

Numeri Quantici degli Elettroni

$n =$ **numero quantico principale** ($n \geq 1$): energia, grandezza

$l =$ **numero quantico (del momento angolare) orbitale**: forma

$l = 0, 1, 2, 3, 4, \dots, n-1$ (in totale n valori interi)

La grandezza del momento angolare orbitale è data da $h/2\pi \times \sqrt{l(l+1)}$

$m_l =$ **numero quantico magnetico**: orientazione

$m_l = -l, -l+1, \dots, 0, \dots, l-1, l$ (in totale $2l+1$ valori interi)

$s =$ **numero quantico di spin**: definisce il momento angolare di spin

$s = 1/2$

La grandezza del momento angolare di spin è data da $h/2\pi \times \sqrt{s(s+1)}$

$m_s =$ **numero quantico magnetico di spin**: orientazione

$m_s = -1/2, +1/2$

Un orbitale atomico è definito in maniera univoca da 3 numeri quantici n , l , e m_l .

Un elettrone in un orbitale atomico è definito in maniera univoca da 4 numeri quantici: n , l , m_l , m_s .

Atomi Polielettronici

Principio di esclusione di Pauli

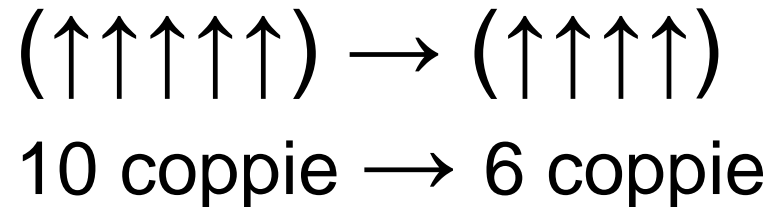
in un dato atomo non vi possono essere 2 elettroni con la stessa quaterna di numeri quantici

Regola di Hund o della massima molteplicità

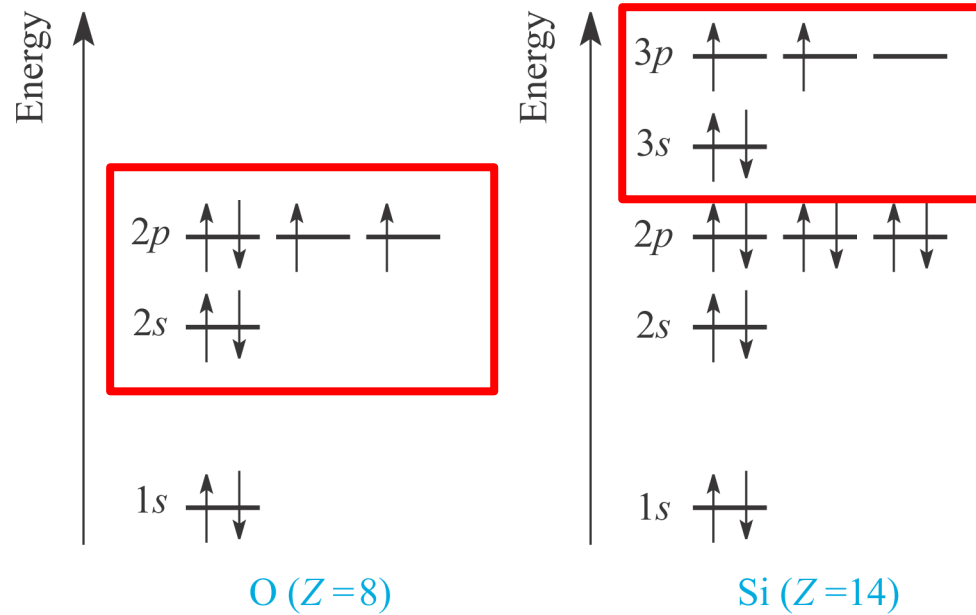
in un set di orbitali degeneri gli elettroni non possono avere spin accoppiati in un orbitale finché ogni orbitale nel set non contenga un elettrone, tutti con spin parallelo

Energia di correlazione ed Energia di scambio

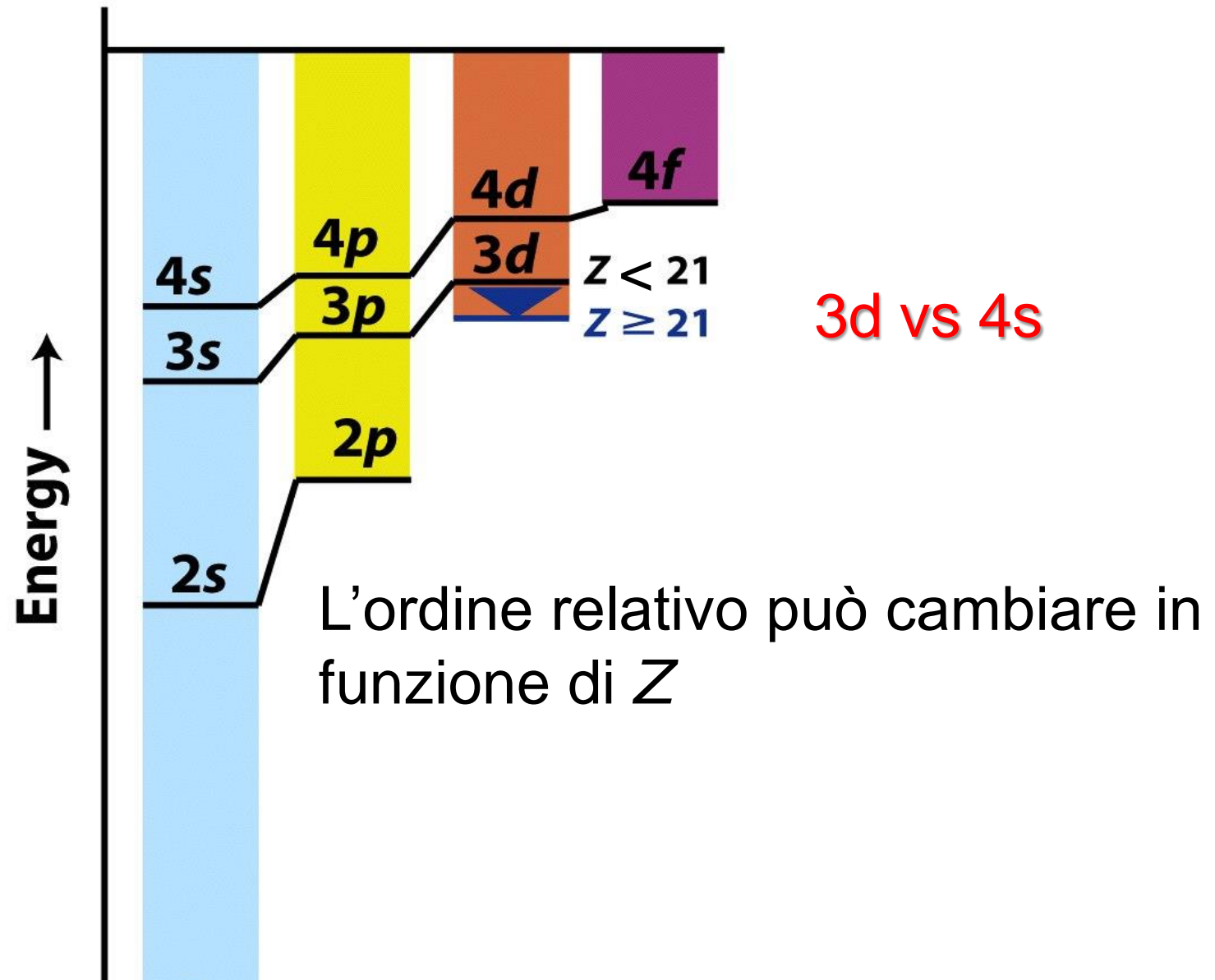
La massima energia di scambio si ottiene nei gusci semi-pieni, nei quali si ha il massimo numero di elettroni a spin paralleli.



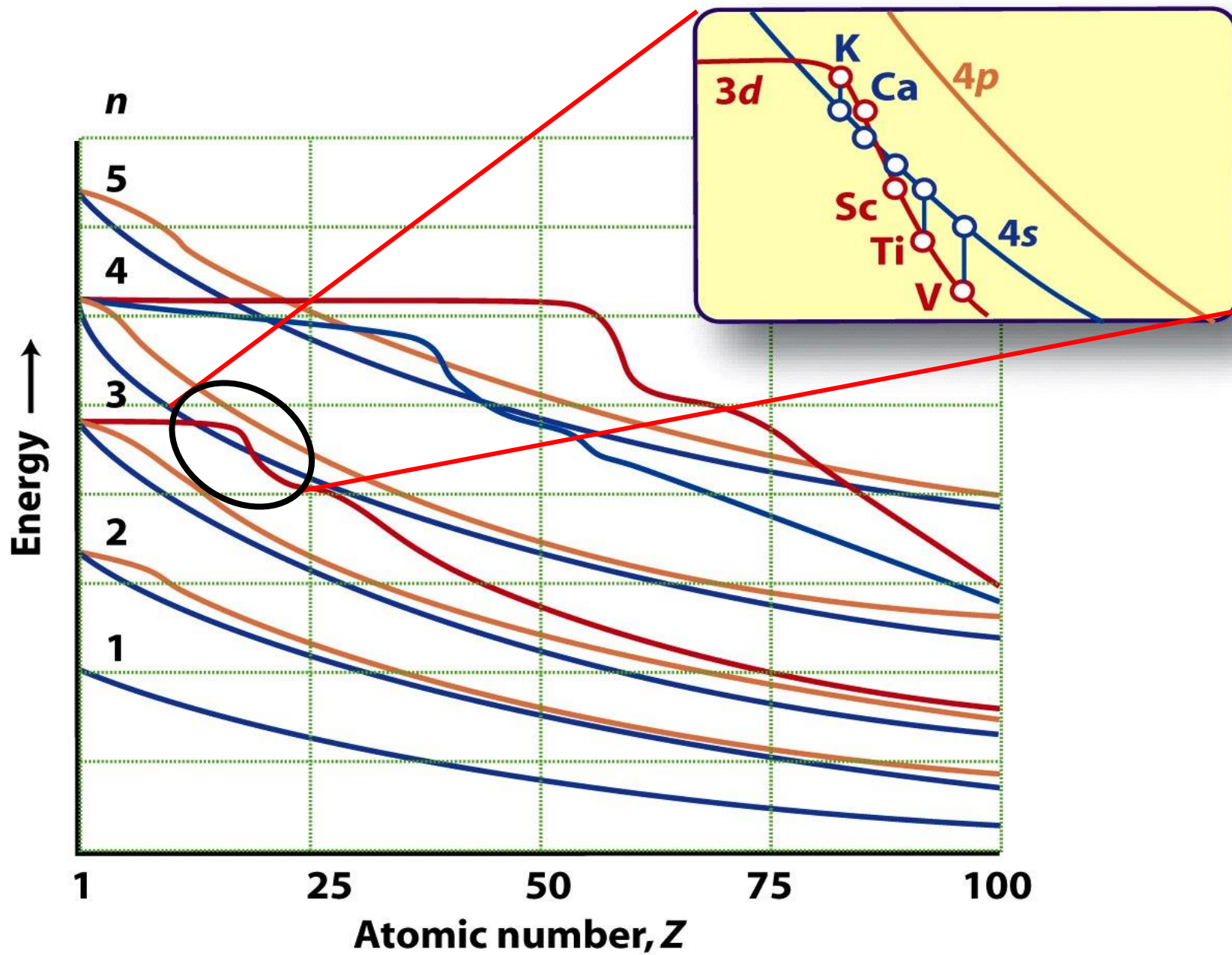
Negli atomi polielettronici l'energia dipende da n e da l



Principio del riempimento progressivo (*Aufbau*)

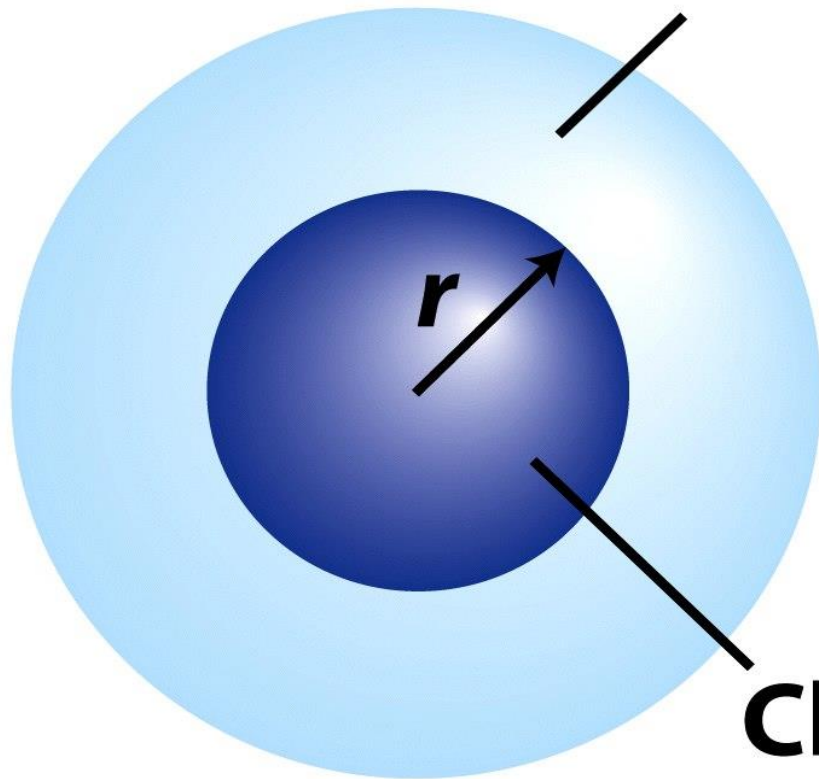


$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 5d \approx 4f < 6p < 7s < 6d \approx 5f$



Penetrazione e schermatura

**Charge does
not contribute**



**Charge
contributes**

Regole di Slater (ca. 1930)

(empiriche) per il calcolo della **costante di schermo S**

$$Z_{\text{eff}} = Z - S$$

1. si scrive la configurazione elettronica dell'elemento nel seguente ordine e con questi raggruppamenti: $(1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) \dots$
2. gli elettroni in ogni gruppo a destra dell'elettrone considerato non contribuiscono a S
3. per un elettrone in un orbitale ns o np :
 - ogni altro elettrone nello stesso gruppo contribuisce $S = 0.35$;
 - ogni elettrone nel livello $n-1$ contribuisce $S = 0.85$;
 - ogni elettrone nei livelli $n-2$ o inferiori contribuisce $S = 1$
4. per un elettrone in un orbitale nd o nf :
 - ogni altro elettrone nello stesso gruppo (nd, nf) contribuisce $S = 0.35$
 - ogni elettrone in un gruppo a sinistra di quello considerato contribuisce $S = 1$.

Valori sperimentali di Z_{eff}

Table 1.3 Effective nuclear charges, Z_{eff}

	H								He
<i>Z</i>	1								2
1 <i>s</i>	1.00								1.69
	Li	Be	B	C	N	O	F		Ne
<i>Z</i>	3	4	5	6	7	8	9	10	10
1 <i>s</i>	2.69	3.68	4.68	5.67	6.66	7.66	8.65	9.64	9.64
2 <i>s</i>	1.28	1.91	2.58	3.22	3.85	4.49	5.13	5.76	5.76
2 <i>p</i>			2.42	3.14	3.83	4.45	5.10	5.76	5.76
	Na	Mg	Al	Si	P	S	Cl		Ar
<i>Z</i>	11	12	13	14	15	16	17	18	18
1 <i>s</i>	10.63	11.61	12.59	13.57	14.56	15.54	16.52	17.51	17.51
2 <i>s</i>	6.57	7.39	8.21	9.02	9.82	10.63	11.43	12.23	12.23
2 <i>p</i>	6.80	7.83	8.96	9.94	10.96	11.98	12.99	14.01	14.01
3 <i>s</i>	2.51	3.31	4.12	4.90	5.64	6.37	7.07	7.76	7.76
3 <i>p</i>			4.07	4.29	4.89	5.48	6.12	6.76	6.76

0.69

0.62

s-block elements

d-block elements

p-block elements

Group 1		Group 2		Group 3	Group 4	Group 5	Group 6	Group 7	Group 8	Group 9	Group 10	Group 11	Group 12	Group 13	Group 14	Group 15	Group 16	Group 17	Group 18	
1 H																				2 He
3 Li	4 Be													5 B	6 C	7 N	8 O	9 F	10 Ne	
11 Na	12 Mg													13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
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			
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			
55 Cs	56 Ba	57–71 La–Lu	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			
87 Fr	88 Ra	89–103 Ac–Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub									

f-block elements

Lanthanoids	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
Actinoids	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

The 32-column version of the periodic table published by IUPAC

H																	He															
Li	Be															B	C	N	O	F	Ne											
Na	Mg															Al	Si	P	S	Cl	Ar											
K	Ca											Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr					
Rb	Sr											Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe					
Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og

The group 3 problem

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

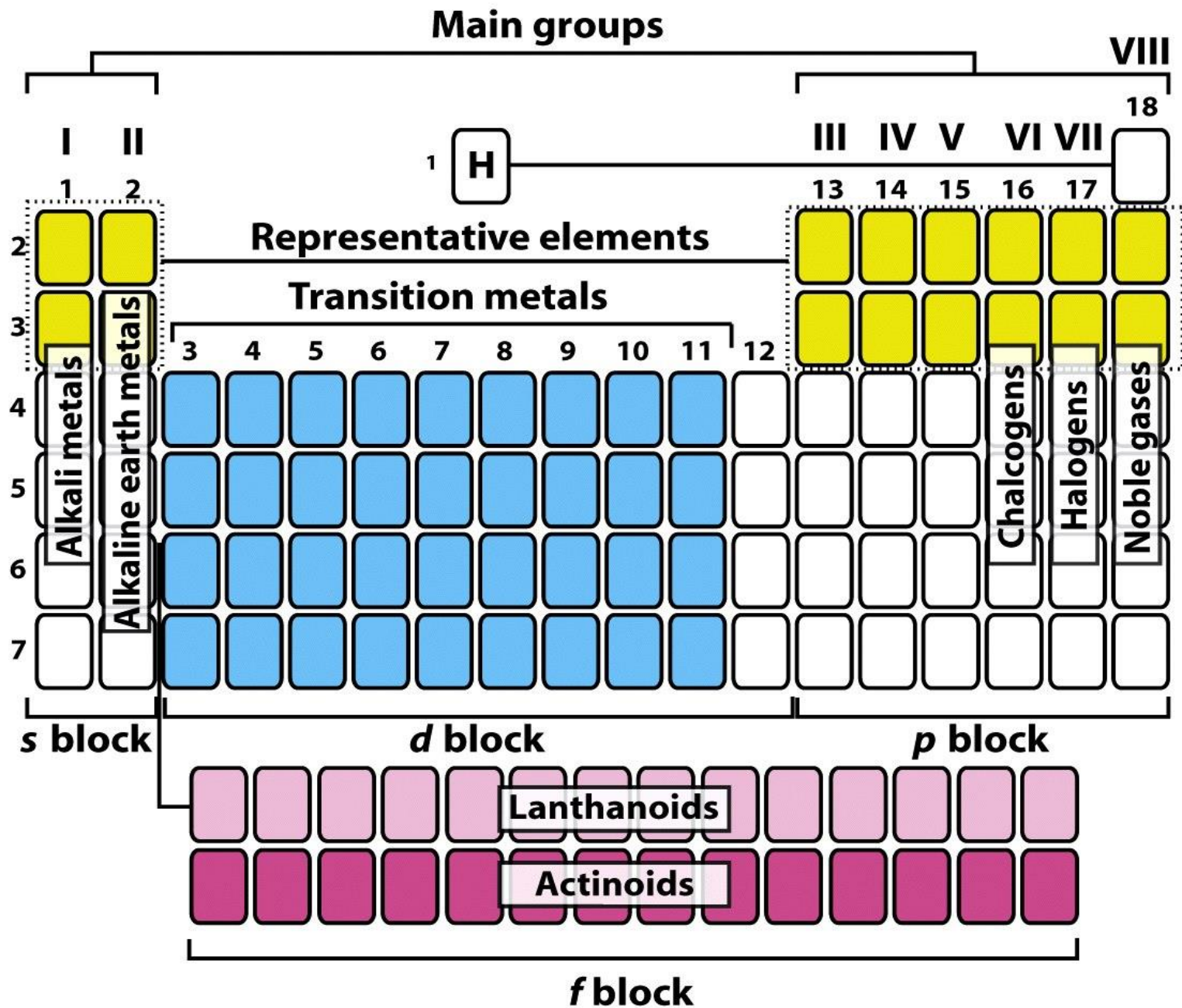
The main periodic table consists of 7 rows and 18 columns. The elements are arranged as follows:

H	He	Li	Be													B	C	N	O
F	Ne	Na	Mg													Al	Si	P	S
Cl	Ar	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn		Ga	Ge	As	Se	
Br	Kr	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd		In	Sn	Sb	Te	
I	Xe	Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg		Tl	Pb	Bi	Po	
At	Rn	Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub		Uut	Uuq	Uup	Uuh	
Uus	Uuo																		

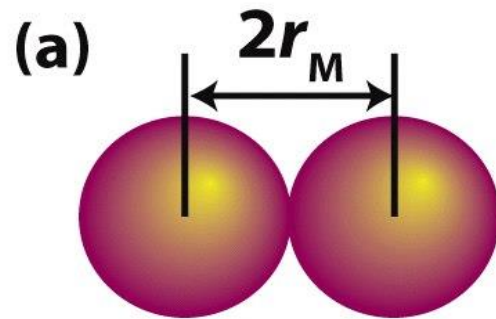
The lanthanide and actinide series are shown in two rows of 14 elements each, colored yellow:

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

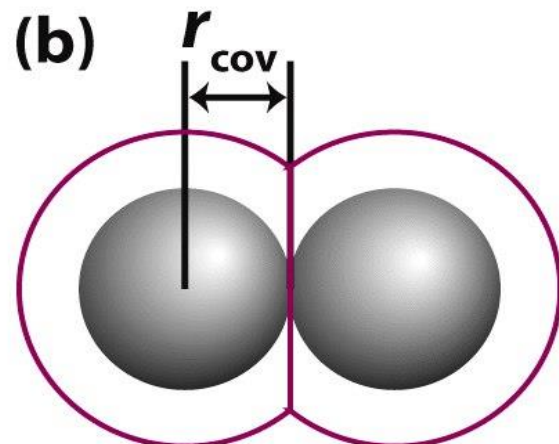
Figure 2 | Scerri's periodic table. Eric Scerri proposes a symmetrical version of the periodic table in which hydrogen is grouped with the halogens, and there are no longer any exceptional periods. Figure adapted with permission from Eric Scerri.



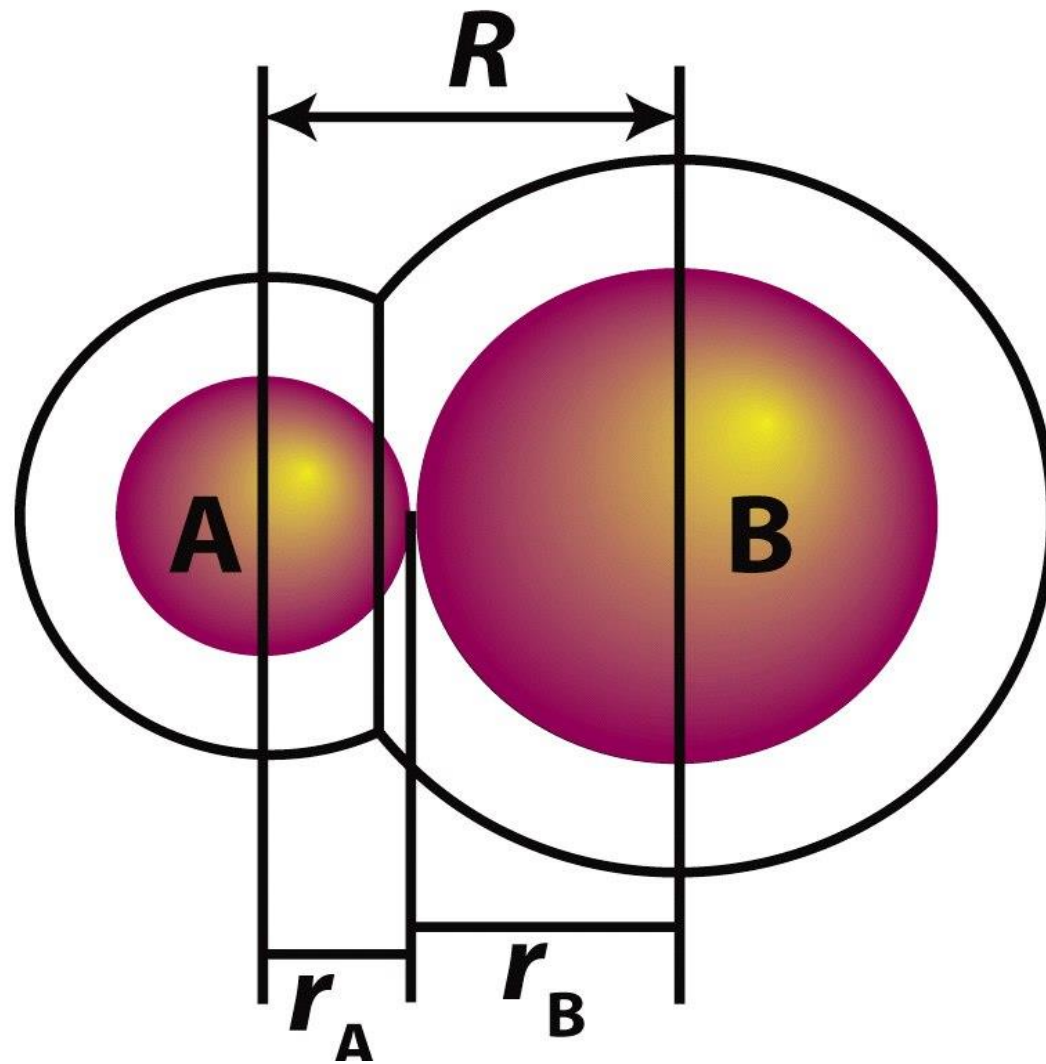
Raggio Atomico



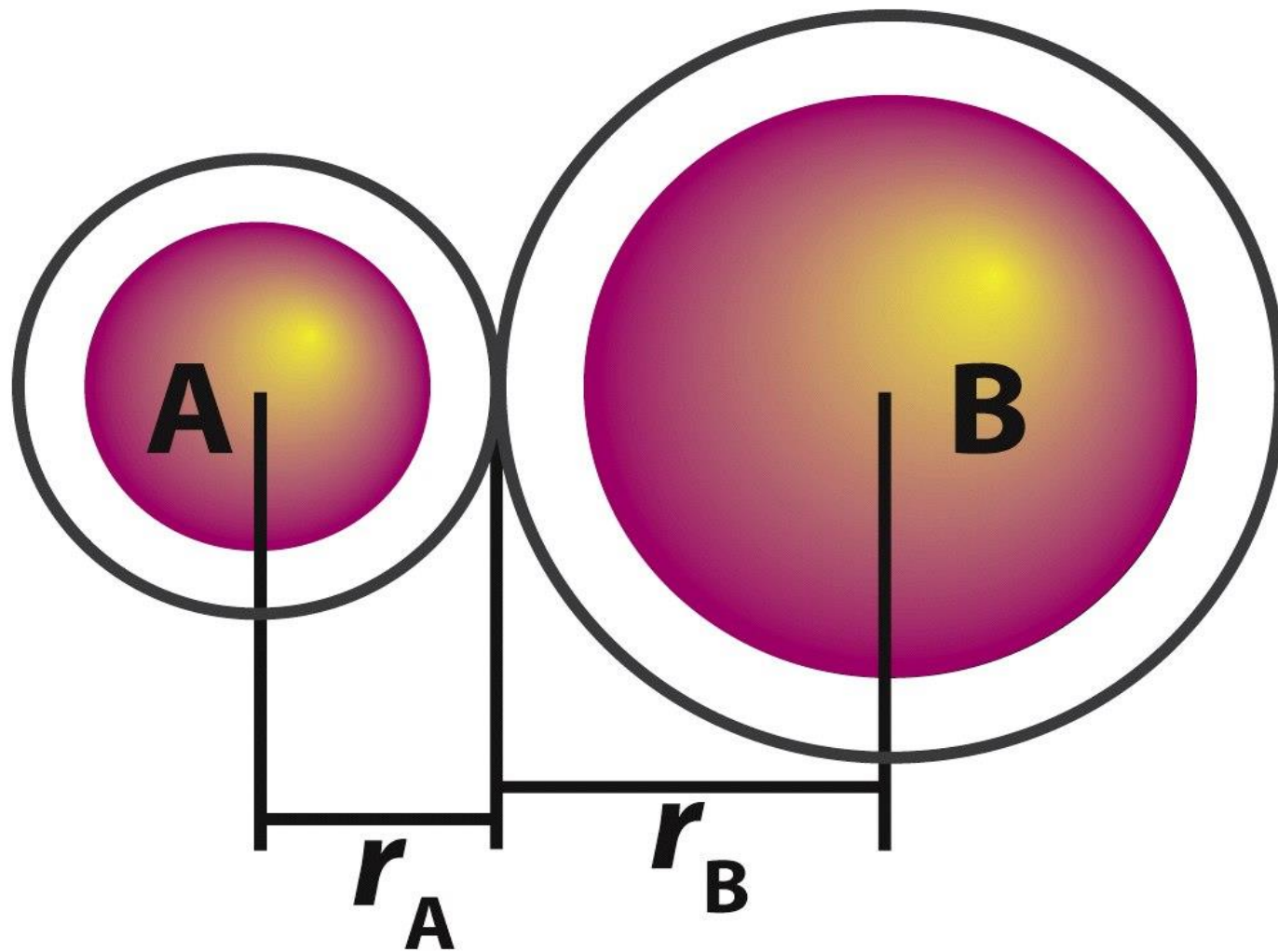
Raggio metallico



Raggio covalente

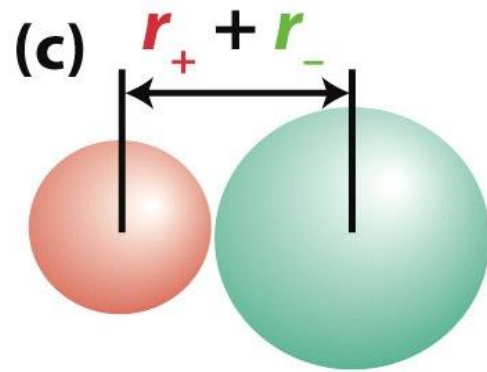


Raggio covalente

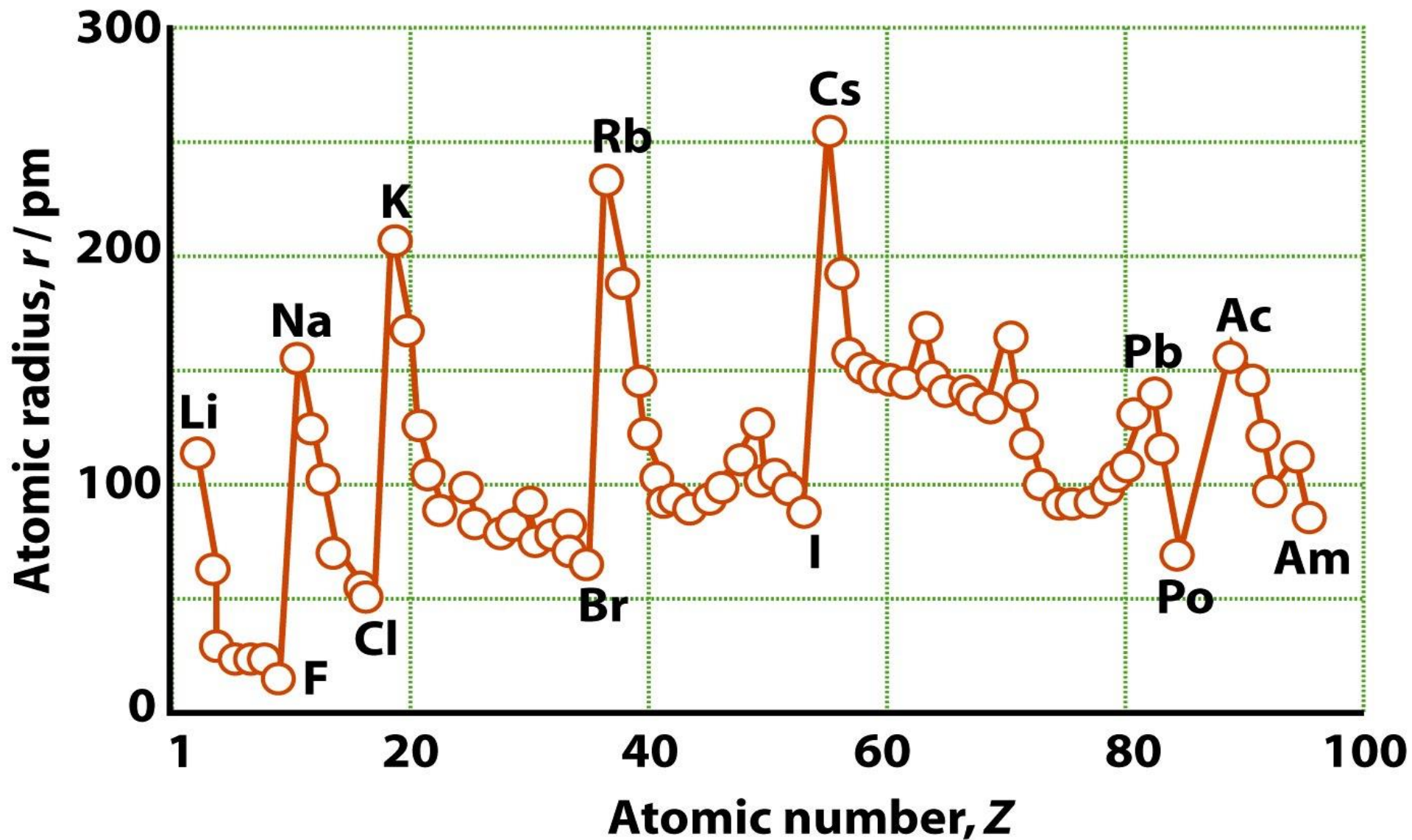


Raggio di van der Waals

Raggio Ionico



$$r_{\text{O}^{2-}} = 140 \text{ pm}$$

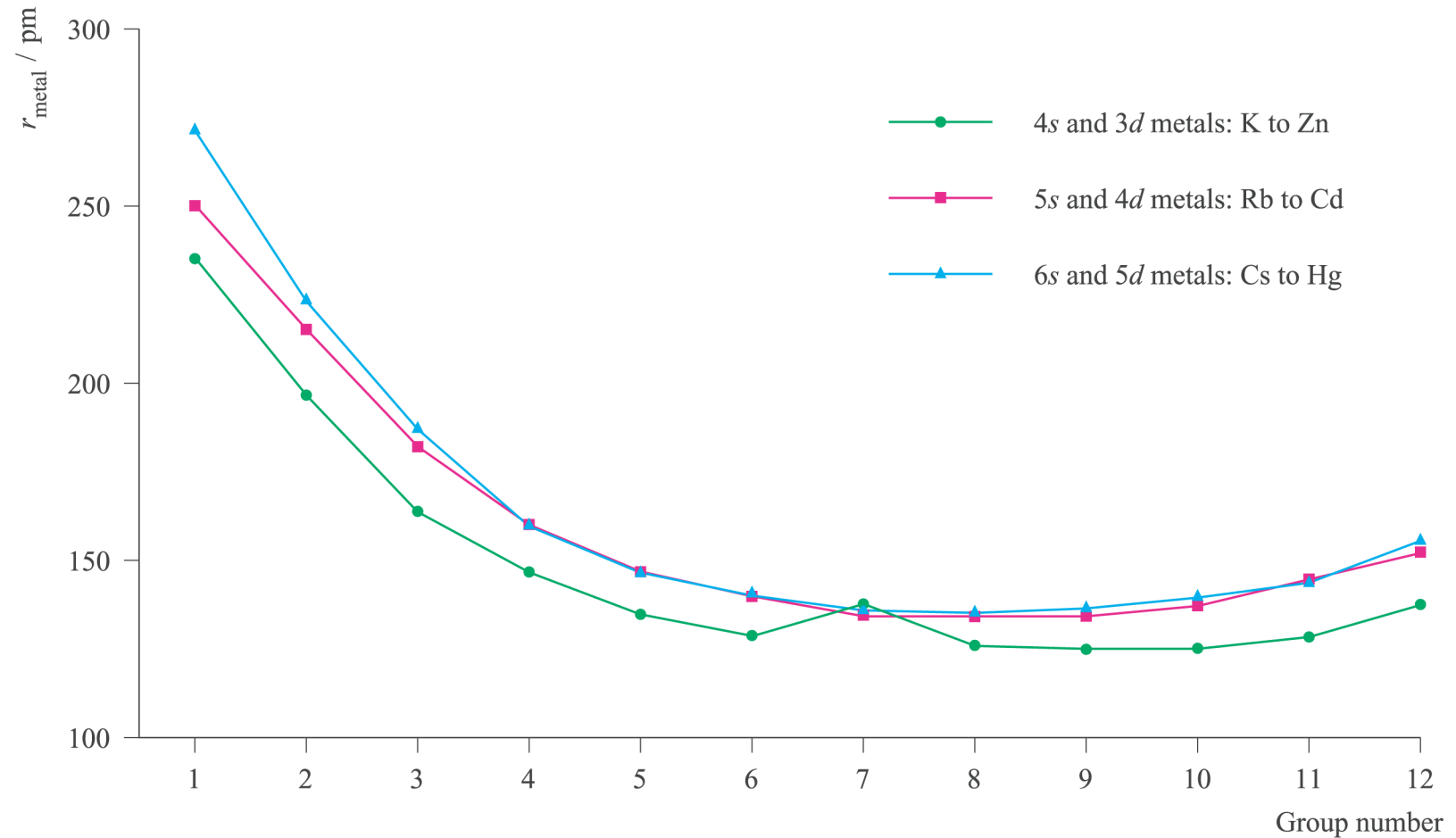


Raggi atomici

The image displays a periodic table with atomic radii trends. The table is organized into 6 rows and 8 columns. The columns are labeled 1 through 18. The rows are labeled 2 through 6. Each element is represented by a colored circle containing its symbol and atomic number. The colors of the circles indicate the trend of atomic radii: yellow for the largest radii (alkali metals), green for intermediate radii, and blue for the smallest radii (halogens). The size of the circles increases from top-left to bottom-right. Overlapping circles are shown on the left side of the table, illustrating the increasing trend of atomic radii down a group.

	1	2	13	14	15	16	17	18
2	Li 152	Be 113	B 83	C 77	N 75	O 73	F 71	Ne
3	Na 180	Mg 160	Al 143	Si 117	P 115	S 104	Cl 99	Ar
4	K 227	Ca 197	Ga 122	Ge 123	As 125	Se 117	Br 114	Kr
5	Rb 248	Sr 215	In 163	Sn 141	Sb 141	Te 143	I 133	Xe
6	Cs 265	Ba 217	Tl 170	Pb 175	Bi 155	Po 167	At	Rn

Raggio metallico



Contrazione lantanidica

Table 1.4 Atomic radii, r/pm^*

Li	Be											B	C	N	O	F
157	112											88	77	74	66	64
Na	Mg											Al	Si	P	S	Cl
191	160											143	118	110	104	99
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
235	197	164	147	135	129	137	126	125	125	128	137	153	122	121	117	114
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
250	215	182	160	147	140	135	134	134	137	144	152	167	158	141	137	133
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi		
272	224	172	159	147	141	137	135	136	139	144	155	171	175	182		

* The values refer to coordination number 12 (see Section 3.2).

Effetti relativistici

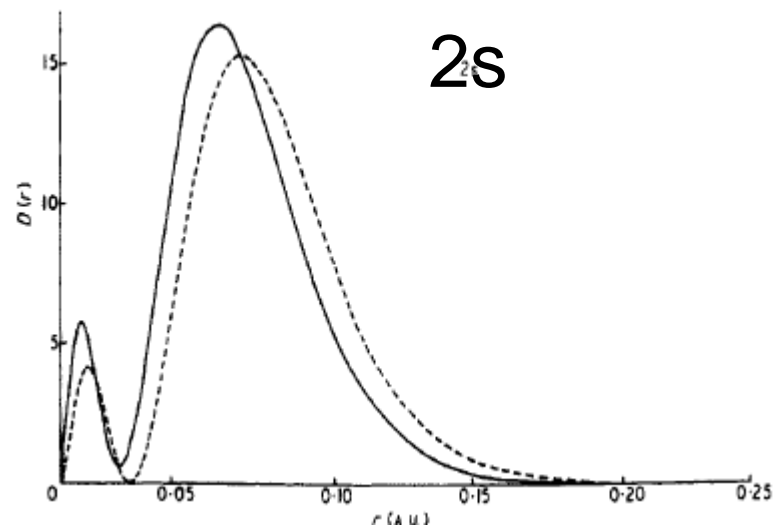
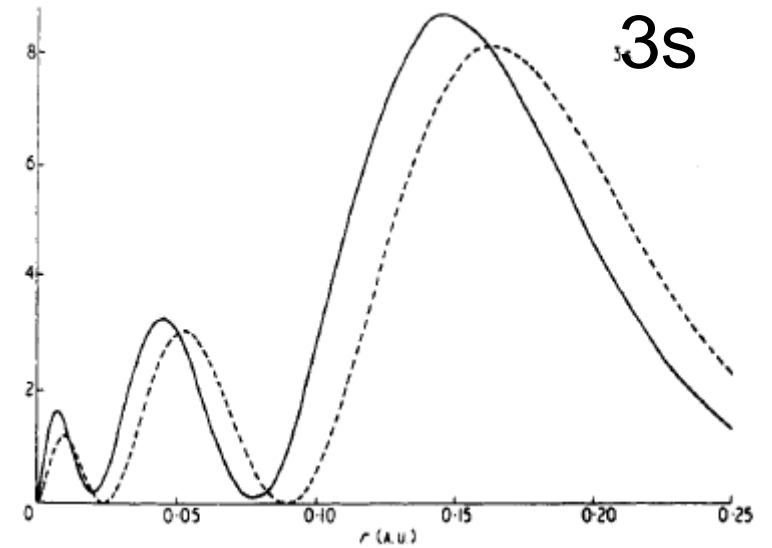
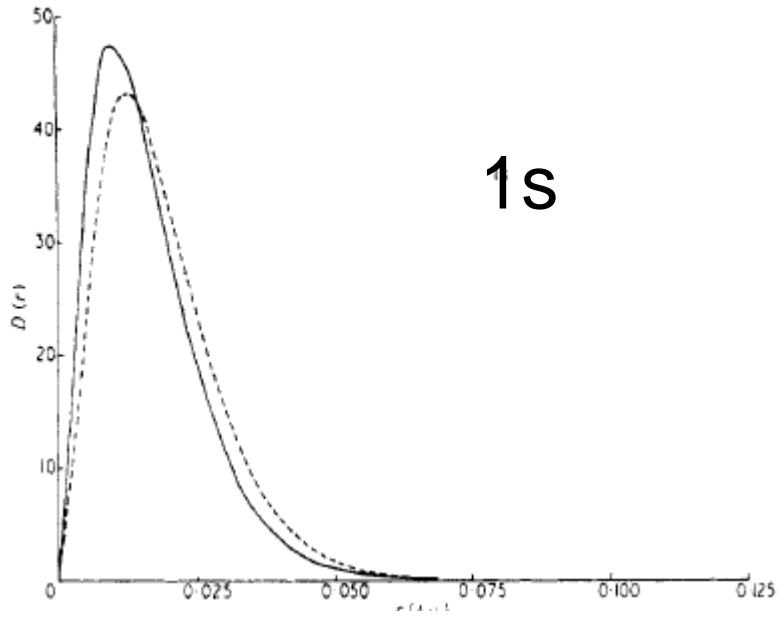
$$m_{\text{rel}} = m_{\text{rest}} / \sqrt{1 - (v/c)^2}$$

Al crescere della velocità degli elettroni, la massa relativistica aumenta rispetto a quella a riposo

$$a_0 = (4\pi\epsilon_0)(\hbar^2 / me^2)$$

L'aumento di massa comporta una contrazione dell'orbitale, che per gli atomi pesanti come Au e Hg può arrivare al 20%

Densità radiale per $Z = 80$





$D(r)$  relativistico
 Non-relativistico

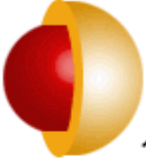

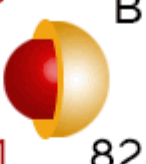
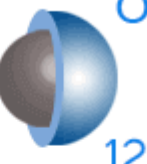
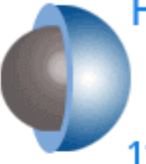
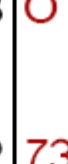
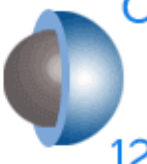

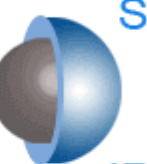





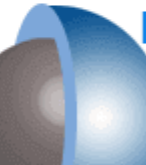
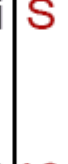
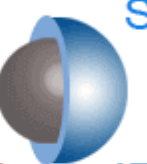





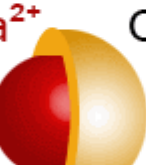




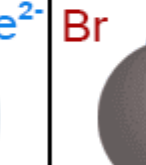

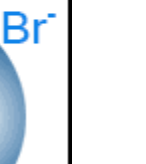


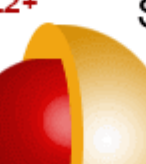



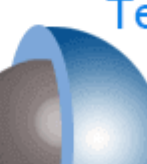
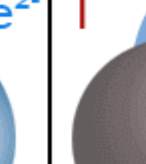

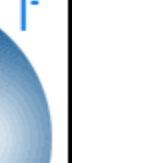
Table 1.5 Ionic radii, r/pm^*

Li⁺ 59(4) 76(6)	Be²⁺ 27(4)	B³⁺ 11(4)			N³⁻ 146	O²⁻ 135(2) 138(4) 140(6) 142(8)	F⁻ 128(2) 131(4) 133(6)
Na⁺ 99(4) 102(6) 118(8)	Mg²⁺ 49(4) 72(6) 89(8)	Al³⁺ 39(4) 53(6)			P³⁻ 212	S²⁻ 184(6)	Cl⁻ 181(6)
K⁺ 138(6) 151(8) 159(10) 160(12)	Ca²⁺ 100(6) 112(8) 123(10) 134(12)	Ga³⁺ 62(6)			As³⁻ 222	Se²⁻ 198(6)	Br⁻ 196(6)
Rb⁺ 152(6) 160(8) 173(12)	Sr²⁺ 118(6) 125(8) 144(12)	In³⁺ 79(6) 92(8)	Sn²⁺ 83(6) 93(8)	Sn⁴⁺ 69(6)		Te²⁻ 221(6)	I⁻ 220(6)
Cs⁺ 167(6) 174(8) 188(12)	Ba²⁺ 149(6) 156(8) 175(12)	Tl³⁺ 88(6)					Tl⁺ 164(6)

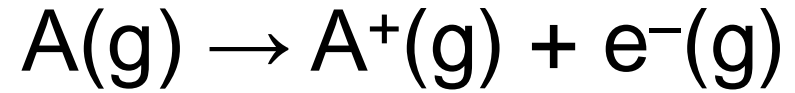
* Numbers in parentheses are the coordination number of the ion. For more values, see *Resource section 1*.

Steps of atoms and their ions in pm

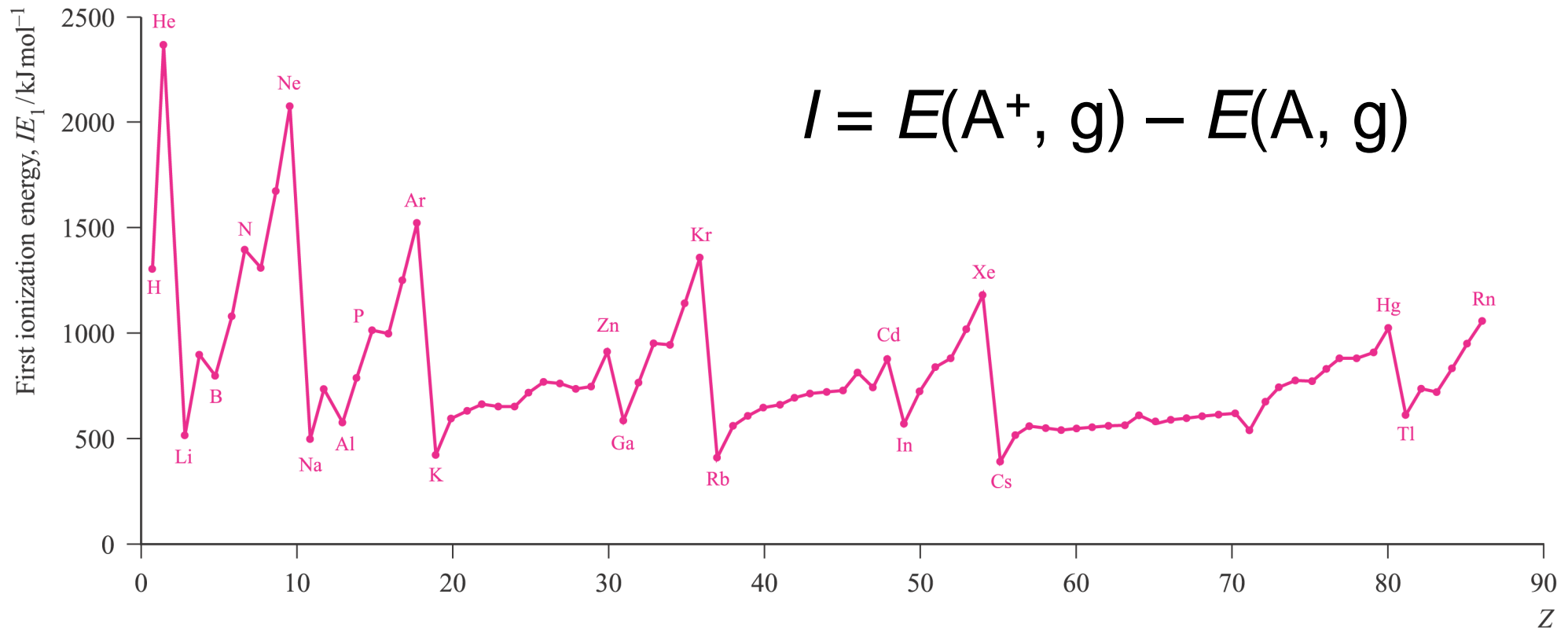
Group 1 Group 2 Group 13 Group 16 Group 17

Li^+  90	Li  134	Be^{2+}  59	Be  90	B^{3+}  41	B  82	O  73	O^{2-}  126	F  71	F^-  119
Na^+  116	Na  154	Mg^{2+}  86	Mg  130	Al^{3+}  68	Al  118	S  102	S^{2-}  170	Cl  99	Cl^-  167
K^+  152	K  196	Ca^{2+}  114	Ca  174	Ga^{3+}  76	Ga  126	Se  116	Se^{2-}  184	Br  114	Br^-  182
Rb^+  166	Rb  211	Sr^{2+}  132	Sr  192	In^{3+}  94	In  144	Te  135	Te^{2-}  207	I  133	I^-  206

Energia di Ionizzazione



$$I = E(A^+, g) - E(A, g)$$



$$1\text{eV} = 96.5 \text{ kJ mol}^{-1}$$

Table 1.6 First and second (and some higher) ionization energies of the elements, $I/(kJ\ mol^{-1})$

H							He
1312							2373
							5259
Li	Be	B	C	N	O	F	Ne
513	899	801	1086	1402	1314	1681	2080
7297	1757	2426	2352	2855	3386	3375	3952
11809	14844	3660	4619	4577	5300	6050	6122
		25018					
Na	Mg	Al	Si	P	S	Cl	Ar
495	737	577	786	1011	1000	1251	1520
4562	1476	1816	1577	1903	2251	2296	2665
6911	7732	2744	3231	2911	3361	3826	3928
		11574					
K	Ca	Ga	Ge	As	Se	Br	Kr
419	589	579	762	947	941	1139	1351
3051	1145	1979	1537	1798	2044	2103	3314
4410	4910	2963	3302	2734	2974	3500	3565
Rb	Sr	In	Sn	Sb	Te	I	Xe
403	549	558	708	834	869	1008	1170
2632	1064	1821	1412	1794	1795	1846	2045
3900	4210	2704	2943	2443	2698	3197	3097
Cs	Ba	Tl	Pb	Bi	Po	At	Rn
375	502	590	716	704	812	926	1036
2420	965	1971	1450	1610	1800	1600	
3400	3619	2878	3080	2466	2700	2900	

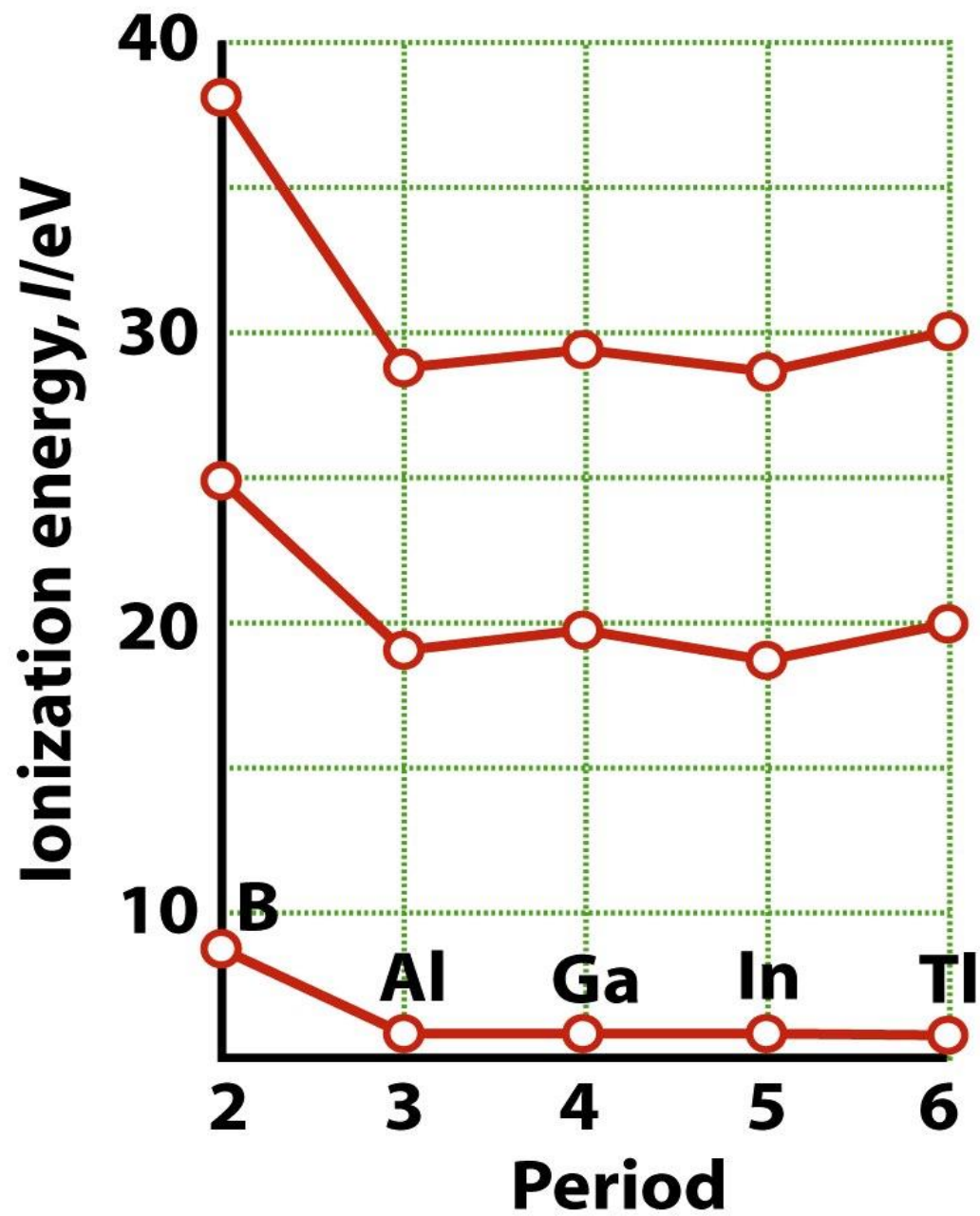


Table 1.7 Electron affinities of the main-group elements, $E_a/(\text{kJ mol}^{-1})^*$

H								He
72								-48
Li	Be	B	C	N	O	F	Ne	
60	≤ 0	27	122	-8	141	328	-116	
					-780			
Na	Mg	Al	Si	P	S	Cl	Ar	
53	≤ 0	43	134	72	200	349	-96	
					-492			
K	Ca	Ga	Ge	As	Se	Br	Kr	
48	2	29	116	78	195	325	-96	
Rb	Sr	In	Sn	Sb	Te	I	Xe	
47	5	29	116	103	190	295	-77	

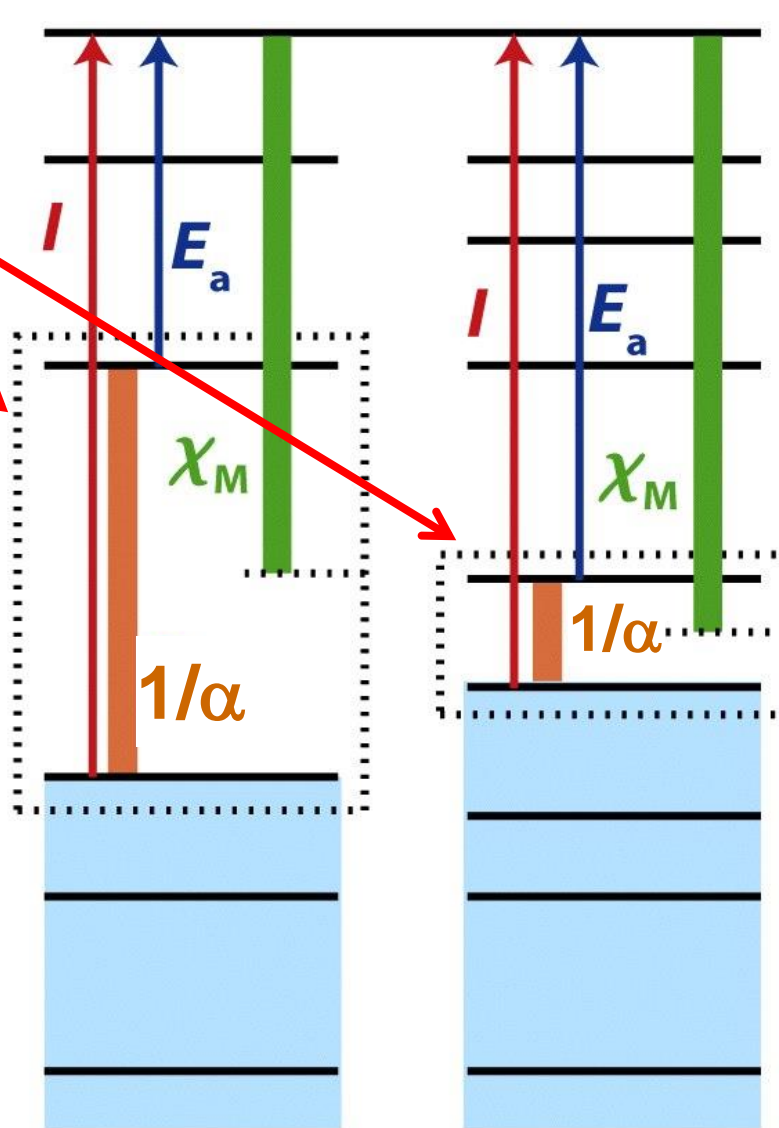
* The first values refer to the formation of the ion X^- from the neutral atom; the second value to the formation of X^{2-} from X^- .

l'affinità elettronica ha segno opposto alla variazione di energia

Ionization limit

Orbitali di
frontiera

Energy ↑



(a)

(b)

Electron affinity/kJ mol⁻¹



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

Polarizzabilità e Regole di Fajans

(per predire se un legame sarà ionico o covalente)

1. cationi piccoli e a carica elevata (e.g. Li^+ , Mg^{2+}) hanno forte **potere polarizzante**
2. anioni larghi e con carica elevata sono **facilmente polarizzabili** (e.g. I^- , Se^{2-} , Te^{2-} , As^{3-} , P^{3-})
3. cationi che non hanno una configurazione elettronica di gas nobile (e.g. quasi tutti quelli dei metalli di transizione) sono più polarizzanti di quelli con guscio chiuso (e.g. cationi dei metalli alcalini o alcalino-terrosi) perché avranno una maggiore Z_{eff} , cioè una carica più alta sulla loro superficie (*cfr* Hg^{2+} e Ca^{2+} , 116 pm).

Fajans at the Bunsen Congress, Munich, 1928



Friedrich Hund

X

X

X

X

X

X X

Oskar von Miller

X

X

X

X

X

X

Walther Kossel

X

Kasimir Fajans

Alwin Mittasch

Franz Eugen Simon

X

Frl. Vohsen

X

X

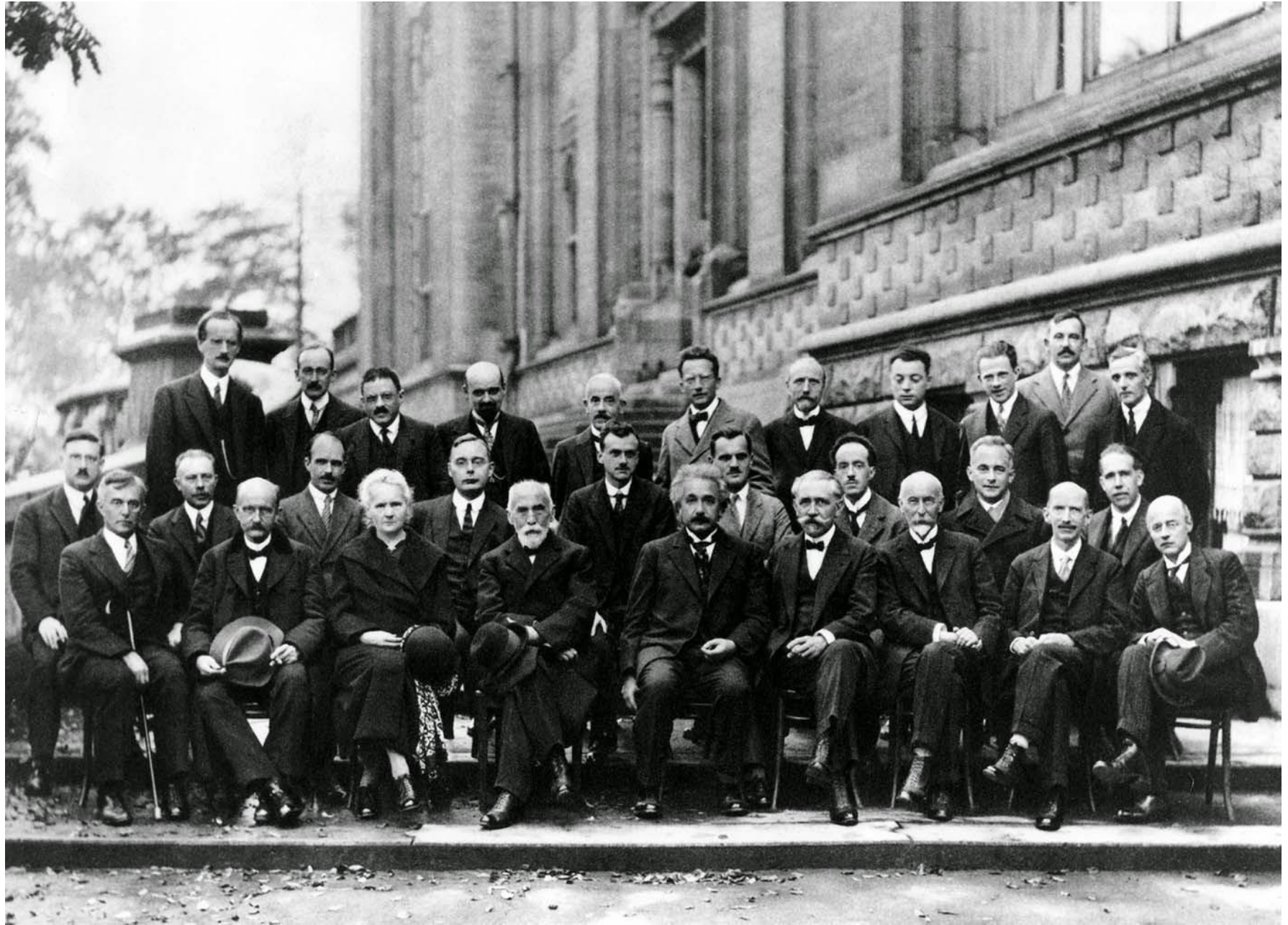
X

Peter Debye

X

Fritz London

The Solvay Conference, 1927



A. PICCARD E. HENRIOT P. EHRENFEST Ed. HERZEN Th. DE DONDER E. SCHRÖDINGER E. VERSCHAFFELT W. PAULI W. HEISENBERG R.H. FOWLER L. BRILLOUIN
 P. DEBYE M. KNUDSEN W.L. BRAGG H.A. KRAMERS P.A.M. DIRAC A.H. COMPTON L. de BROGLIE M. BORN N. BOHR
 I. LANGMUIR M. PLANCK Mme CURIE H.A. LORENTZ A. EINSTEIN P. LANGEVIN Ch.E. GUYE C.T.R. WILSON O.W. RICHARDSON

Absents : Sir W.H. BRAGG, H. DESLANDRES et E. VAN AUBEL

