Describe e^- with 4 quantum numbers

each electron in atom needs a unique set of QN

Pauli exclusion principle { "orbitals" only use first 3 QN; so each orbitals can "accomodate" 2 e^- → one with $m_s = +\frac{1}{2}$ other $m_s = -\frac{1}{2}$

He atom has 2 e^-

n	ℓ	m_ℓ	m_s
1	0	0	$+\frac{1}{2}$
1	0	0	$-\frac{1}{2}$

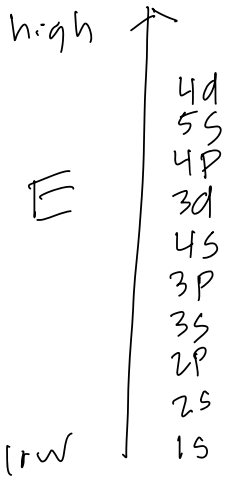
How do we decide how electrons are distributed among the possible orbitals? → Energy

* lower energy is "preferable"

n, ℓ are related to energy → smaller values = lower energy

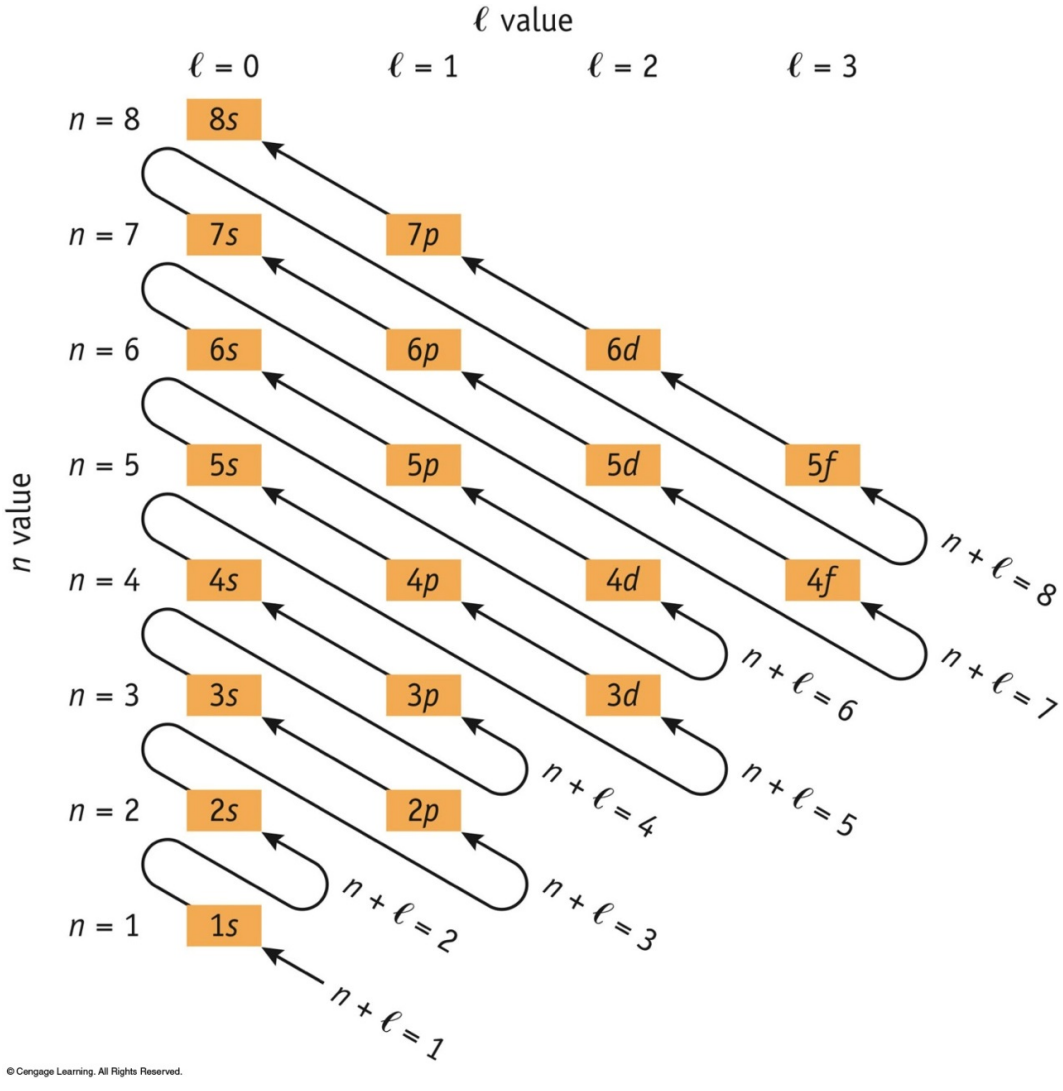
(n+ℓ) is a good measure of relative energy

orbital	n	ℓ	n+ℓ	
1s	1	0	~~1~~	tiebreaker is n
2s	2	0	~~2~~	
2p	2	1	~~3~~	2p lower in energy
3s	3	0	~~3~~	than 3s
3p	3	1	~~4~~	
3d	3	2	~~5~~	lower
4s	4	0	~~4~~	
4p	4	1	~~5~~	middle
4d	4	2	6	
4f	4	3	7	
5s	5	0	~~5~~	higher

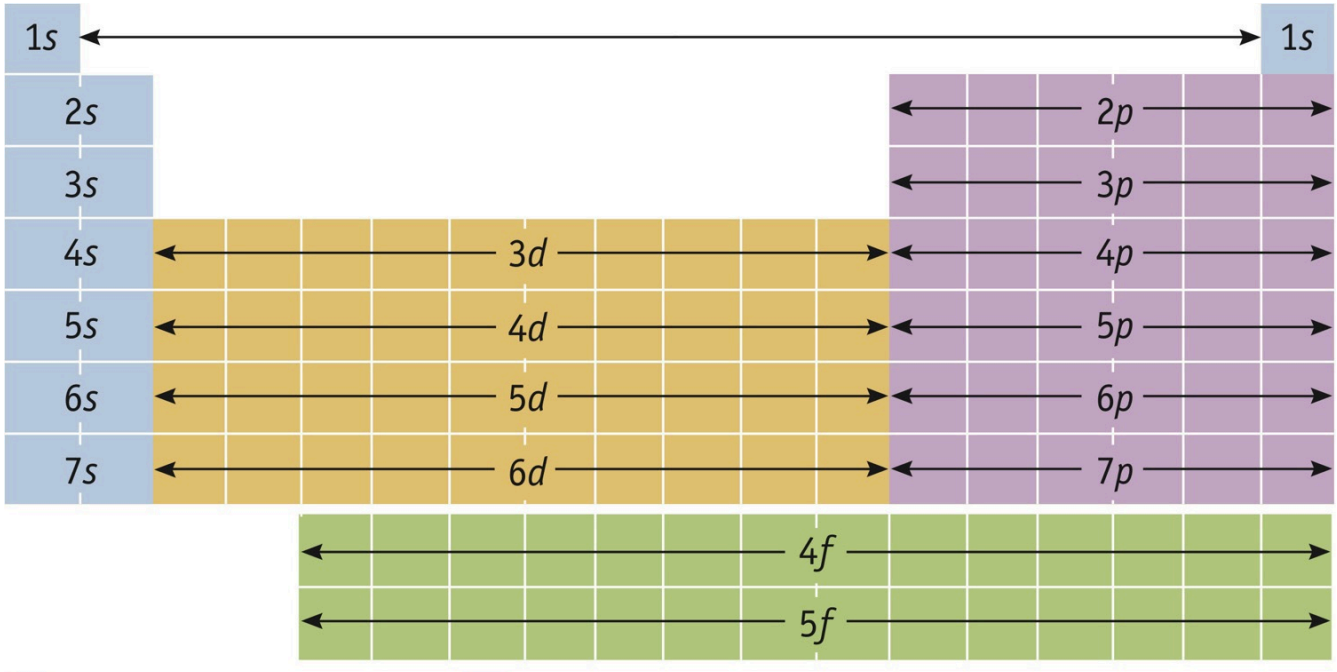


"aufbau principle"
using energy to describe order

Subshell Filling Order

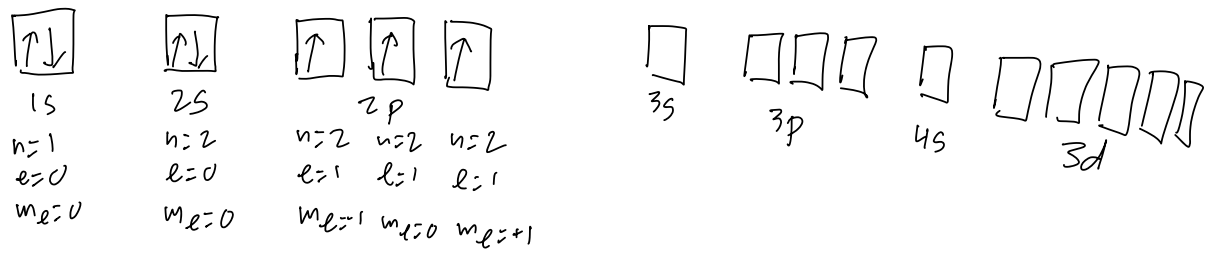


Orbital Filling of Electrons



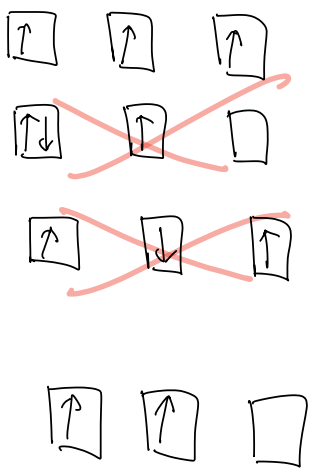
How to represent electron configurations

- write out quantum numbers
- Box diagram



For $N - 7e^- \rightarrow 1s^2 2s^2 2p^3$

* Hund's rule = maximize $\sum m_s$ as long as not having electrons in higher energy orbital



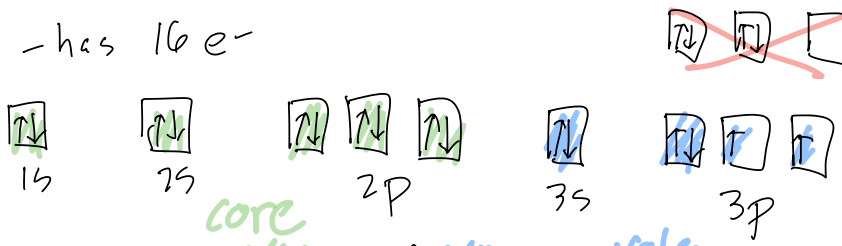
Interaction between positively charged nucleus and negatively charged electrons is what determines energy of orbital

stronger + − interaction = lower energy situation

e^- closer to nucleus have stronger interactions
hence orbitals describing regions of space closer to nucleus will be lower in energy

e⁻s farther from nucleus are "screened" by e⁻s closer to nucleus and feel is a smaller "effective nuclear charge"

S - has 16 e⁻



core

valence

$1s^2 2s^2 2p^6 3s^2 3p^4$

$[Ne]\ 3s^2 3p^4$

$1s^2 2s^2 2p^6$

valence e⁻ → highest n

core e⁻ → all others

Mg: $1s^2 2s^2 2p^6 (3s^2)$ ← valence

K: $1s^2 2s^2 2p^6 3s^2 3p^6 (4s^1)$

Na: $1s^2 2s^2 2p^6 (3s^1)$

Table 7.4 Orbital Box Diagrams for the Elements Ca Through Zn

		3*d*	4*s*
Ca	[Ar]$4s^2$	☐ ☐ ☐ ☐ ☐	↑↓
Sc	[Ar]$3d^1 4s^2$	↑ ☐ ☐ ☐ ☐	↑↓
Ti	[Ar]$3d^2 4s^2$	↑ ↑ ☐ ☐ ☐	↑↓
V	[Ar]$3d^3 4s^2$	↑ ↑ ↑ ☐ ☐	↑↓
Cr*	[Ar]$3d^5 4s^1$	↑ ↑ ↑ ↑ ↑	↑
Mn	[Ar]$3d^5 4s^2$	↑ ↑ ↑ ↑ ↑	↑↓
Fe	[Ar]$3d^6 4s^2$	↑↓ ↑ ↑ ↑ ↑	↑↓
Co	[Ar]$3d^7 4s^2$	↑↓ ↑↓ ↑ ↑ ↑	↑↓
Ni	[Ar]$3d^8 4s^2$	↑↓ ↑↓ ↑↓ ↑ ↑	↑↓
Cu*	[Ar]$3d^{10} 4s^1$	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑
Zn	[Ar]$3d^{10} 4s^2$	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓

why not $3d^4 4s^2$

half full d orbital is special and low energy

*See *A Closer Look: Questions about Transition Element Electron Configurations*, page 263.

Electron configs for ions

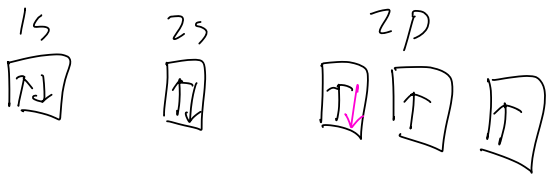
Cl^- has one more e^- than Cl atom

Mg^{2+} has two less e^- than Mg atom

N vs N^{-1}

$\downarrow$ $\downarrow$

7e 8e



$1s^2 2s^2 2p^3$ $1s^2 2s^2 2p^4$

N^{+1} has 6e $1s^2 2s^2 2p^2$

Transition metal ion - always cations

- always lose s before d

Fe: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$ or $3d^6 4s^2$ - lose these first

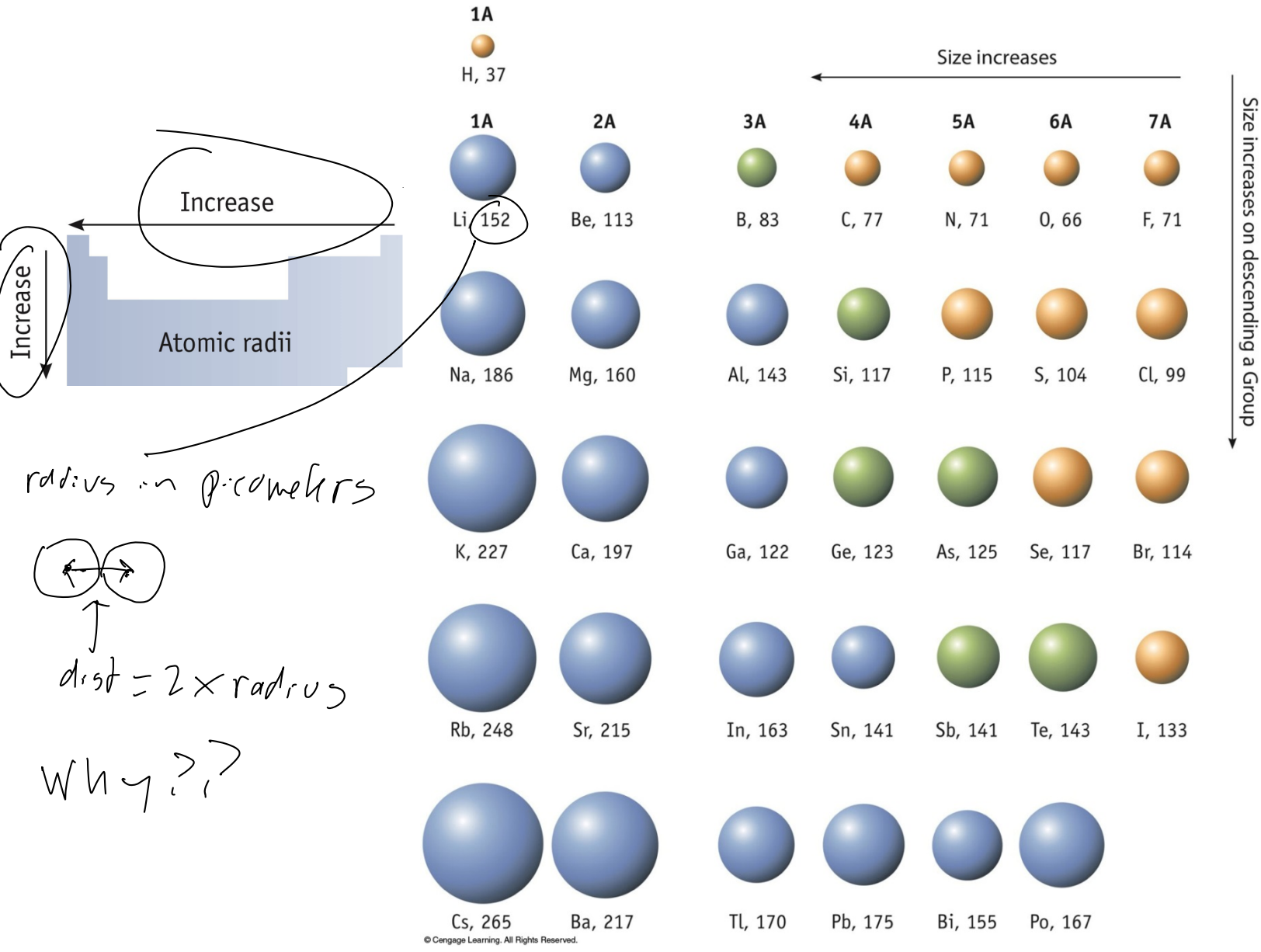
Fe^{2+}: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$

Fe^{3+}: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$

Atom properties depend on electron configs (periodic table placement)

Atom size (atomic radius)

Atomic Radii of Elements



radius in picometers

dist = 2 × radius

Why??

Why does size increase going down a column?

- more electrons as we go down
- more electrons at greater distance from nucleus

Why does size decrease L→R across a row?

- all atoms in a row have same n value for valence e^- → all about same distance from nucleus
- L→R charge of nucleus is increasing so electrons pulled closer to nucleus and atom is smaller

Cations are smaller neutral - same nuc. charge fewer e-

Anions larger than neutral - same nuc. charge more e-

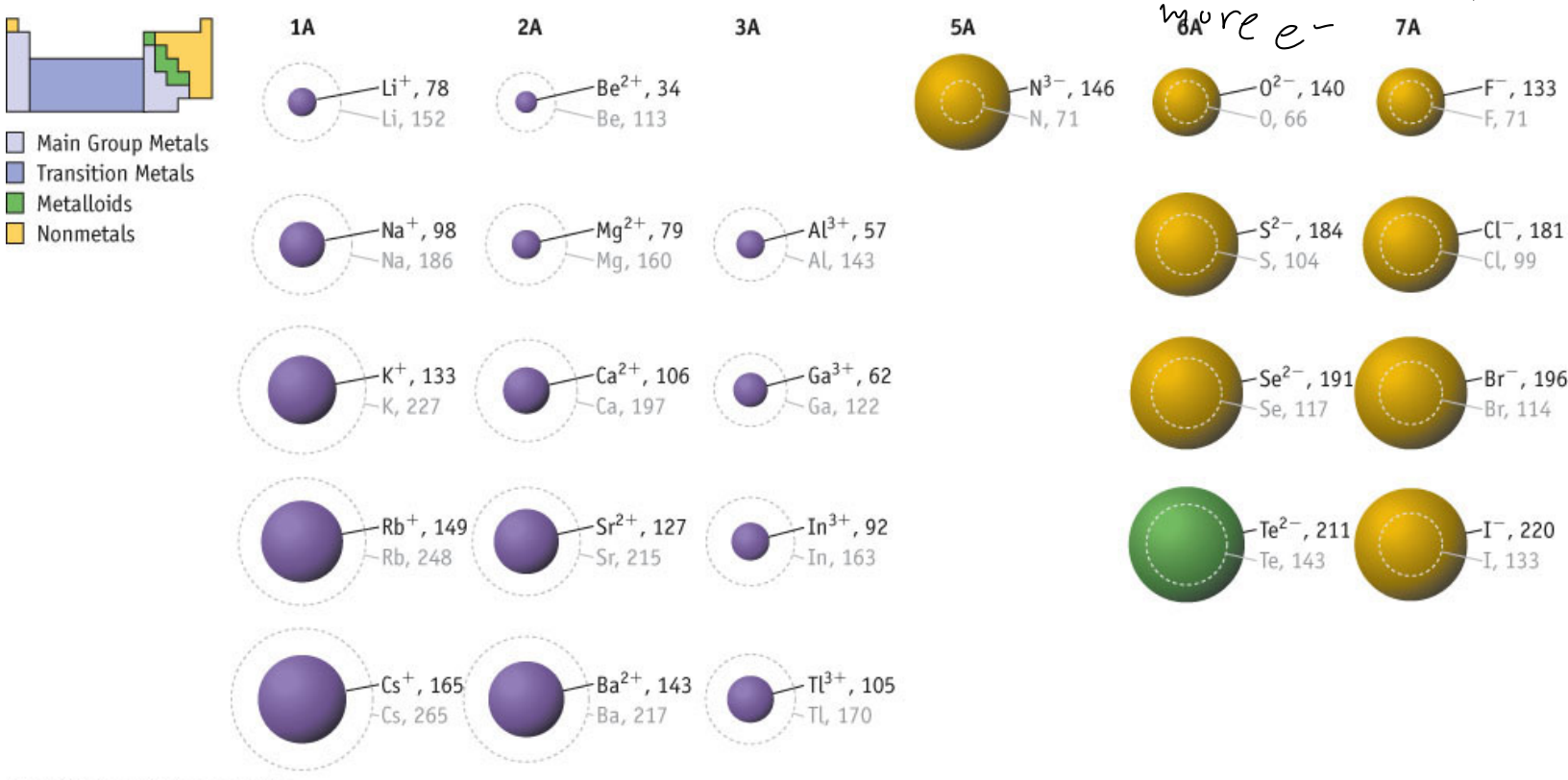


Fig. 7-12, p. 326

In general highly charged anions bigger than lower charged

highly charged cations smaller than lower charge

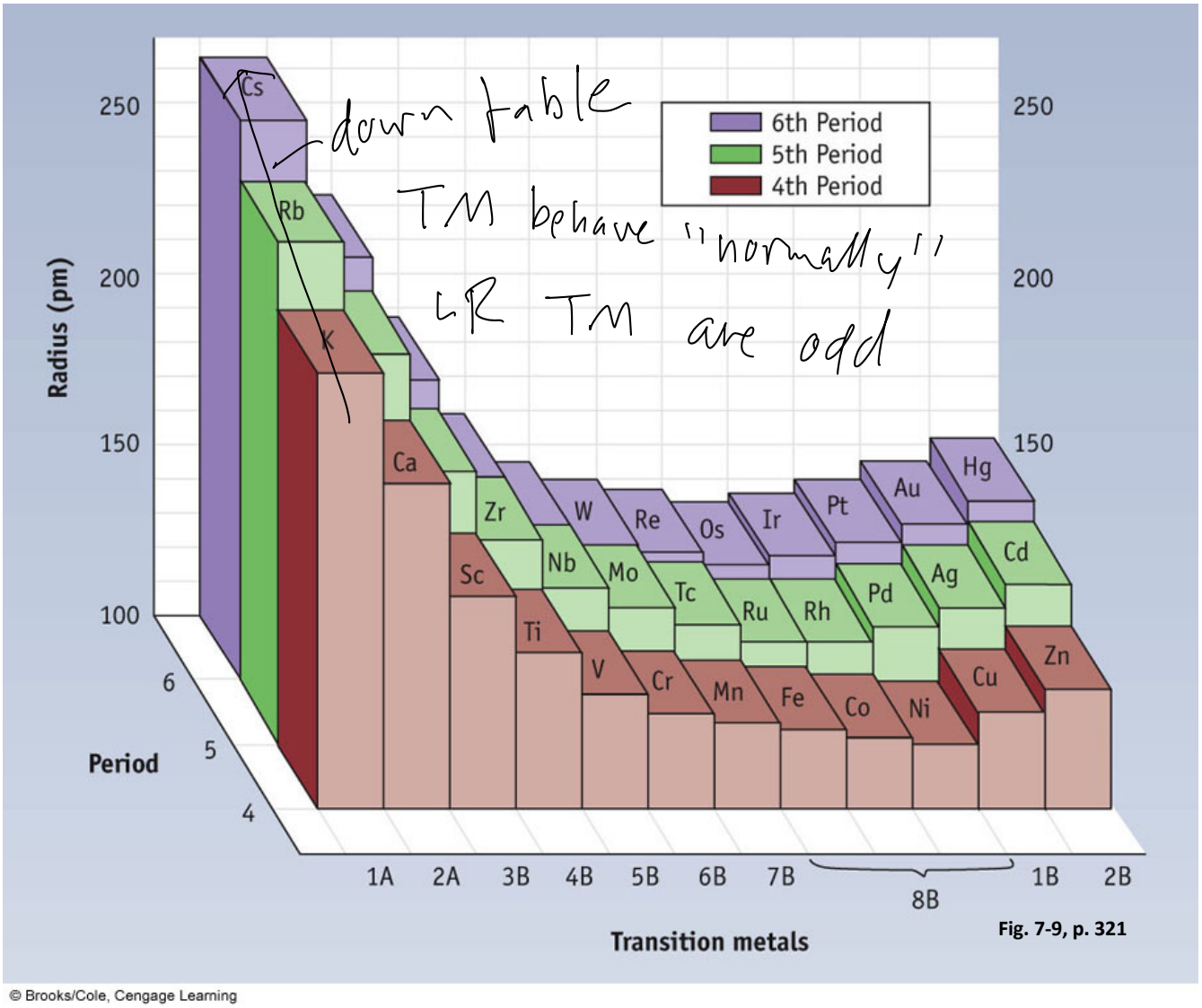


Fig. 7-9, p. 321

competition btw incr nuclear charge and increasing e-e repulsion

Ionization energy - amt of energy required to remove e⁻ from atom

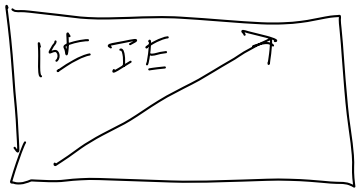


TABLE 7.5 First, Second, and Third Ionization Energies for the Main Group Elements in Periods 2–4 (kJ/mol)

2nd Period	Li	Be	B	C	N	O	F	Ne
1st	513	899	801	1086	1402	1314	1681	2080
2nd	7298	1757	2427	2352	2856	3388	3374	3952
3rd	11815	14848	3660	4620	4578	5300	6050	6122
3rd Period	**Na**	**Mg**	**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
1st	496	738	577	787	1012	1000	1251	1520
2nd	4562	1451	1817	1577	1903	2251	2297	2665
3rd	6912	7732	2745	3231	2912	3361	3826	3928
4th Period	**K**	**Ca**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
1st	419	590	579	762	947	941	1140	1351
2nd	3051	1145	1979	1537	1798	2044	2104	2350
3rd	4411	4910	2963	3302	2735	2974	3500	3565

Be: $1s^2 2s^2$ remove e⁻ from 2s (lower energy) (harder to do)

B: $1s^2 2s^2 2p^1$ remove e⁻ from 2p (easier to do) (higher energy)

Table 7-5, p. 322

Li vs Be 2nd ionization

Li: $1s^2 2s^1$ — 2nd e⁻ removed is core

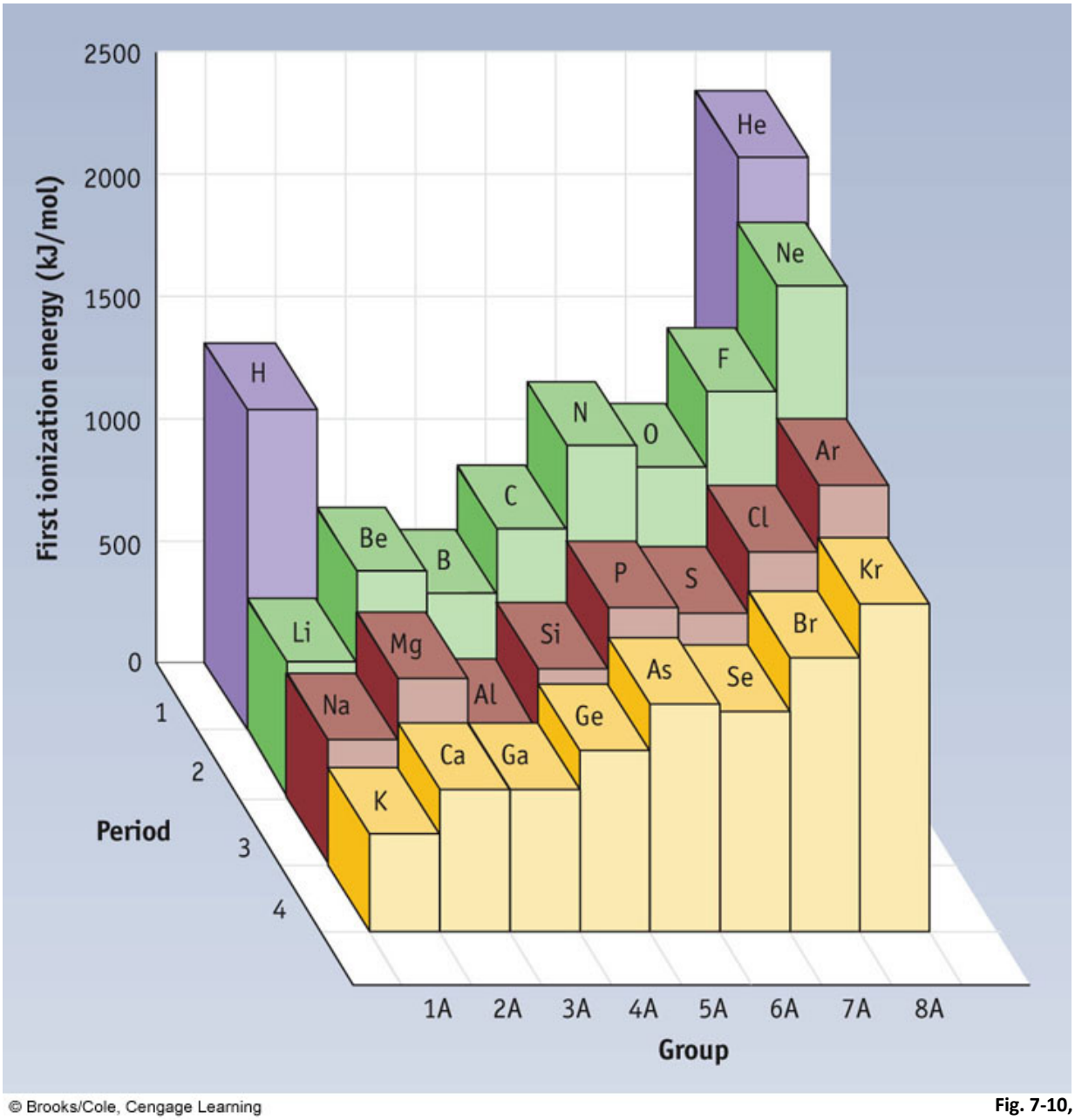
Be: $1s^2 2s^2$ — 2nd e⁻ removed is still valence

N vs O 1st ionization

N: $1s^2 2s^2 2p^3$ ↑ ↑ ↑

O: $1s^2 2s^2 2p^4$ ↑↓ ↑ ↑

e-e⁻ repulsion makes this easier to remove



Top → bott
IE decrease
b/c e⁻
are further
away + less
strongly
held

Fig. 7-10, p. 323

Electron affinity – energy when e⁻ is added to neutral atom – always exothermic

Roughly increases L → R

Roughly decreases top → bottom

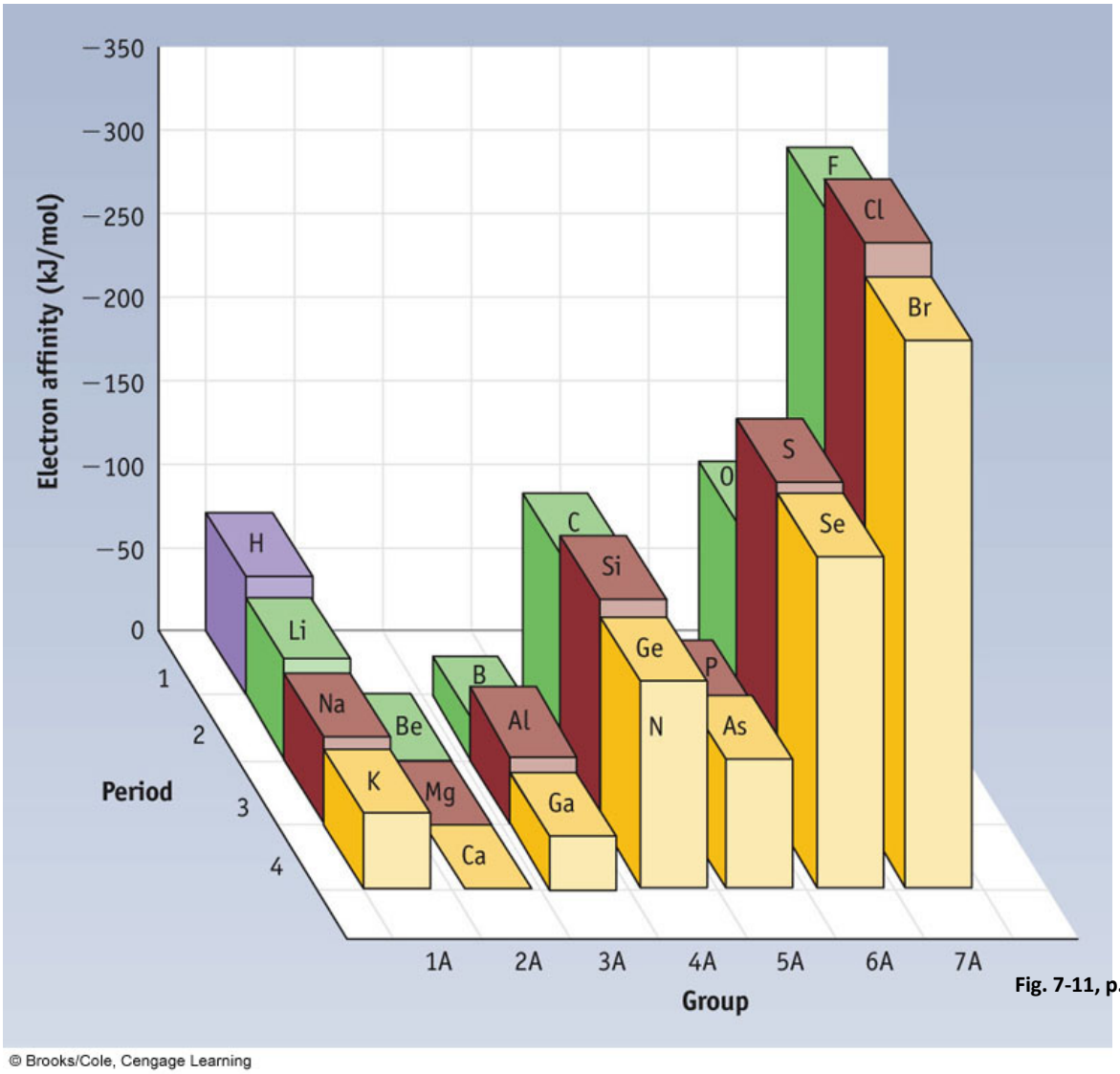


Fig. 7-11, p. 324

Atoms on right more likely to want to be anions – gets closer to noble gas config

Atoms on bottom less likely to want to be anions – added e⁻ is farther from nucleus and doesn't have a bit benefit

Atoms on left get to noble gas config by losing e^-

Atoms on right get to noble gas config by gaining electrons

Atoms in middle share = covalent bond