Describe electrons with 4 quantum #s

n
ℓ
m_ℓ
m_s

each electron in an atom needs a unique set of 4 quantum numbers

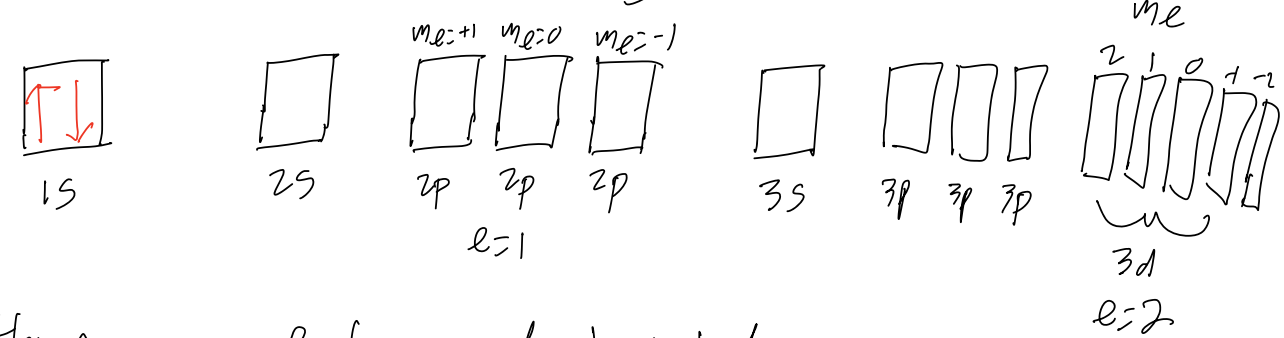
so each orbital (defined by n, ℓ, m_ℓ) can "accomodate" 2 e⁻ ($+\frac{1}{2}; -\frac{1}{2}$)

Pauli exclusion principle – up to 2 e⁻ in an orbital as long as one is spin up ($m_s = +\frac{1}{2}$) and other is spin down ($m_s = -\frac{1}{2}$)

He atom – has 2 e⁻

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

} describe w/ quantum #s



How are electrons distributed amongst the possible orbitals – e⁻ want to be at lower energy

n tells us about energy – smaller n = lower energy

ℓ tells us a bit about energy smaller ℓ = lower energy

n+l gives us good energy ranking (n will be tiebreaker)

orbital	n	l	n+l
1s	1	0	1
2s	2	0	2
2p	2	1	3
3s	3	0	3
3p	3	1	4
3d	3	2	5
4s	4	0	4
4p	4	1	5
4d	4	2	6
4f	4	3	7
5s	5	0	5

n is tiebreaker

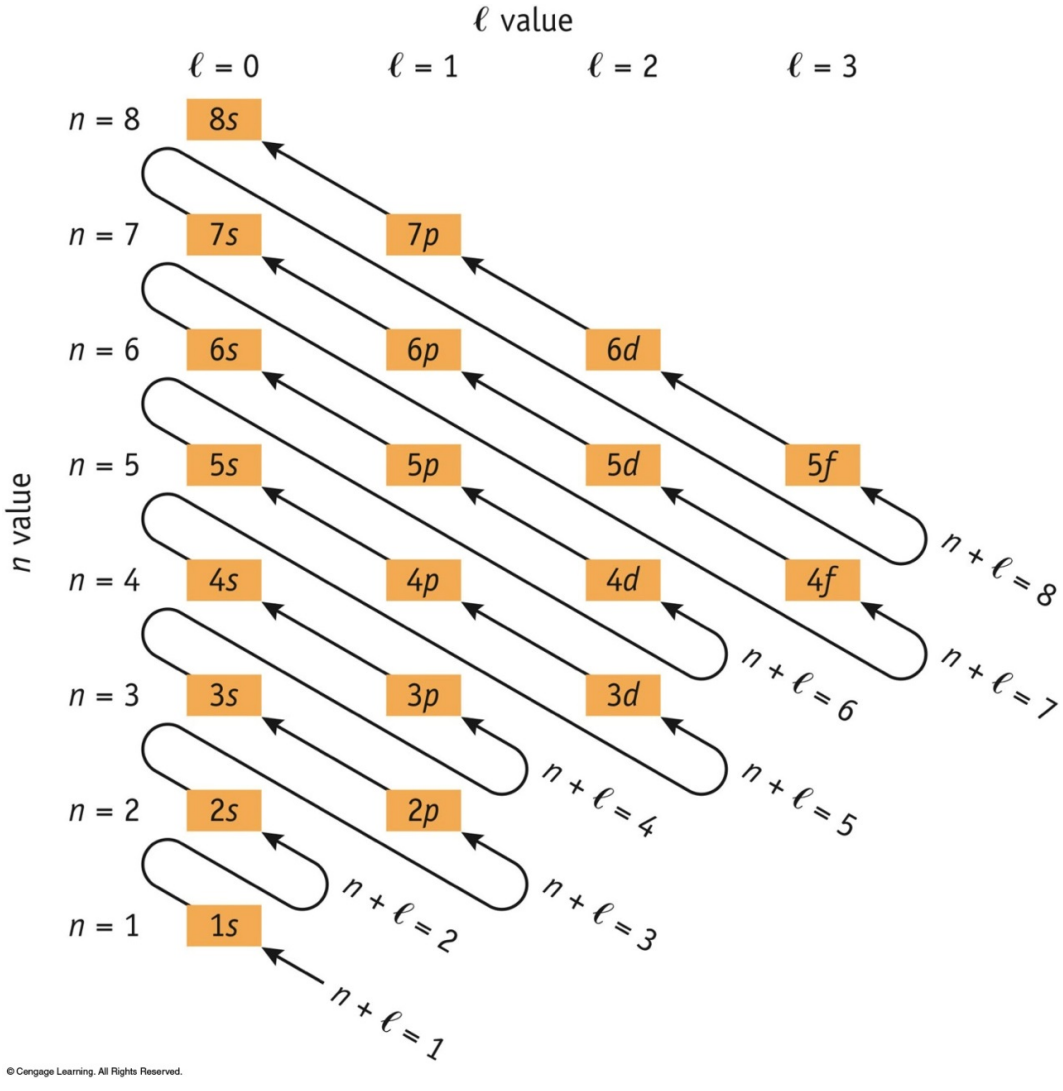
1s
2s
2p
3s
3p
4s
3d
4p
~~4d~~
5s

lowest E

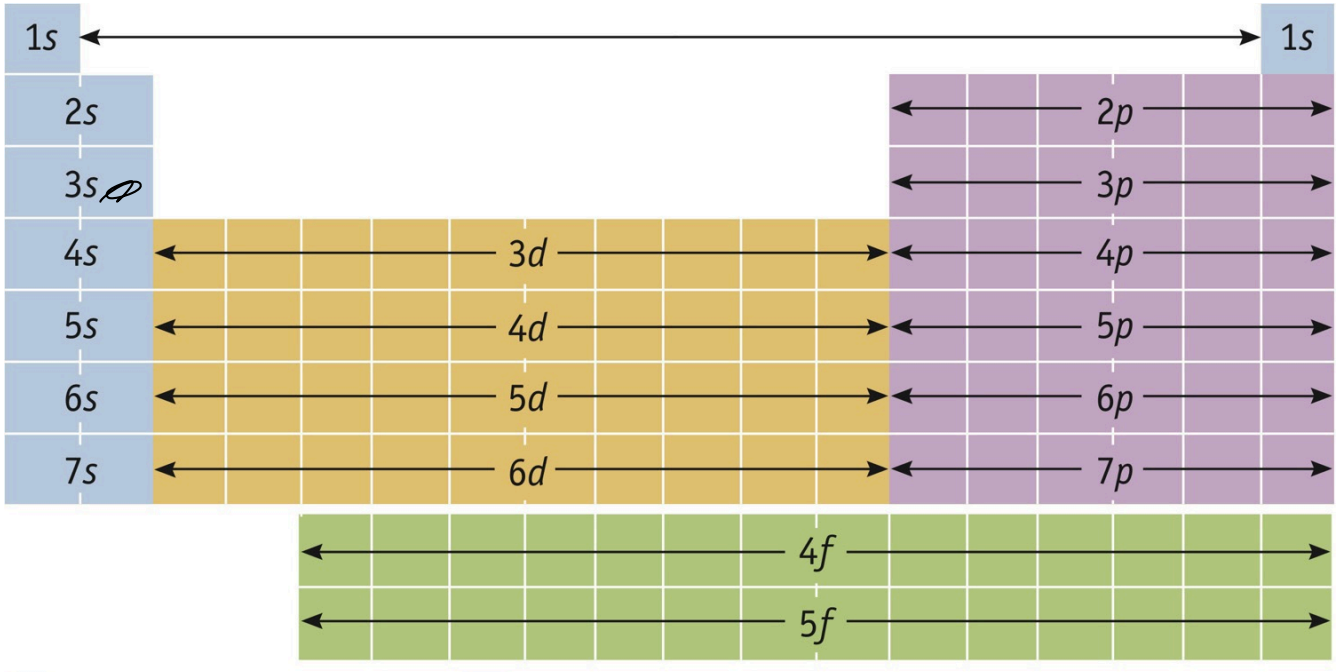
highest E

"aufbau principle"

Subshell Filling Order



Orbital Filling of Electrons



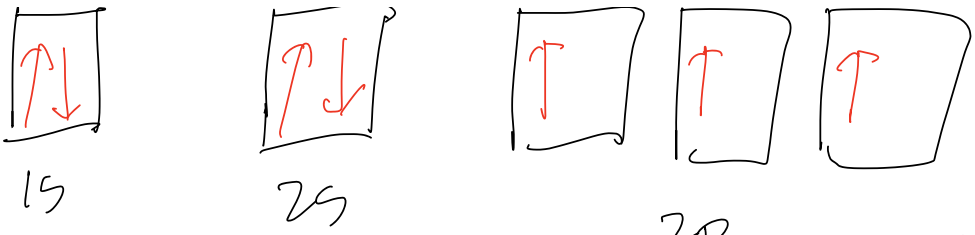
Effective nuclear charge helps explain energies of orbitals

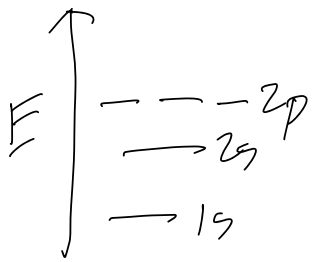
electron interacting w/ nucleus is "good"
stronger interaction = lower energy

- electrons closer to nucleus will have stronger interaction → lower energy
- electrons farther from nucleus are "screened" by electrons closer to nucleus and feel less of positive charge of nucleus
- effective nuclear charge is what charge on nucleus "looks like" to an e^- far away + screened

electrons in 2p experience smaller effective nuclear charge than 2s electrons
so less attraction to nucleus → 2p is higher energy than 2s

N atom - 7e⁻





When given a choice, e⁻ prefer to have own room to minimize e⁻-e⁻ repulsion
"Hund's Rule"
* better to have more unpaired spins

shorthand electron config for N atom
$1s^2 2s^2 2p^3$
$[He]\ 2s^2 2p^3$
↑ electron config of He atom

S atom – 16 e⁻
$1s^2 2s^2 2p^6 3s^2 3p^4$
$[Ne]\ 3s^2 3p^4$

core
N: $1s^2 2s^2 2p^3$ ← valence
S: $1s^2 2s^2 2p^6 3s^2 3p^4$

valence e⁻ – in highest n level
core e⁻ – all the non-valence e⁻
* Chemistry happens b/c of valence –

Mg: $1s^2 2s^2 2p^6 3s^2$ ← valence e⁻

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

similar valence e⁻ config → similar properties

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 $3d^4 4s^2$

2 half full

Why not $3d^9 4s^2$

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

Electron configurations for ions

anion - add more e-

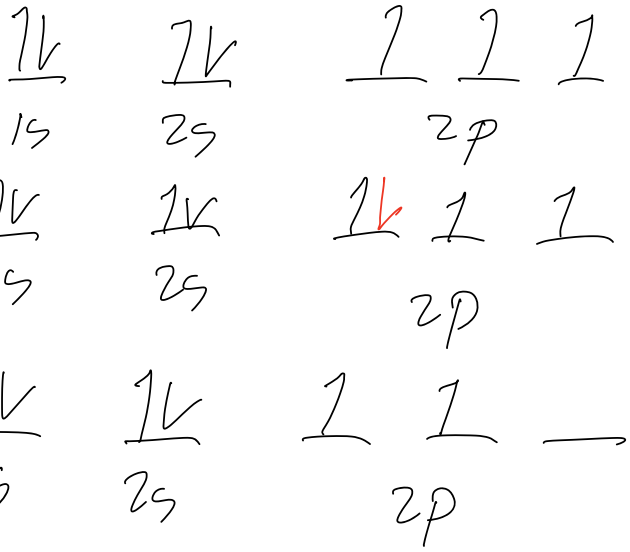
cation - remove e-

N vs N^{-1}

N: $1s^2 2s^2 2p^3$

N^{-1}: $1s^2 2s^2 2p^4$

N^{+1}: $1s^2 2s^2 2p^2$



Transition metal ions - always cations

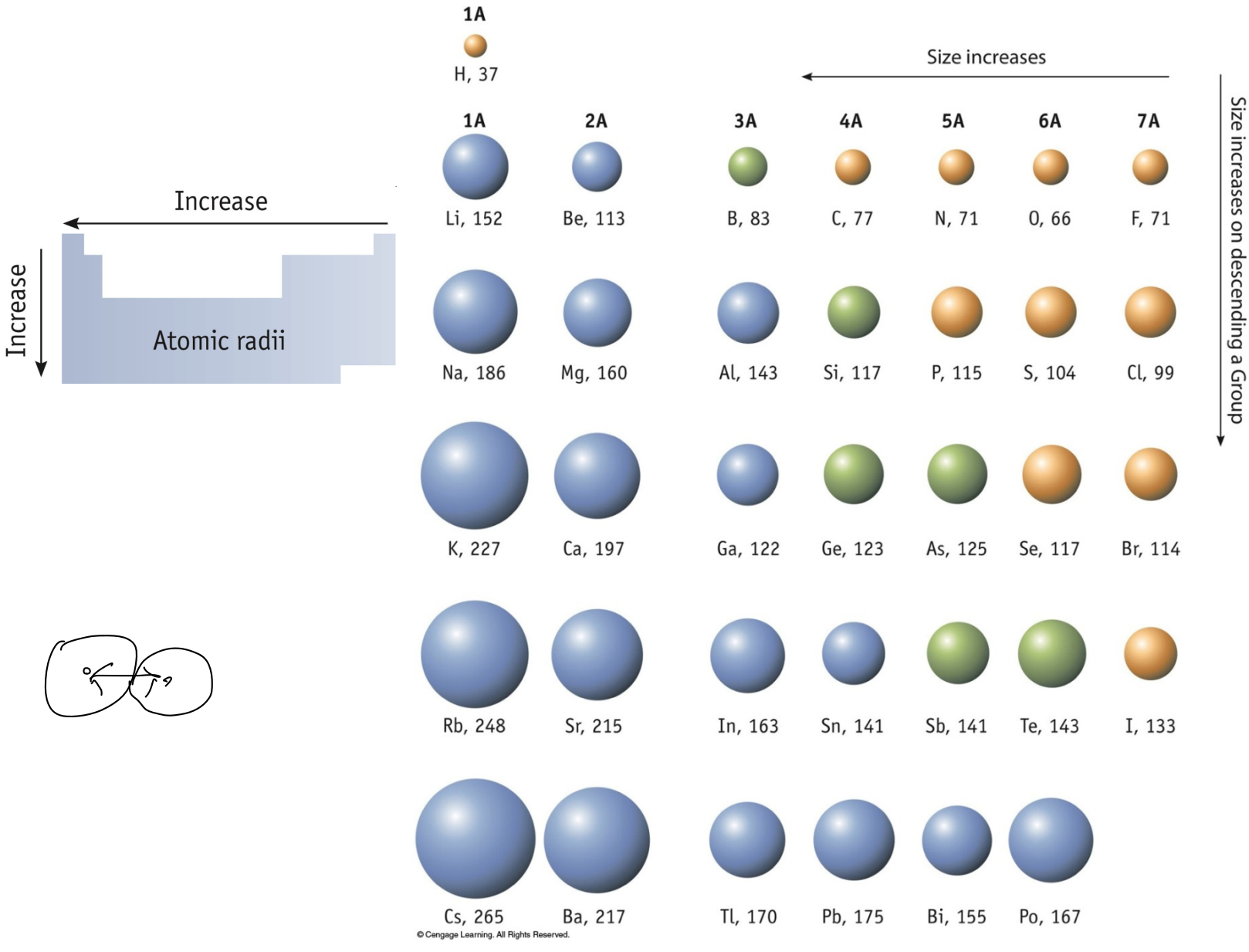
remove 4s electrons before 3d electrons

Fe: $1s^2 2s^2 2p^6 3s^2 3p^6 \cancel{4s^2} 3d^6$ $[Ar]\, 4s^2 3d^6$

Fe^{2+}: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$ $[Ar]\, 3d^6$

Fe^{3+}: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$ $[Ar]\, 3d^5$

Atomic Radii of Elements



why does size increase going down a column - more electrons and they are farther from nucleus

why does size decrease L → R across row - all electrons in a row are same n so all are about same distance from nucleus

- charge on ~~outer~~ nucleus is increasing
- so electrons get pulled in closer

Ion sizes

Ion smaller than neutral for cation

Ion bigger than neutral for anion

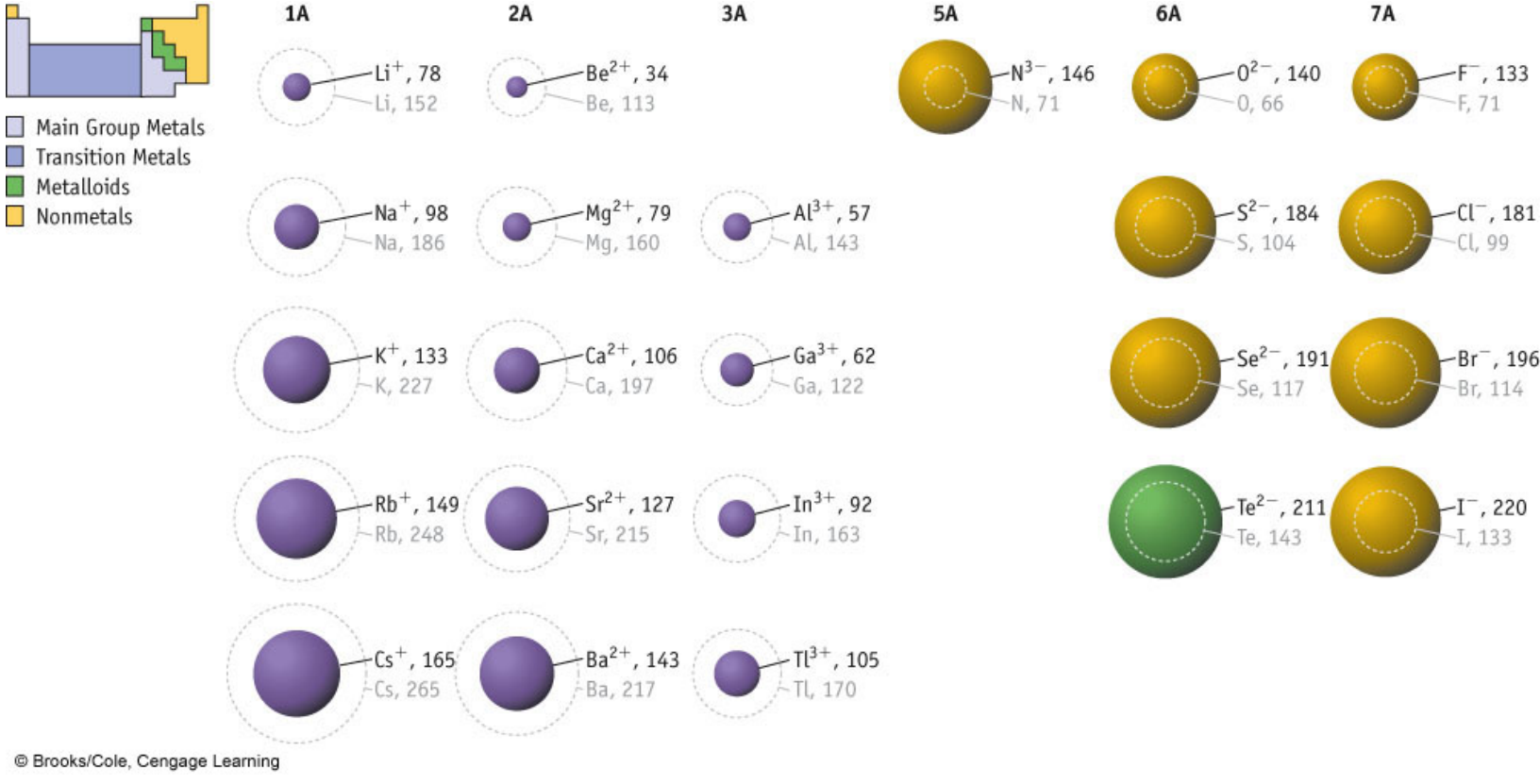


Fig. 7-12, p. 326

cation – same nucleus but fewer e⁻
pulls them closer

anion – same nucleus, more e⁻
can't hold them as tightly

cations – larger charge → smaller ion

Competition btw increasing nuclear charge and increasing e-e repulsion

getting bigger L→R

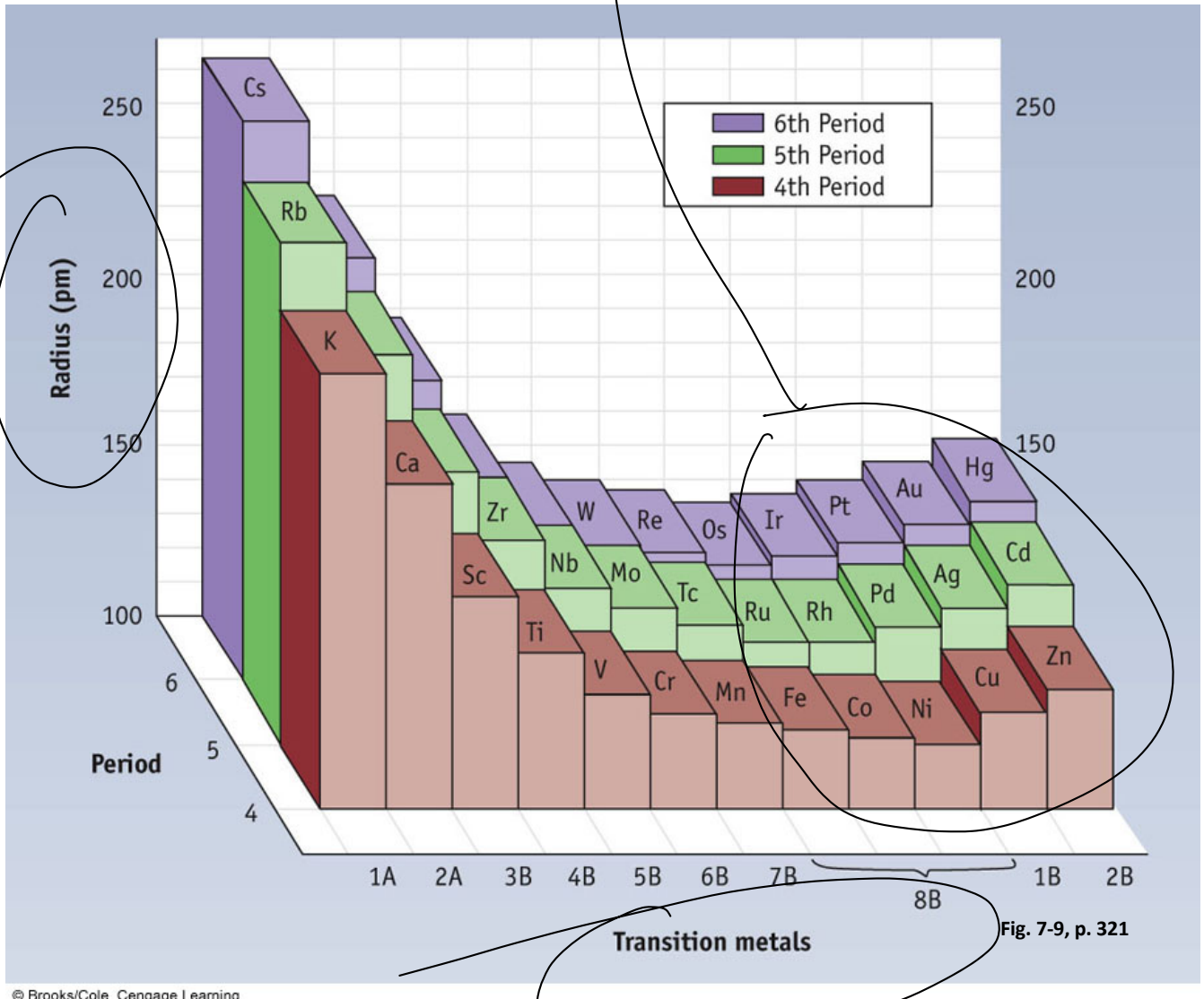


Fig. 7-9, p. 321

Ionization energy – amt of energy needed to remove e⁻ from atom

1st IE [increases]

→ to remove 1 more e⁻

→ to remove 1 more e⁻

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

easier to remove 4s than 3s etc b/c farther from nucleus – less strongly held

Table 7-5, p. 322

L→R, electrons held more tightly b/c increasing nuclear charge

1st → 2nd → 3rd IE increases due to nucleus holding remaining e⁻ more strongly

compare O vs N 1st IE

O: $1s^2 2s^2 2p^4$ ↑↓ ↑ ↑ ↑↓

N: $1s^2 2s^2 2p^3$ ↑↓ ↑ ↑ ↑ ↑

easier to remove this e⁻ than a N p e⁻ b/c of e⁻-e⁻ repulsion

Li 1st IE → 2nd IE

factor ~ 14

Be 1st IE → 2nd IE

factor ~ 2

Li: $1s^2 2s^1$ ~~↑↓~~ ~~↑~~

Be: $1s^2 2s^2$ ↑↓ ~~↑↓~~

2nd electron removed from Li is 1s e⁻

2nd electron removed from Be is 2s e⁻

core e⁻

valence e⁻

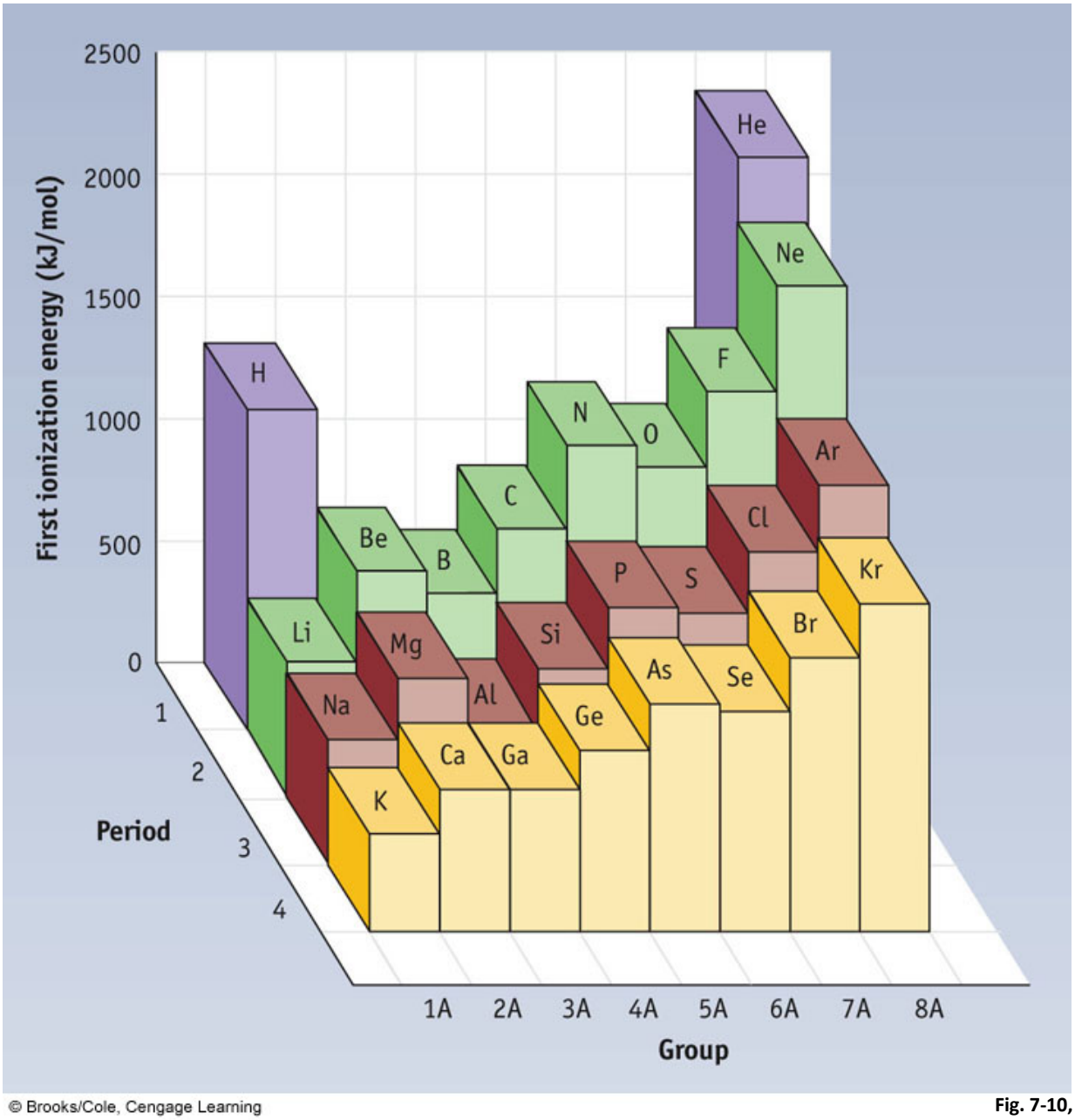


Fig. 7-10, p. 323

Electron affinity - energy when e- added to neutral atom. Always exothermic

Increases L → R things on right more likely to become anions

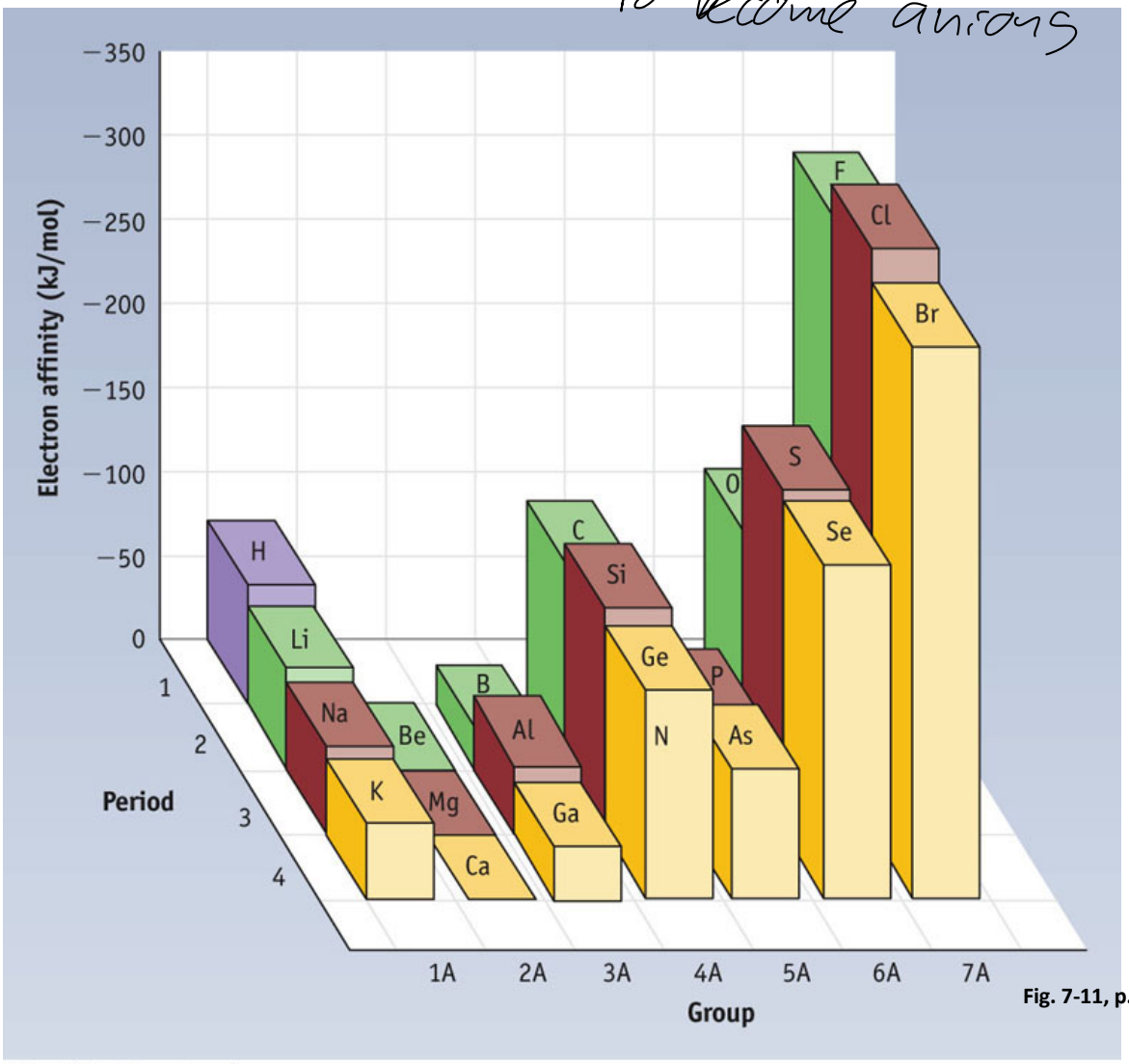


Fig. 7-11, p. 324

In general lower on per. table means smaller EA

larger atom - when it adds e-, frate- will be farther from nucleus and EA will be smaller

Atoms on left side of periodic table get lower energy by losing electrons

Atoms on right get to lower energy by gaining electrons

* trying to get to "noble gas" configuration entirely full/empty n-level

Atoms on middle of table - share electrons to get to noble gas config

smaller

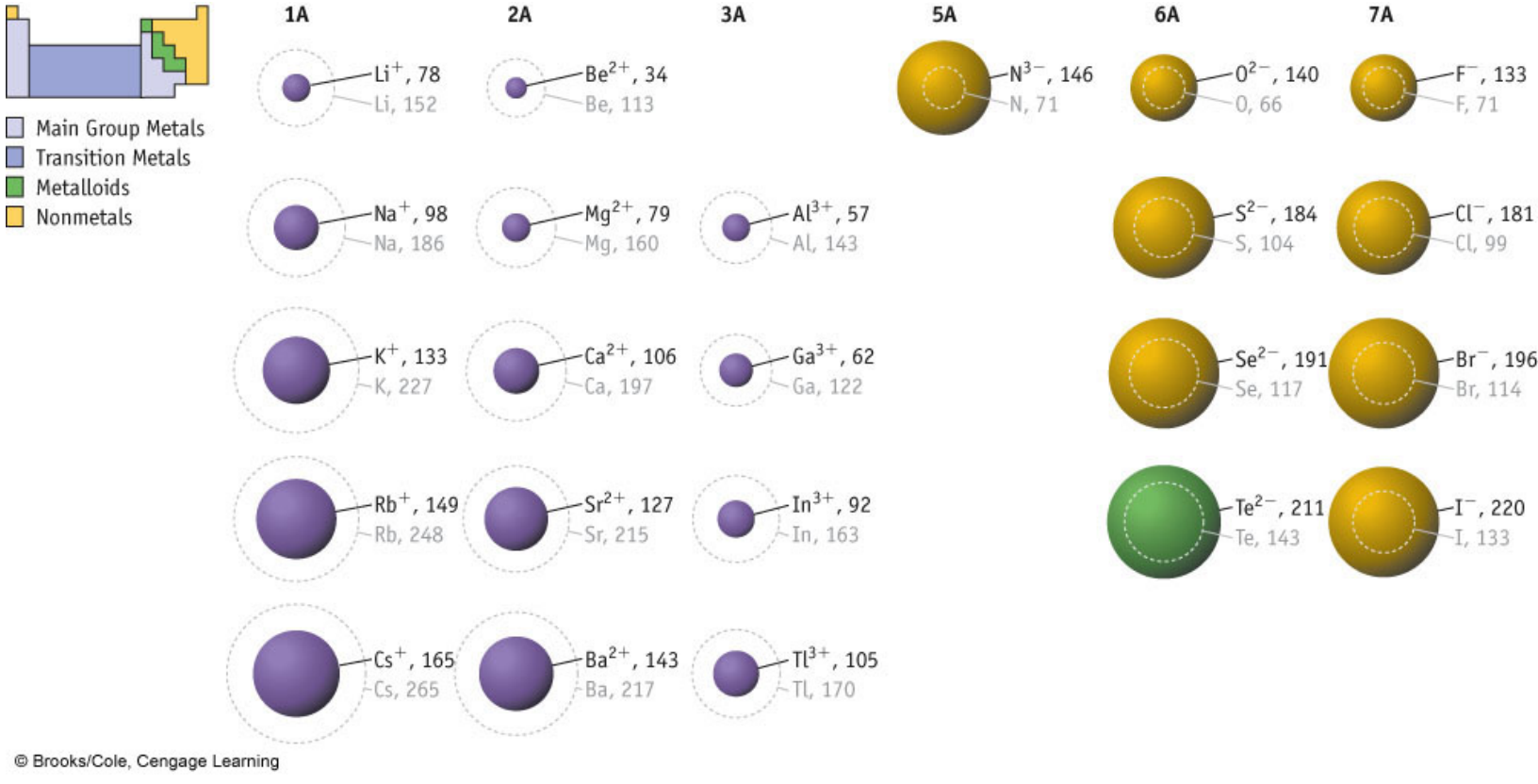


Fig. 7-12, p. 326