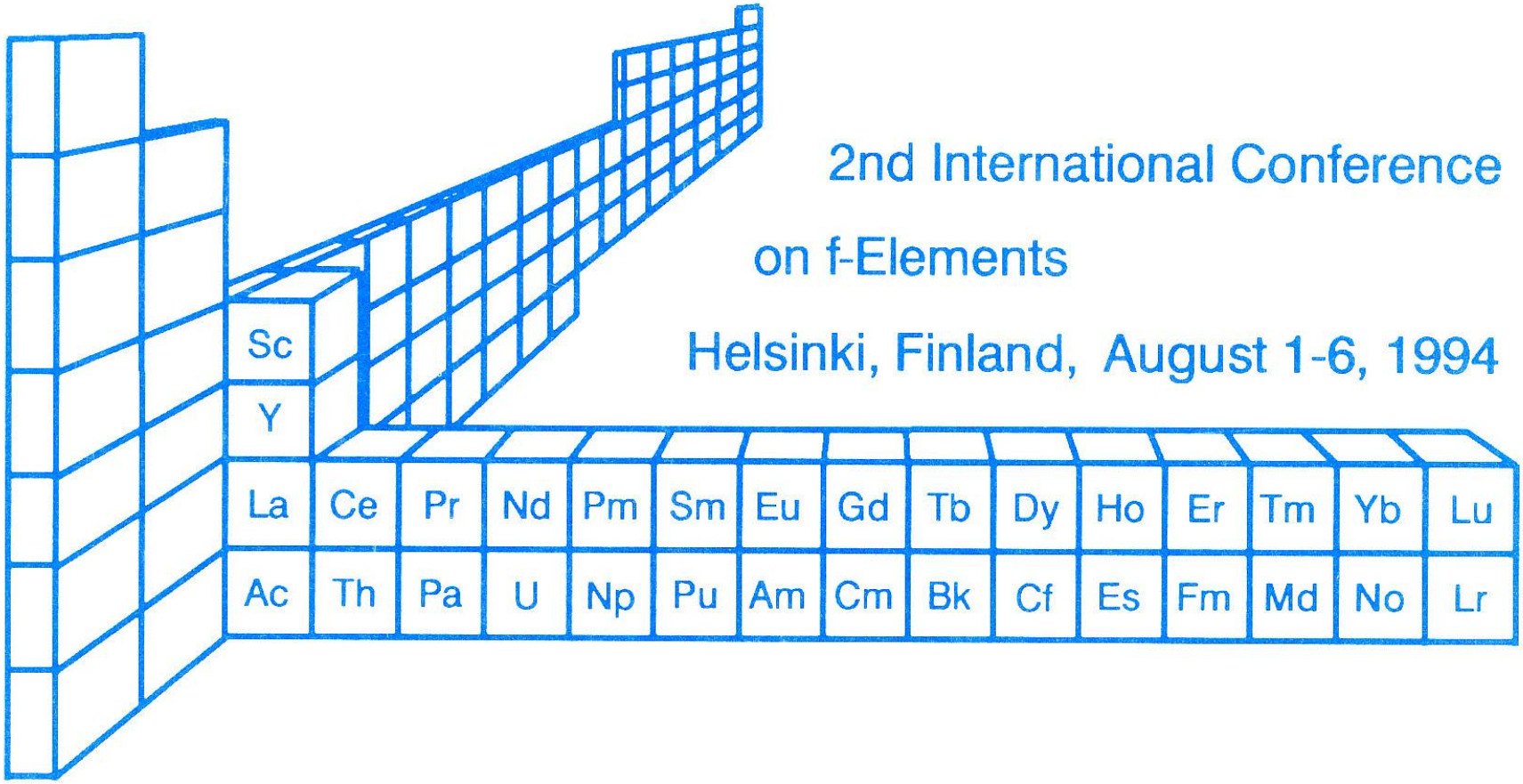


Fig. 10. The Periodic System in the continuation up to element $Z = 172$. The chemical symbols and the proton number are given as well as the outer electrons which are drawn schematically

FROM 6d TO 5f: DARMSTADT GSI PT



HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI



2nd International Conference on f-Elements

Helsinki, Finland, August 1-6, 1994

WHAT WAS ACTUALLY DONE?

- P. Pyykkö: ”A suggested Periodic Table up to Z ≤ 172, based on Dirac-Fock calculations on atoms and ions”,
  Phys. Chem. Chem. Phys. 13 (2011) 161-168.
- Average-of-configuration Dirac-Fock calculations on atoms and ions. [No Breit, no QED. The new Desclaux-Indelicato code.] The last valence electron determines the character of an element.
- Example: In Group 7, $(E125)^{6+}$ is $5g^1$. $(E124)^{5+}$ still $6f^1$. $(E136)^{6+}$ is $5g^{12}$. Then 8s, $8p_{½}$ compete.
- Indeed, $(E125)F_6$ is calculated to be $5g^1$.

M. A. Makhyoun, *J. Chim. Phys.* 85 (1988) 917. (QR MS Xα)

- Compare with NpF_6 which is $5f^1$.
- Note that the earlier members of the nominal 5g series can have other occupations, especially as more neutral atoms.
- Essential conclusion for Z = 119-172 (overlaps may occur):

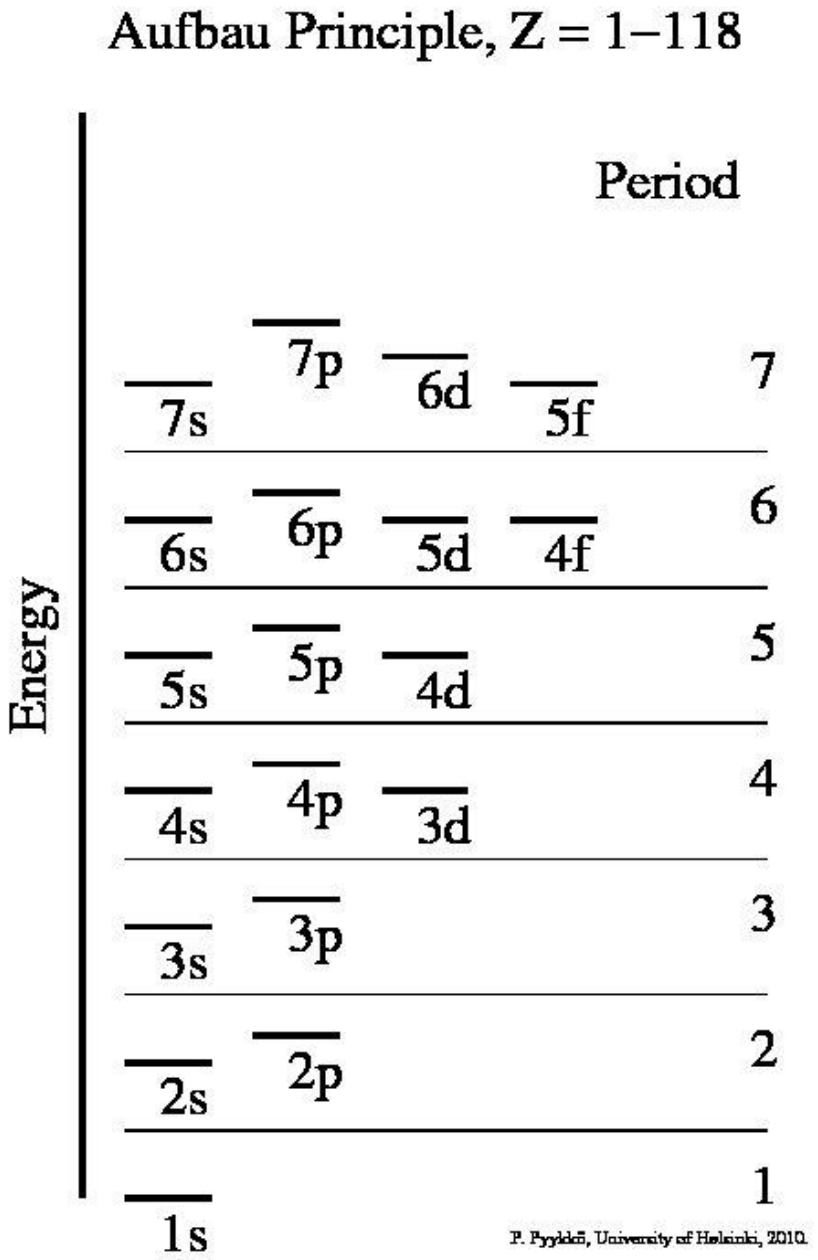
$$8s < 5g \leq 8p_{½} < 6f < 7d < 9s < 9p_{3/2} < 8p_{3/2}.$$

LATER MCDF COMPARISON

- P. Indelicato, J. Bieroń, P. Jönsson, ”Are MCDF calculations 101% correct in the super-heavy elements range? *Theor. Chem. Acc*. 129 (2011) 495-505.
- Yes, QED effects on the IP are of the order of 1% of the Dirac-level relativistic effects, up to Z=173.
- MCDF on E140: At ’Average Level (AL)’, confirm the $8s^2 8p^2 7d\ 6f^3 5g^{14}$ configuration of V.I. Nefedov, M.B. Trzhaskovskaya and V. G. Yarzhemskiii, *Doklady Phys. Chem*. 408 (2006) 149.
- At ’Optimal Level (OL)’: The lowest practical level $8s^2\ 8p^4\ 6f\ 5g^{15}$, J = 8.
- The filled-shell J=0, $8s^2\ 8p^2\ 5g^{18}$ is reached at (E143) $^{3+}$.
- For E140 – E142^{2+}, mix 8p-6f-5g .
- Essential conclusion for Z = 119-172 (overlaps may occur):

$$8s < 5g \leq 8p_{½} < 6f < 7d < 9s < 9p_{3/2} < 8p_{3/2}.$$

THE SEVEN PREVIOUS PERIODS



The Dirac-Coulomb-Breit Hamiltonian: A 'Theory of everything'

$$H = \sum_i h_i + \sum_{i<j} h_{ij}. \tag{1}$$

The one-particle Hamiltonian

$$h_{\rm D} = c\alpha \cdot \mathbf{p} + \beta c^2 + V_n, \quad \mathbf{p} = -i\nabla, \tag{2}$$

The two-particle Hamiltonian

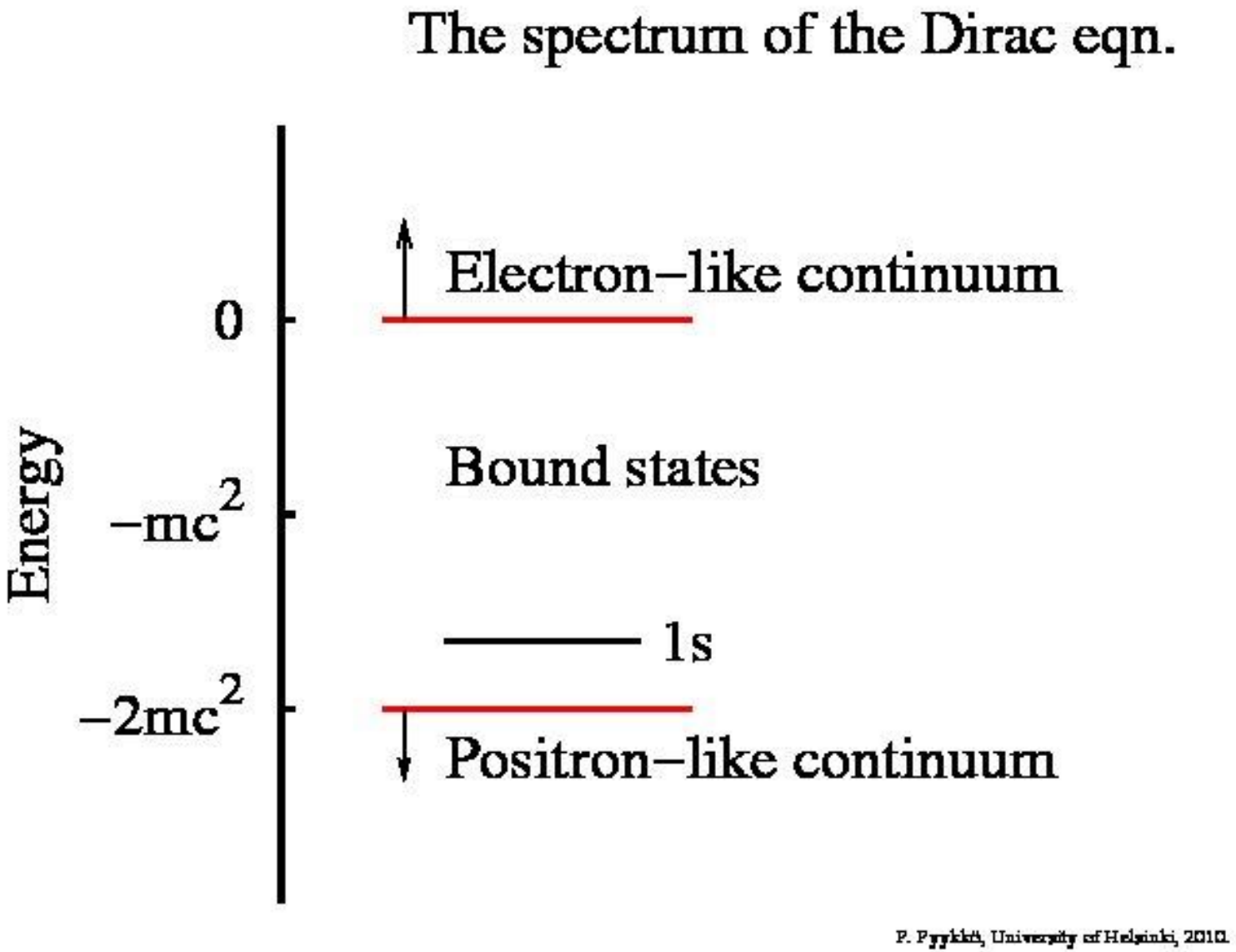
$$h_{ij} = 1/r_{ij} + h_{\rm B}, \tag{3}$$

$$h_{\rm B} = -\frac{1}{2r_{ij}}[\alpha_i \cdot \alpha_j \ + (\alpha_i \cdot \mathbf{r}_{ij})(\alpha_j \cdot \mathbf{r}_{ij})/r_{ij}^2]. \tag{4}$$

In correlated calculations, add electron-like projection operators, P:

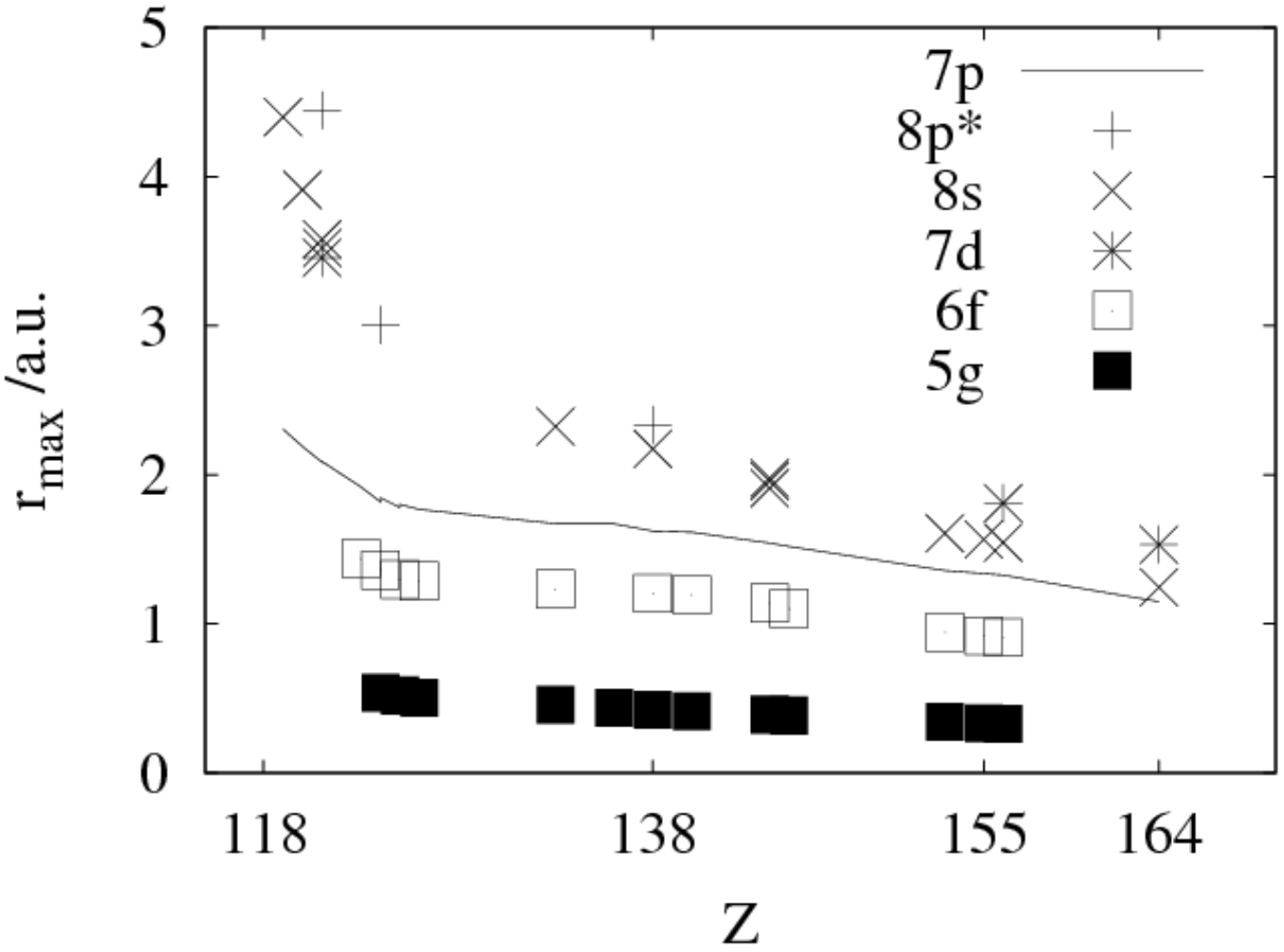
$$h_{ij}^{eff} = P h_{ij} P. \tag{5}$$

In *Coulomb gauge* the next term is the *Araki-Sucher* one, H. Araki, Progr. Theor. Phys. 17 (1957) 619. See I. lindgren, IJQC 106 (2006) 2833.



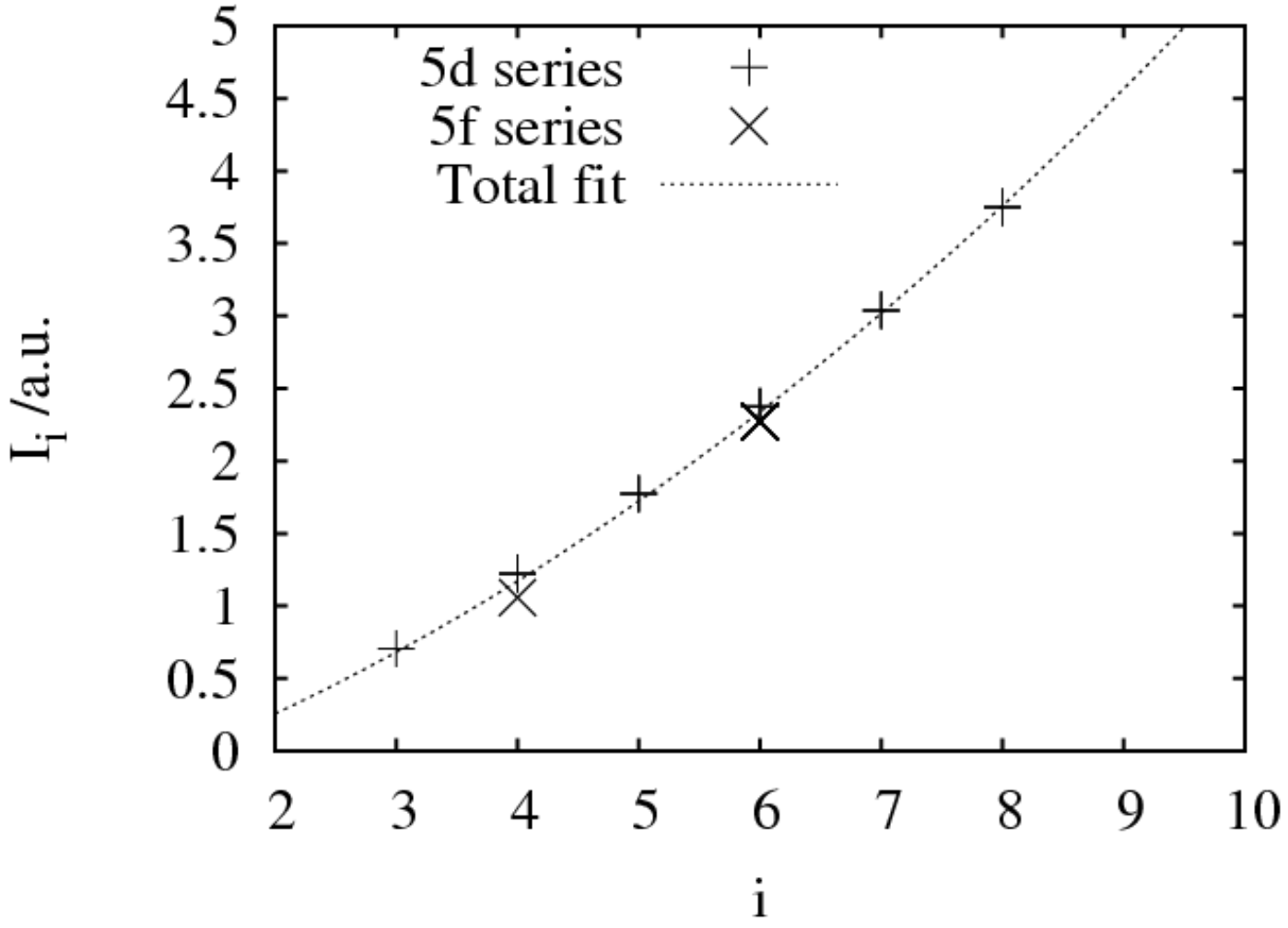
- For a point nucleus, the 1s solution disappears at Z = 137.036.
- For a finite nucleus, that happens around Z = 172.

1) THE NODELESS 5g SHELL IS VERY COMPACT .
2) THE 7p SHELL IS A PERSISTENT OUTER-CORE ORBITAL



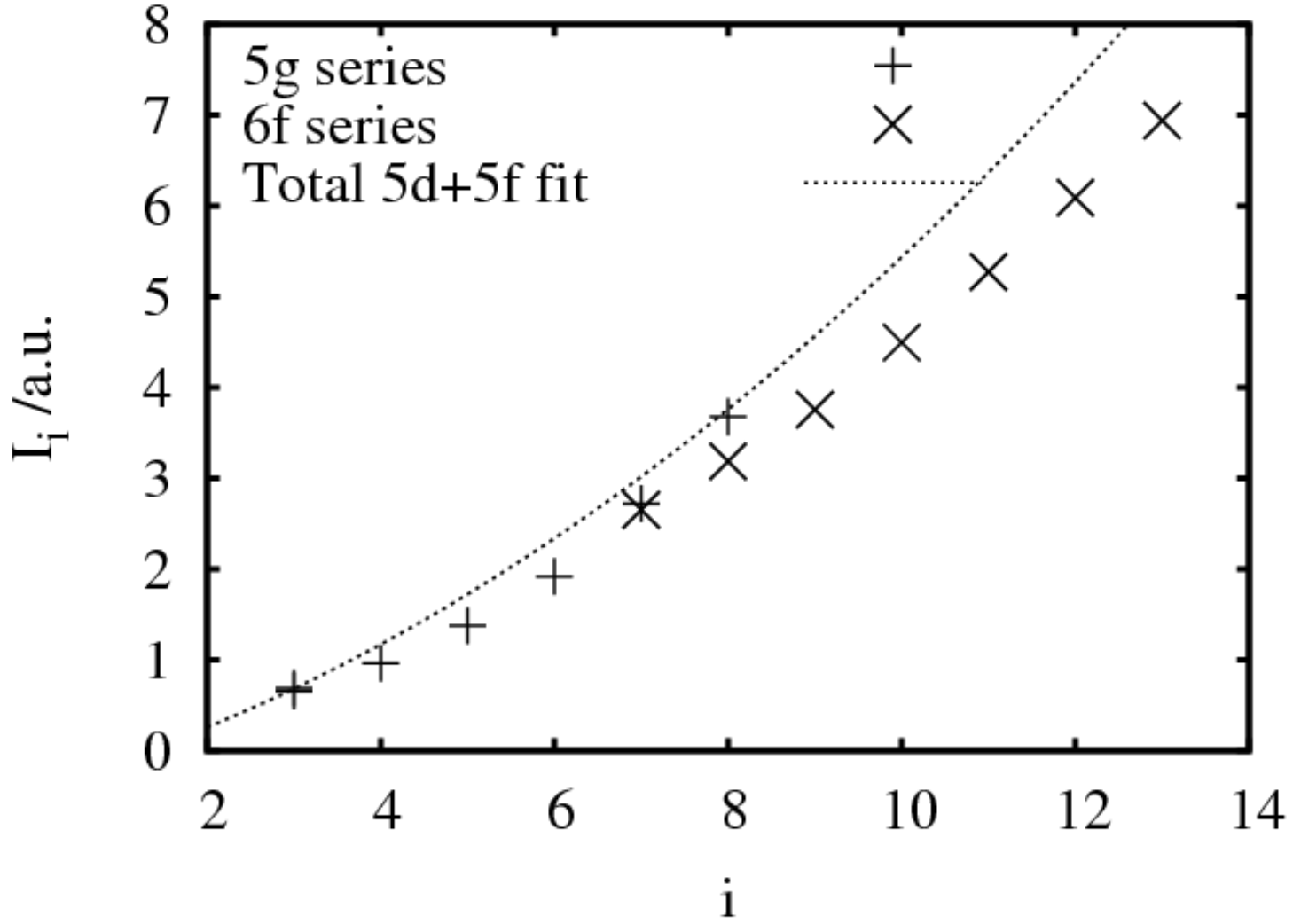
P. Pyykkö, PCCP 13 (2011) 161-168.

HOW ABOUT OXIDATION STATES?
USE THE 5d AND 5f ELEMENTS FOR COMPARISON



P. Pyykkö, PCCP 13 (2011) 161-168.

HOW ABOUT OXIDATION STATES/2 ?
USE THE 5d AND 5f ELEMENTS FOR COMPARISON



P. Pyykkö, PCCP 13 (2011) 161-168.

POSSIBLE NEW MOLECULES

Class	Molecule	Analogs
$8s^0\ 5g^1$	$(E125)X_6$	
$8s^2\ 5g^{18}$	$(E142)X_4$	ThF_4
	$(E146)X_6$	UF_6
$8s^0\ 5g^{18}$	$(E144)X_8$	PuF_8
	$(E144)O_4$	PuO_4
	$(E148)O_6$	UO_6
$8s^2\ 7d^0\ 6f^{14}\ 5g^{18}$	$(E158)X_6$	WF_6
$7d^8$	$(E164)X_4$	HgF_4

SIMPLEST PREDICTIONS FOR CHEMICAL BONDING: Molecular, self-consistent covalent radii

$$R(AB) = r_A + r_B.$$

SINGLE-, DOUBLE- AND TRIPLE-BOND COVALENT RADII UP TO Z = 118. Mean deviation 3 pm.

P. Pyykkö, M. Atsumi, CEJ 15 (2009) 12770.

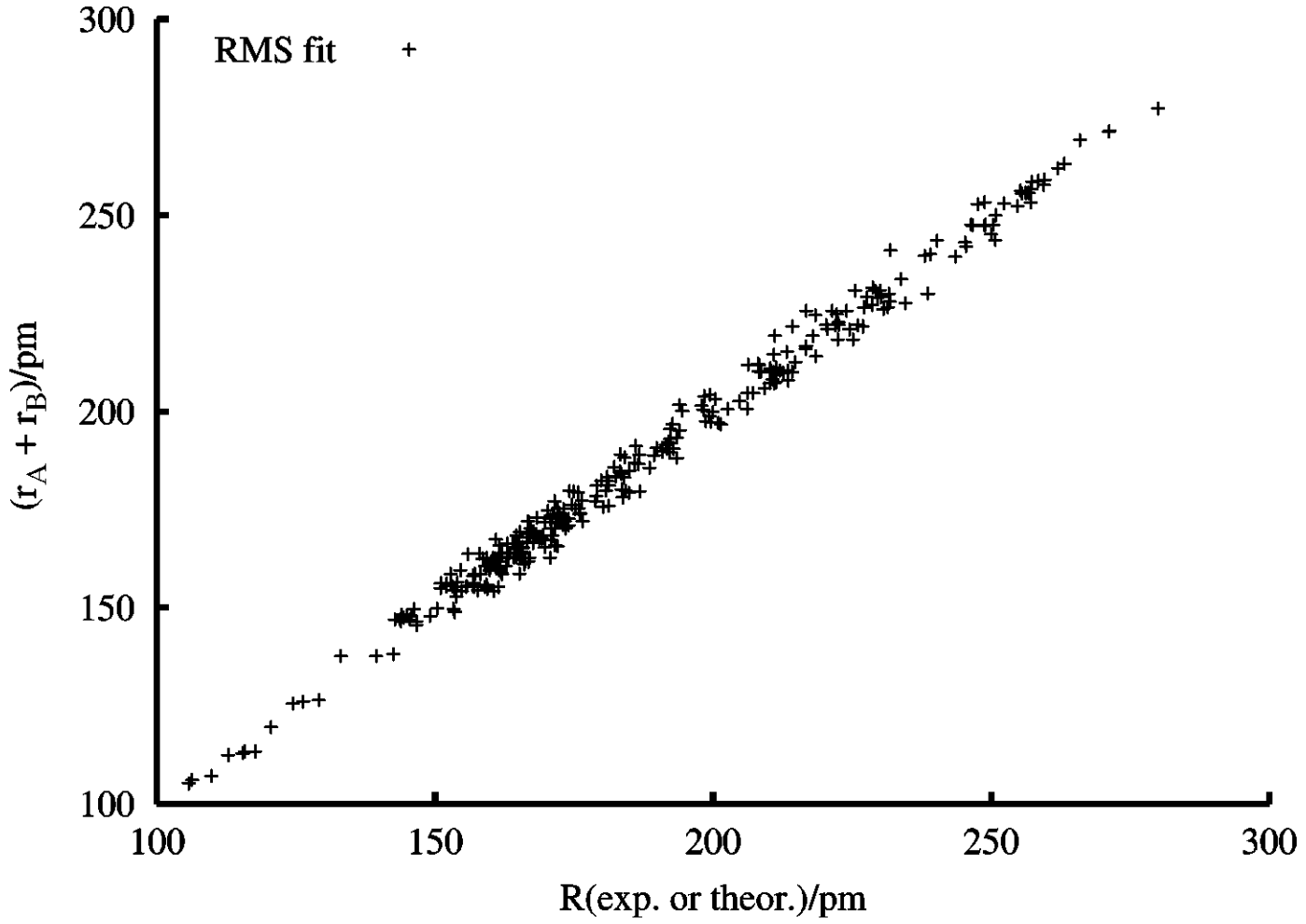
Self-Consistent, Year-2009 Covalent Radii

r/pm (=10^{-12} m)

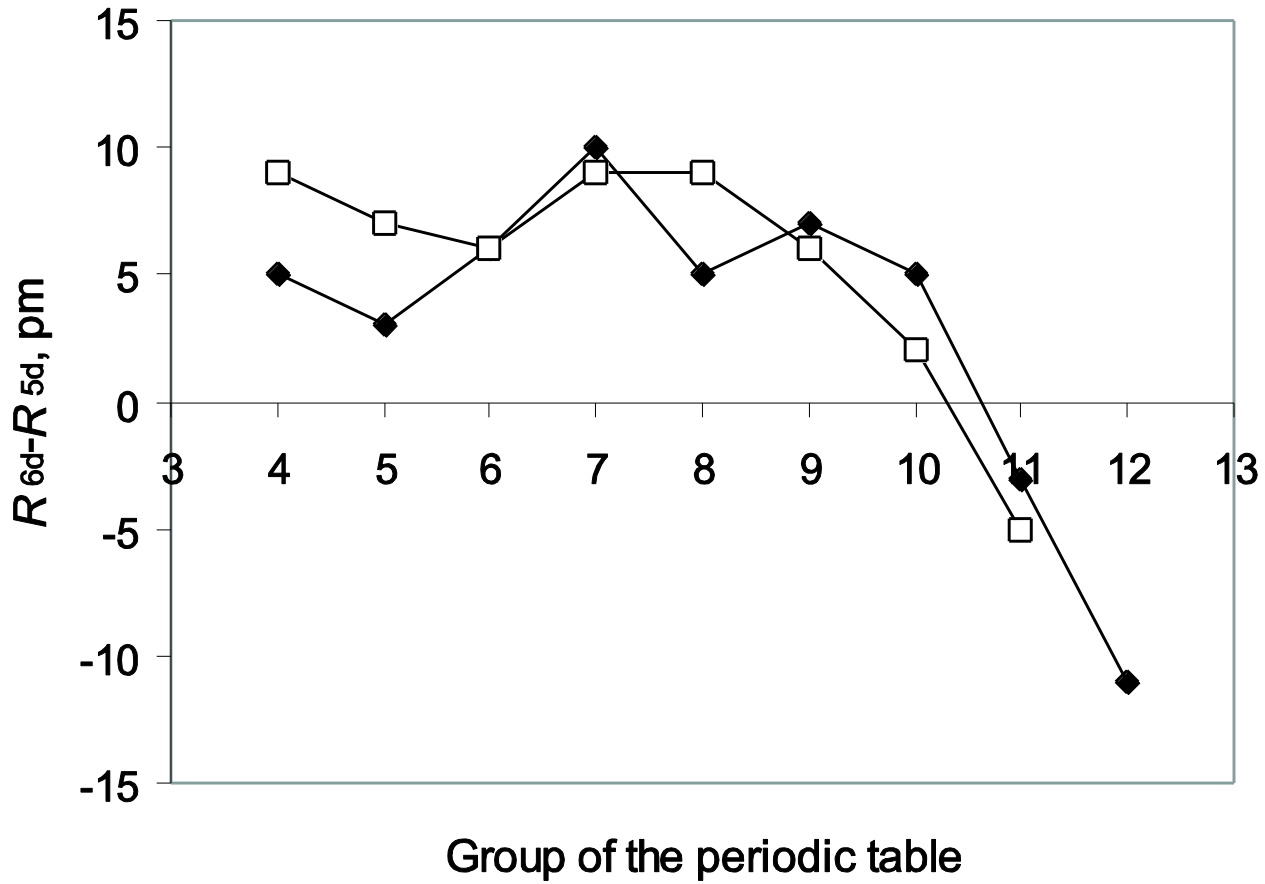
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H **32** - -																	2 He **46** - -
3 Li **133** **124** -	4 Be **102** **90** **85**				Z Radius, r_n: Symbol $\mathbf{r}_1$ $\mathbf{r}_2$ $\mathbf{r}_3$							5 B **85** **78** **73**	6 C **75** **67** **60**	7 N **71** **60** **54**	8 O **63** **57** **53**	9 F **64** **59** **53**	10 Ne **67** **96** -
11 Na **155** **160** -	12 Mg **139** **132** **127**											13 Al **126** **113** **111**	14 Si **116** **107** **102**	15 P **111** **102** **94**	16 S **103** **94** **95**	17 Cl **99** **95** **93**	18 Ar **96** **107** **96**
19 K **196** **193** -	20 Ca **171** **147** **133**	21 Sc **148** **116** **114**	22 Ti **136** **117** **108**	23 V **134** **112** **106**	24 Cr **122** **111** **103**	25 Mn **119** **105** **103**	26 Fe **116** **109** **102**	27 Co **111** **103** **96**	28 Ni **110** **101** **101**	29 Cu **112** **115** **120**	30 Zn **118** **120** -	31 Ga **124** **117** **121**	32 Ge **121** **111** **114**	33 As **121** **114** **106**	34 Se **116** **107** **107**	35 Br **114** **109** **110**	36 Kr **117** **121** **108**
37 Rb **210** **202** -	38 Sr **185** **157** **139**	39 Y **163** **130** **124**	40 Zr **154** **127** **121**	41 Nb **147** **125** **116**	42 Mo **138** **121** **113**	43 Tc **128** **120** **110**	44 Ru **125** **114** **103**	45 Rh **125** **110** **106**	46 Pd **120** **117** **112**	47 Ag **128** **139** **137**	48 Cd **136** **144** -	49 In **142** **136** **146**	50 Sn **140** **130** **132**	51 Sb **140** **133** **127**	52 Te **136** **128** **121**	53 I **133** **129** **125**	54 Xe **131** **135** **122**
55 Cs **232** **209** -	56 Ba **196** **161** **149**	La–Lu	72 Hf **152** **128** **122**	73 Ta **146** **126** **119**	74 W **137** **120** **115**	75 Re **131** **119** **110**	76 Os **129** **116** **109**	77 Ir **122** **115** **107**	78 Pt **123** **112** **110**	79 Au **124** **121** **123**	80 Hg **133** **142** -	81 Tl **144** **142** **150**	82 Pb **144** **135** **137**	83 Bi **151** **141** **135**	84 Po **145** **135** **129**	85 At **147** **138** **138**	86 Rn **142** **145** **133**
87 Fr **223** **218** -	88 Ra **201** **173** **159**	Ac–Lr	104 Rf **157** **140** **131**	105 Db **149** **136** **126**	106 Sg **143** **128** **121**	107 Bh **141** **128** **119**	108 Hs **134** **125** **118**	109 Mt **129** **125** **113**	110 Ds **128** **116** **112**	111 Rg **121** **116** **118**	112 **122** **137** **130**	113 **136**	114 **143**	115 **162**	116 **175**	117 **165**	118 **157**

57 La	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
180	**163**	**176**	**174**	**173**	**172**	**168**	**169**	**168**	**167**	**166**	**165**	**164**	**170**	**162**
139	**137**	**138**	**137**	**135**	**134**	**134**	**135**	**135**	**133**	**133**	**133**	**131**	**129**	**131**
139	**131**	**128**					**132**							**131**
89 Ac	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
186	**175**	**169**	**170**	**171**	**172**	**166**	**166**	**168**	**168**	**165**	**167**	**173**	**176**	**161**
153	**143**	**138**	**134**	**136**	**135**	**135**	**136**	**139**	**140**	**140**		**139**		**141**
140	**136**	**129**	**118**	**116**										

MEAN-SQUARE DEVIATION ONLY 3 pm
for both single-, double- and *triple*-bond radii, $r_1 - r_3$



THE COLLAPSE OF COVALENT RADII AT GROUP 10 (♦ SINGLE, □ TRIPLE BONDS) .



The Kumpula Campus, University of Helsinki, Finland

- Faculty of Science.
- Government labs:
  - Meteorology
  - Marine Research
- Including students, about 9000 people.
- Entire U of H: 38000 students.
- 8 national CoE:s, including ’Finnish Centre of Excellence of Computational Molecular Science’ (2006-2011). (CMS)
- CMS groups: Pyykkö-Sundholm, Halonen, Räsänen, Nordlund. About 60 people.
- Nordic ’umbrella’ of CoE:s.