

Chapter 7

Periodic Properties of the Elements

- In **periodic table**, elements in the same column contain the same number of electron in their **valence orbitals**, which are the occupied orbitals that hold the electrons involved in bonding.

N $1s^2 \textcolor{red}{2s^2 2p^3}$

P $1s^2 2s^2 2p^6 \textcolor{red}{3s^2 3p^3}$

As $1s^2 2s^2 2p^6 3s^2 3p^3 3d^{10} \textcolor{red}{4s^2 4p^3}$

Ga $1s^2 2s^2 2p^6 3s^2 3p^3 3d^{10} \textcolor{red}{4s^2 4p^1}$



N₂ gas



P



As

- Electron configurations can be used to explain differences as well as similarities in the properties of elements.

➤ The periodic table

- An arrangement of the chemical elements, organized on the basis of their **atomic number, electron configurations and recurring(重复) chemical properties.**
- Elements are presented in order of increasing atomic number.
- The standard form of the table consists of a grid of elements, with rows called periods(周期) and columns called groups(族).

<http://www.rsc.org/periodic-table>

<http://www.rsc.org/periodic-table>

Periodic Table

ROYAL SOCIETY OF CHEMISTRY

Home History Alchemy Podcast Video Trends

Visual Elements images Temperature 0 K - + 6000 K Classification Metal Non-metal Clear filters

Groups 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 Blocks s p d f Periods 1 2 3 4 5 6 7 Lanthanides Actinides

G+1

Newsletter Feedback

Periodic Table

The Royal Society of Chemistry's interactive periodic table features history, alchemy, podcasts, videos, and data trends across the periodic table. Click the tabs at the top to explore each section. Use the buttons above to change your view of the periodic table and view Murray Robertson's stunning Visual Elements artwork. Click each element to read detailed information.

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

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Periodic Table

Visual Elements images

Temperature 0 K



6000 K

Classification

Metal

Non-metal

Clear filters

Groups 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

Blocks s p d f

Periods 1 2 3 4 5 6 7 Lanthanides Actinides

| H 1 | Copper | | | | | | | | | | | | Supply risk | He 2 |
|----------|----------|---|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-------------|---|
| Li 3 | Be 4 |  <div>Key isotopes</div> <div>⁶³Cu</div> <div>Electron configuration</div> <div>[Ar] 3d¹⁰ 4s¹</div> <div>Density (g cm⁻³)</div> <div>8.96</div> <div>1st ionisation energy</div> <div>745.482 kJ mol⁻¹</div> | | | | | | | | | | | | ■ High supply risk ■ Medium supply risk ■ Low supply risk ■ Unknown |
| Na 11 | Mg 12 | <div>Cu</div> <div>Copper</div> <div>29</div> <div>63.546</div> | | | | | | | | | | | | B 5 |
| 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 | N 7 |
| 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 | O 8 |
| Cs 55 | Ba 56 | La 57 | Hf 72 | Ta 73 | W 74 | Re 75 | Os 76 | Ir 77 | Pt 78 | Au 79 | Hg 80 | Tl 81 | Pb 82 | F 9 |
| Fr 87 | Ra 88 | Ac 89 | Rf 104 | Db 105 | Sg 106 | Bh 107 | Hs 108 | Mt 109 | Ds 110 | Rg 111 | Cn 112 | Nh 113 | Fl 114 | Ne 10 |
| 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 | |
| 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 | |

Newsletter

Feedback

[Move to Neon](#)[Move to Magnesium](#) >

Sodium



| | |
|--------------------|---|
| Discovery date | 1807 |
| Discovered by | Humphry Davy |
| Origin of the name | The name is derived from the English word 'soda'. |
| Allotropes | |

Na

Sodium

11

22.990

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Fact box

| | | | |
|--------------------------|-------------------------|--|--------------------------------------|
| ■ Group | 1 | ■ Melting point | 97.794°C, 208.029°F, 370.944 K |
| ■ Period | 3 | ■ Boiling point | 882.940°C, 1621.292°F, 1156.090 K |
| ■ Block | s | ■ Density (g cm ⁻³) | 0.97 |
| ■ Atomic number | 11 | ■ Relative atomic mass | 22.990 |
| ■ State at 20°C | Solid | ■ Key isotopes | ²³ Na |
| ■ Electron configuration | [Ne] 3s ¹ | ■ CAS number | 7440-23-5 |
| ■ ChemSpider ID | 4514534 | ChemSpider is a free chemical structure database | |

Uses and properties



History



Atomic data



Oxidation states and isotopes



Supply risk



Pressure and temperature data – advanced



Podcasts



Video

➤ Element Discovery Timeline(时间表)

- Here's a helpful table chronicling(载入编年史) the discovery of the elements. The date is listed for when the element was first isolated. In many cases, the presence of a new element was suspected years or even thousands of years before it could be purified. Click on an element's name to see its entry in the Periodic Table and get facts for the element.

<http://chemistry.about.com/od/elementfacts/a/timeline-element-discovery.htm>

Screenshot of a web browser showing the Element Discovery Timeline page on About Education.

The page title is "Element Discovery Timeline" and the subtitle is "When Were the Elements Discovered?".

By Anne Marie Helmenstine, Ph.D.
Chemistry Expert

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Ads Element Chemistry Analytical Chemistry Lab Atom Periodic Table

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 Some elements have been discovered recently or are man-made. Others, like gold, were known to ancient man. Aramgutan, Wikipedia Commons

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Here's a helpful table chronicling the discovery of the elements. The date is listed for when the element was first isolated. In many cases, the presence of a new element was suspected years or even thousands of years before it could be purified. Click on an element's name to see its entry in the [Periodic Table](#) and get facts for the element.

Ancient Times - Prior to 1 A.D.

What's Your English Level Test
Wall Street English

TODAY'S TOP 5 PICKS IN EDUCATION

5 [8 Proven Strategies to Help Reluctant Readers](#)
By Janelle Cox
Elementary Education Expert

22:18 2014/9/29

- **Ancient Times - Prior to 1 A.D.**

Gold, Silver, Copper, Iron, Lead, Tin, Mercury, Sulfur, Carbon

- **Time of the Alchemists(炼金术士) - 1 A.D. to 1735**

Arsenic (Magnus ~1250) 砷

Antimony (17th century or earlier) 锑

Phosphorus (Brand 1669)

Zinc(13th Century India)



- **1955 to 1965**

Nobelium (Ghiorso, Sikkeland, Walton, and Seaborg 1958) 镨

Lawrencium (Ghiorso et al. 1961) 锫

Rutherfordium (L Berkeley Lab, USA - Dubna Lab, Russia 1964) 鐤



- **1995 to 2005**

Ununbium (Hofmann, Ninov et al. GSI-Germany 1996) 第112号元素

➤ Development of Periodic Table

| | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| H | | | | | | | | | | | | | | | | He | |
| Li | Be | | | | | | | | | | | | | | | | |
| Na | Mg | | | | | | | | | | | | | | | | |
| 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 | | | | | | |

| | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 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 |

Ancient Times

(9 elements)

Middle Ages–1700

(6 elements)

1735–1843

(42 elements)

1843–1886

(18 elements)

1894–1918

(11 elements)

1923–1961

1965–

(9 elements)

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Dmitrij Ivanovič Mendeleev (Russian chemist and inventor) and Lothar Meyer (German chemist) independently came to the same conclusion about how elements should be grouped.

➤ Mendeleev's 1871 periodic table

| 门捷列夫的第二张元素周期表(1871年12月) | | | | | | | | |
|-------------------------|------------------|-----------|-------------------------------|-----------------|-------------------------------|--|-------------------------------|--|
| 最高氢化物 | I族 | II族 | III族 (RH ₅ ?) | IV族 | V族 | VI族 | VII族 | VIII族 |
| 最高氧化物 | R ₂ O | RO | R ₂ O ₃ | RO ₂ | R ₂ O ₅ | RO ₃ 或 R ₂ O ₆ | R ₂ O ₇ | RO ₄ 或R ₂ O ₈ |
| | H=1 | - | - | - | - | - | - | - |
| 典型元素 | Li=7 | Be=9.4 | B=11 | C=12 | N=14 | O=16 | F=19 | |
| 第一周期 [1类 2类] | Na=23 | Mg=24 | Al=27.3 | Si=28 | P=31 | S=32 | Cl=35.5 | Fe=56 Co=59 |
| K=39 | Ce=40 | -=44 | Ti=50? | V=51 | Cr=52 | Mn=55 | Cu=63 Ni=59 | |
| 第二周期 [3类 4类] | (Cu=63) Zn=65 | -=68 | -=72 | As=75 | Se=78 | Br=80 | Ru=104 Rh=104 | |
| Rb=85 | Sr=87 | (?Yt=88?) | Zr=90 | Nb=94 | Mo=96 | -=100 | Ag=108 d=104 | |
| 第三周期 [5类 6类] | (Ag=108) Cd=112 | In=113 | Sn=118 | Sb=122 | Te=128? | I=127 | | |
| Cs=133 | Ba=137 | -=137 | Ce=138? | - | - | - | Os=199? Ir=198? | |
| 第四周期 [7类 8类] | (-) | - | - | - | - | - | Pt=197 Au=197 | |
| - | - | - | - | Ta=182 | W=184 | - | | |
| 第五周期 [9类 10类] | (Au=197) Hg=200 | Tl=204 | Pb=207 | Bi=208 | - | - | Ur=240 | - |
| | - | - | Th=232 | - | | | | |

On 6 March 1869, Mendeleev made a formal presentation to the , entitled *The Dependence between the Properties of the Atomic Weights of the Elements*, which described elements according to both atomic weight and valence.

➤ Development of Periodic Table

Chemists mostly credit Mendeleev because he also used chemical properties to organize the table and predicted some missing elements and their expected properties, including germanium.

TABLE 7.1 • Comparison of the Properties of Eka-Silicon Predicted by Mendeleev with the Observed Properties of Germanium

| Property | Mendeleev's Predictions for Eka-Silicon (made in 1871) | Observed Properties of Germanium (discovered in 1886) |
|---------------------------------------|--|---|
| Atomic weight | 72 | 72.59 |
| Density (g/cm ³) | 5.5 | 5.35 |
| Specific heat (J/g-K) | 0.305 | 0.309 |
| Melting point (°C) | High | 947 |
| Color | Dark gray | Grayish white |
| Formula of oxide | XO ₂ | GeO ₂ |
| Density of oxide (g/cm ³) | 4.7 | 4.70 |
| Formula of chloride | XCl ₄ | GeCl ₄ |
| Boiling point of chloride (°C) | A little under 100 | 84 |

➤ Atomic Number

- Mendeleev's table was based on atomic masses. It was the most fundamental property of elements known at the time.
- About 35 years later, the nuclear atom was discovered by Ernest Rutherford.
- Henry Moseley developed the concept of atomic number experimentally. The number of protons was considered the basis for the periodic property of elements.

Henry Moseley (1913)

Used X-Ray diffraction to determine how many protons are in an atom of an element.



- Grouped elements by similar chemical properties.
- Arranged elements by increasing atomic number.

Lead to the discovery of previous unknown elements

Periodic Table of the Elements

| | |
|---------------|---------------|
| Atomic Number | Boiling Point |
| | Symbol |
| | Name |
| | Atomic Mass |

Normal boiling points are in °C.
SP = Triple Point
Pressure is listed if not 1 atm.
Allotrope is listed if more than one allotrope.

Normal boiling points are in °C

SP = Triple Point

Pressure is listed if not 1 atm.

Allotrope is listed if more than one allotrope.

Alkali

Alkaline

transition

Basic

Comments

Next

11

10

Noble

Lanthanide

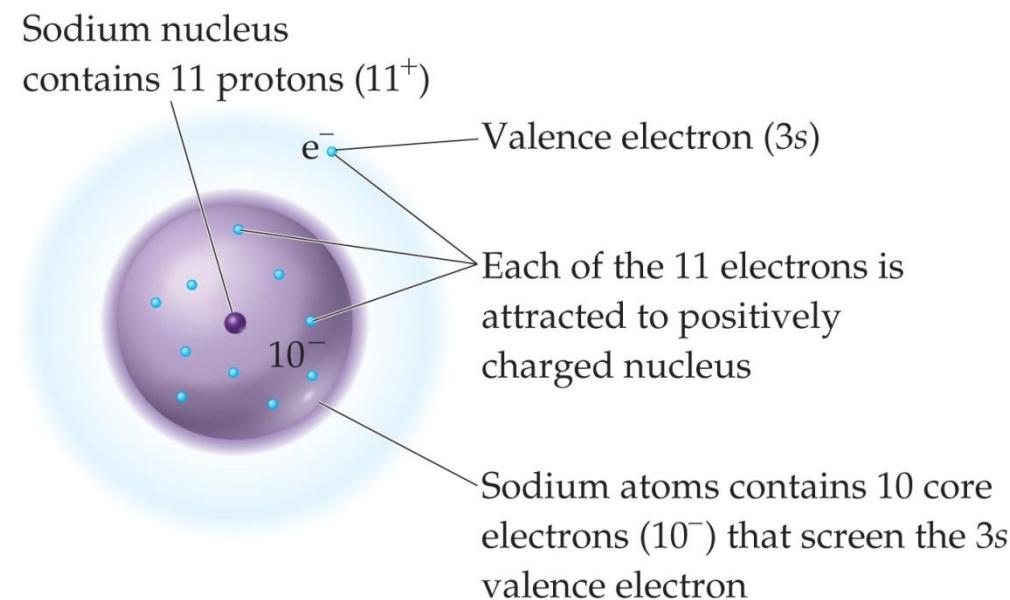
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➤ Periodicity (元素周期性)

- In this chapter, we will rationalize the observed trends in
 - ✓ Effective Nuclear Charge(有效核电荷)
 - ✓ Sizes of atoms and ions
 - ✓ Ionization energy(电离能)
 - ✓ Electron affinity(电子亲和势)
 - ✓ Some group chemical property trends

➤ Effective Nuclear Charge

- In a many-electron atom, electrons are both attracted to the nucleus and repelled by other electrons
- The nuclear charge that an electron experiences depends on both factors



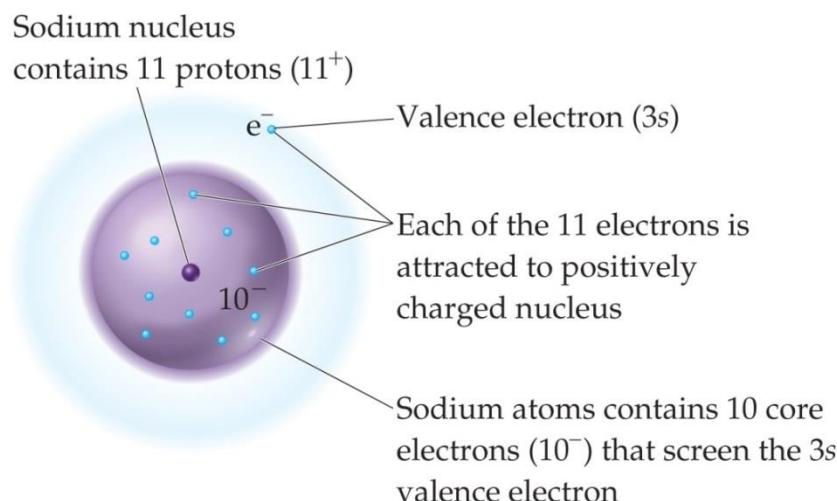
➤ Effective Nuclear Charge

- The effective nuclear: net electric field acting on the electron in an atom

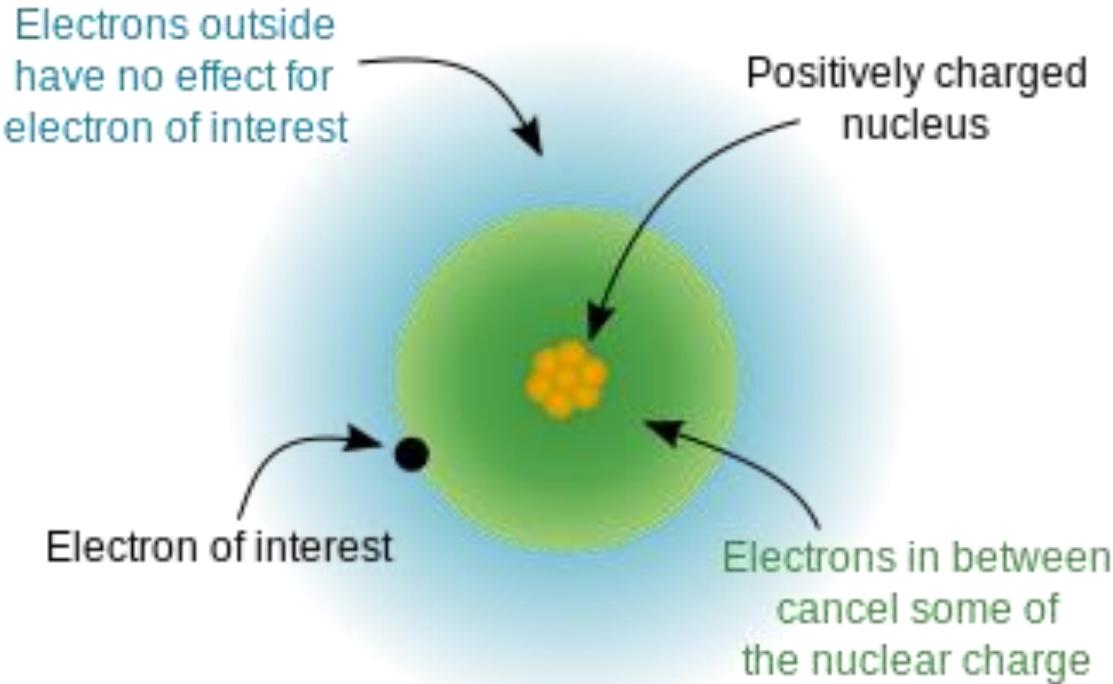
The effective nuclear charge, Z_{eff} , is found this way:

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

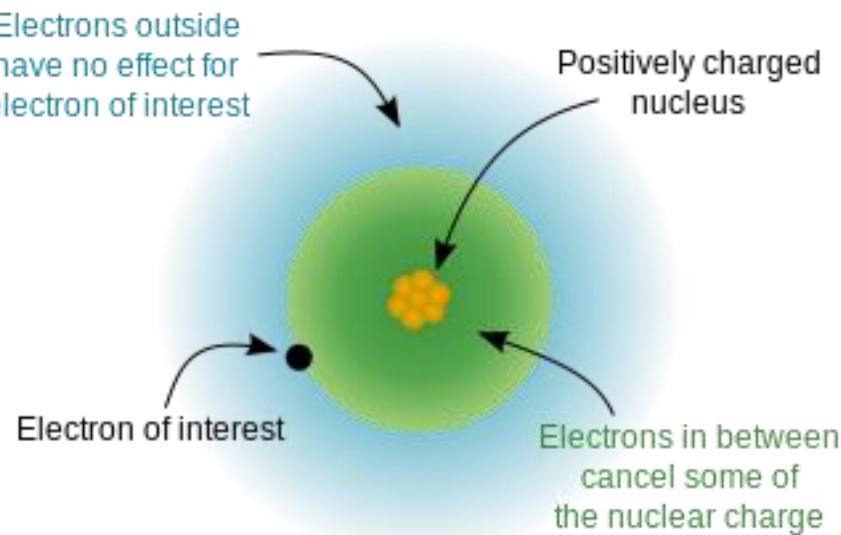
where Z is the atomic number and S is a screening constant,
usually close to the number of core electrons



- The **effective nuclear charge** (often symbolized as Z_{eff} or Z^*) is the net positive charge experienced by an electron in a multi-electron atom.



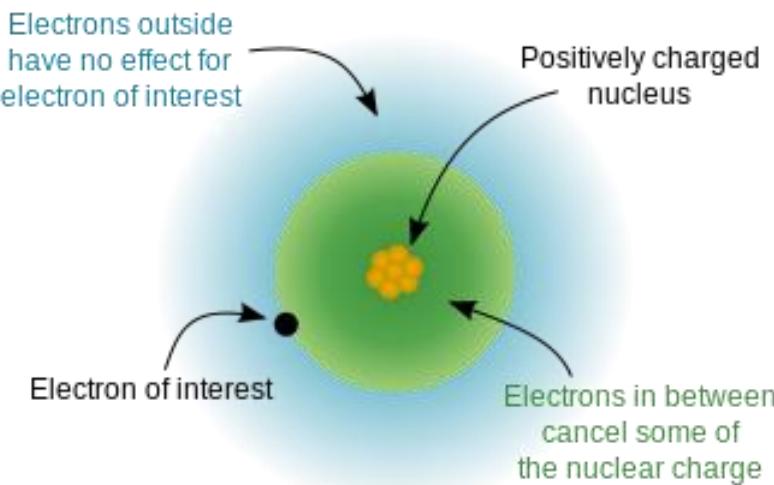
- The term "effective" is used because the **shielding/screening effect(屏蔽效应)** of negatively charged electrons prevents higher orbital electrons from experiencing the full nuclear charge by the repelling effect of inner-layer electrons. The effective nuclear charge experienced by the outer shell electron is also called the core charge.



➤ 有效核电荷

- 多电子原子中，某一个电子所受的净正电荷。这个概念是基于屏蔽作用理论而存在：由于共同带有负电荷的内外层电子之间存在排斥力，内层电子“阻挡”了一部分外层电子与原子核之间的正负电荷吸引力。应用这个概念，可以直接根据原子的氧化值判断核电荷的强度。
- 在单电子原子中，电子受到原子核中全部正电荷的吸引（即屏蔽作用不存在）。这种情况下，有效核电荷可以直接应用库伦定律计算。然而，在多电子原子中，处于外层的电子既受到正电荷的吸引，同时也被处于内层带负电荷的电子排斥。此时，其中一个电子所受的有效核电荷可以用以下公式求得：

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



➤ Effective Nuclear Charge

- The effective nuclear charge, Z_{eff} , increases from left to right across any period of the periodic table. Because the number of protons increases across the period, while the number of core electrons stays the same.

| $Z_{\text{eff}} = Z - S$ | | | |
|--------------------------|----|------------------------------------|--------------------------------------|
| e.g. | Si | $1s^2 2s^2 2p^6 \boxed{3s^2 3p^2}$ | $Z_{\text{eff}} \approx 14 - 10 = 4$ |
| | P | $1s^2 2s^2 2p^6 \boxed{3s^2 3p^3}$ | $Z_{\text{eff}} \approx 15 - 10 = 5$ |
| | S | $1s^2 2s^2 2p^6 \boxed{3s^2 3p^4}$ | $Z_{\text{eff}} \approx 16 - 10 = 6$ |

➤ Effective Nuclear Charge

- Going down a column, the effective nuclear charge experienced by valence electrons changes far less than it does across a period
- For example,

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



$$Z_{\text{eff}} \approx 3 - 2 = 1$$

$$Z_{\text{eff}} \approx 11 - 10 = 1$$

?

➤ Effective Nuclear Charge

- In fact, effective nuclear charge increases slightly as we go down a column because the more diffuse(发散) core electron cloud is less able to screen the valence electrons from the nuclear charge. In the case of the alkali metals, Z_{eff} increases from $\sim 1.3+$ for lithium, to $\sim 2.5+$ for sodium, to $\sim 3.5+$ for potassium.

Slater's Rules

<http://calistry.org/calculate/slaterRuleCalculator>

The screenshot shows a web browser window with the URL <http://calistry.org/calculate/slaterRuleCalculator> in the address bar. The page title is "Slater's Rule : Effective nuclear charge calculator". The main content area features a lightbulb icon and the formula $Z_{eff} = Z - \sigma$. Below the formula, text defines Z as Effective nuclear charge, Z as Atomic Number, and σ as Shielding. A text input field shows "Number of Protons in the Nucleus : 11". Below it, a row of buttons lists electron configurations: 1s2, 2s2, 2p6, and 3s1. A dropdown menu indicates "Calculate Z_{eff} on the : 3s electron". A result box shows "Z_{eff}: 2.2". To the right, there are "Sponsorships" sections for "Fast & Safe VPN 4 China" and "ExpressVPN". The bottom of the screen shows the Windows taskbar with various pinned icons.

http://calistry.org/calculate/slaterRuleCalculator

K的有效核荷数_百度搜索 Slater's Rule : Effective n... Wikipedia 【大学】关于斯莱特规则关于...

CALISTRY

Home Physical Chemistry Inorganic Chemistry Computational Chemistry

Slater's Rule : Effective nuclear charge calculator

$Z_{eff} = Z - \sigma$

Z = Effective nuclear charge; Z = Atomic Number ; σ = Shielding

Number of Protons in the Nucleus : 11

1s2 2s2 2p6 3s1

Calculate Z_{eff} on the : 3s electron

Z_{eff}: 2.2

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□ Shielding (Screening) Constant – Slater's Rules

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

1. The electronic structure of the atom is written in groupings as follows:

(1s)(2s,2p)(3s,3p)(3d)(4s,4p)(4d)(4f)(5s,5p), etc.

2. Electrons in higher groups (to the right in the list above) do not shield those in lower groups.

only shield those in much higher groups.

□ Shielding (Screening) Constant – Slater's Rules

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

3. For ns or np valence electrons:

a. Electrons in the same ns or np group contribute 0.35,
except the 1s, where 0.30 works better.

b. Electrons in the n–1 group contribute 0.85.

c. Electrons in the n–2 or lower groups contribute 1.00.

4. For nd and nf valence electrons:

a. Electrons in the same nd or nf group contribute 0.35.

b. Electrons in groups to the left contribute 1.00.

□ Shielding (Screening) Constant – Slater's Rules

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

e.g. Oxygen

$$\begin{aligned} &1s^2 2s^2 2p^4 \\ &(1s^2)(2s^2 2p^4) \end{aligned}$$

屏蔽常数的计算方法 —— Slater规则：

Slater根据光谱实验资料提出以下计算屏蔽常数 σ 的近似规则。
利用这个规则可以粗略地估计电子在不同轨道上的能量。将原子的电子层结构用括号分成下列小组：

(1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) ...

- (1) 在某小组[以()表示]右边任何小组内的电子对该组电子的屏蔽效应可忽略不计；
- (2) 在各小组中的每一个电子屏蔽同组价电子的程度是0.35，如果同在1s层上则为0.30；
- (3) 在主量子数为n的某小组左边同层小组中及n-1内层小组中的每一个电子对该组价电子屏蔽程度为0.85；
- (4) 在n-2层或更内层中的小组内每一个电子屏蔽外层(n层)价电子的程度都为1.00；
- (5) 被屏蔽的电子在(nd)或(nf)组中，则(1)、(2)两条仍适用，但在其以下各组电子屏蔽程度都为1.00。

For each of the 2p electron,

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

$$= 8 - (2 \times 0.85) - (5 \times 0.35) = 4.55$$



Electrons in the same ns

or np group contribute

0.35



Electrons in the n-1 group contribute 0.85

□ Shielding (Screening) Constant – Slater's Rules

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

Nickel $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
 $(1s^2)(2s^2 2p^6)(3s^2 3p^6)$ **$(3d^8)$** $(4s^2)$

For each of the 3d electron,

$$\begin{aligned} Z_{\text{eff}} &= Z - S \\ &= 28 - (18 \times 1.00) - (7 \times 0.35) = 7.55 \end{aligned}$$



Electrons in groups to
the left contribute 1.00

屏蔽常数的计算方法 —— Slater规则:

Slater根据光谱实验资料提出以下计算屏蔽常数 σ 的近似规则。利用这个规则可以粗略地估计电子在不同轨道上的能量。将原子的电子层结构用括号分成下列小组:

(1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) ...

- (1) 在某小组[以()表示]右边任何小组内的电子对该组电子的屏蔽效应可忽略不计;
- (2) 在各小组中的每一个电子屏蔽同组价电子的程度是0.35, 如果同在1s层上则为0.30;
- (3) 在主量子数为n的某小组左边同层小组中及n-1内层小组中的每一个电子对该组价电子屏蔽程度为0.85;
- (4) 在n-2层或更内层中的小组内每一个电子屏蔽外层(n层)价电子的程度都为1.00;
- (5) 被屏蔽的电子在(nd)或(nf)组中, 则(1)、(2)两条仍适用, 但在其以下各组电子屏蔽程度都为1.00。

Electrons in the same nd or
nf group contribute 0.35

□ Shielding (Screening) Constant – Slater's Rules

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

Nickel $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
 $(1s^2)(2s^2 2p^6)(3s^2 3p^6)(3d^8)(4s^2)$

For each of the 4s electron,

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

$$= 28 - (10 \times 1.00) - (16 \times 0.85) - (1 \times 0.35) = 4.05$$

$1s^2 2s^2 2p^6$ $3s^2 3p^6 3d^8$

$4s^1$

Electrons in the $n-2$ or
lower groups
contribute 1.00

Electrons in the same
ns or np group
contribute 0.35

Electrons in the $n-1$
group contribute
0.85

Principal quantum
number

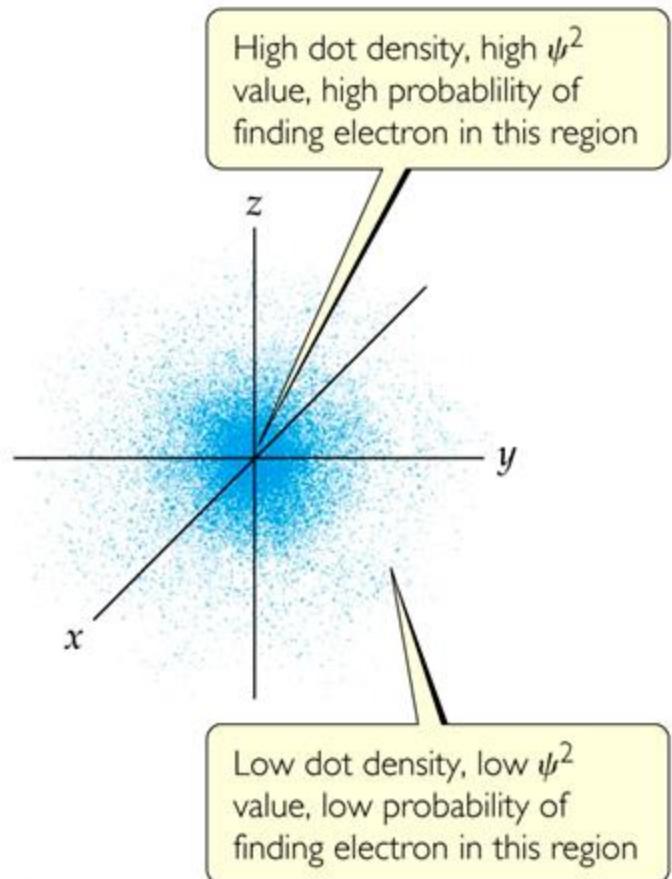
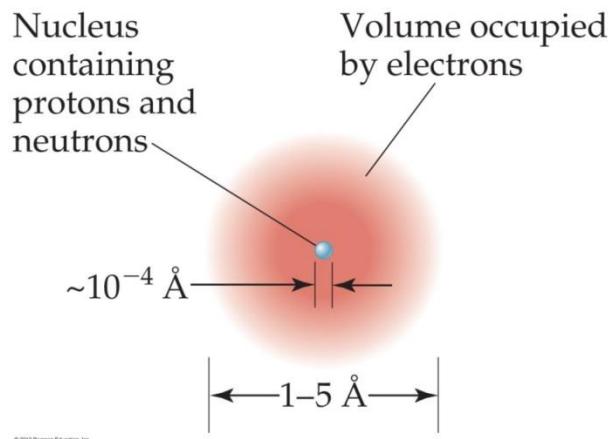
屏蔽常数的计算方法 —— Slater规则：

Slater根据光谱实验资料提出以下计算屏蔽常数 σ 的近似规则。
利用这个规则可以粗略地估计电子在不同轨道上的能量。将原子的电子层结构用括号分成下列小组：

- (1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) ...
- (1) 在某小组[以()表示]右边任何小组内的电子对该组电子的屏蔽效应可忽略不计；
 - (2) 在各小组中的每一个电子屏蔽同组价电子的程度是0.35，如果同在1s层上则为0.30；
 - (3) 在主量子数为 n 的某小组左边同层小组中及 $n-1$ 内层小组中的每一个电子对该组价电子屏蔽程度为0.85；
 - (4) 在 $n-2$ 层或更内层中的小组内每一个电子屏蔽外层(n 层)价电子的程度都为1.00；
 - (5) 被屏蔽的电子在(nd)或(nf)组中，则(1)、(2)两条仍适用，但在其以下各组电子屏蔽程度都为1.00。

➤ Sizes of Atoms and Ions

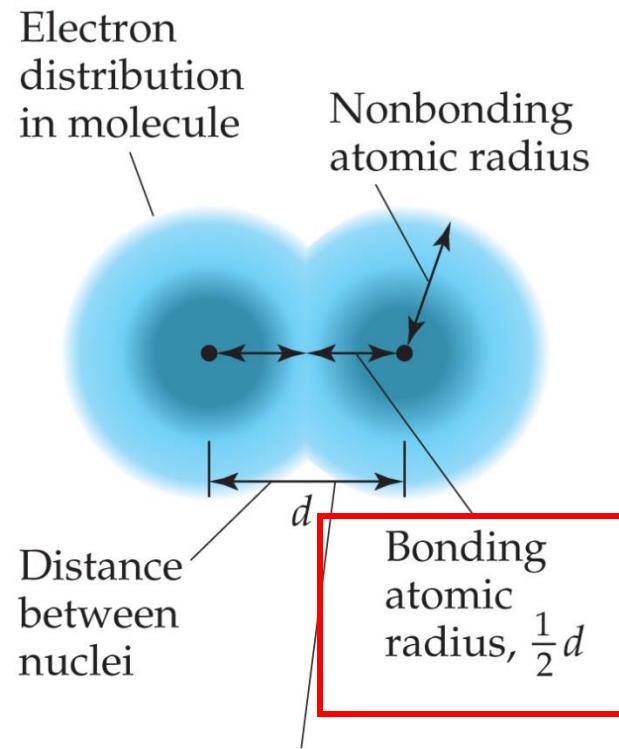
- Atoms do not have sharply defined boundaries at which the electron distribution becomes zero.
- How to define size of atoms?



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➤ What is the Size of an Atom?

- The **bonding atomic radius(半径)** is defined as one-half of the distance between covalently bonded(共价键合) nuclei(原子核复数) within a molecule



Nuclei cannot get any closer to each other because of electron–electron repulsion

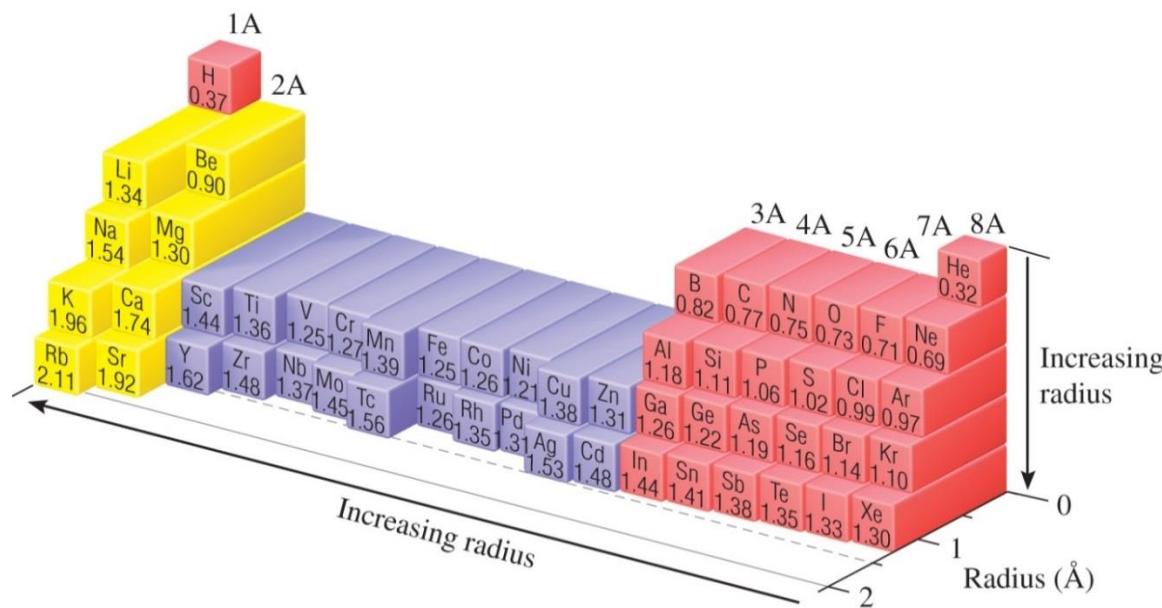
- Atomic radii allows to estimate bond lengths in molecules.

Bonding atomic radius C-0.99 Å
 Cl-0.77 Å  C-Cl bond is 1.77 Å



GO FIGURE

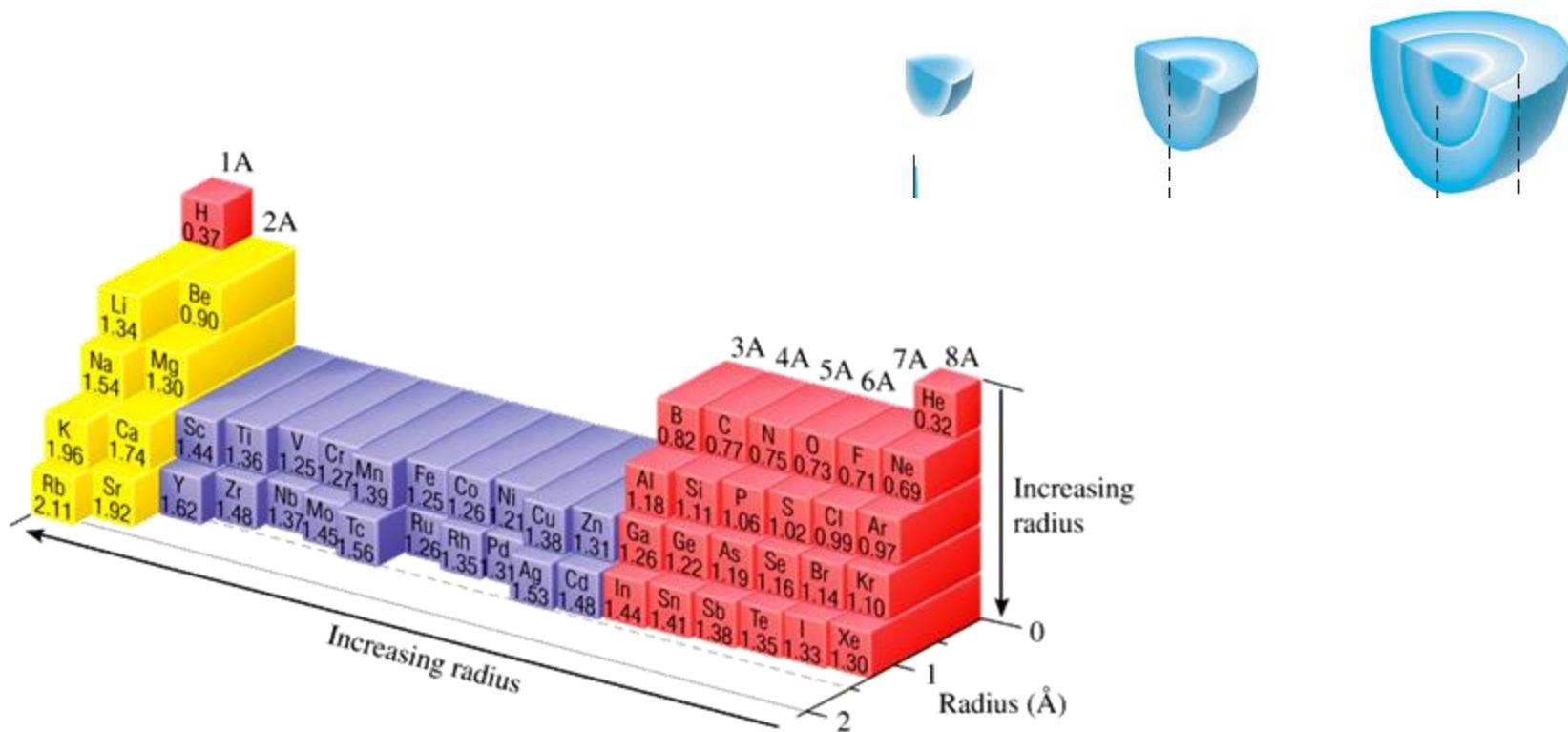
Which part of the periodic table (top/bottom, left/right) has the elements with the largest atoms?



◀ FIGURE 7.6 Trends in bonding atomic radii for periods 1 through 5.

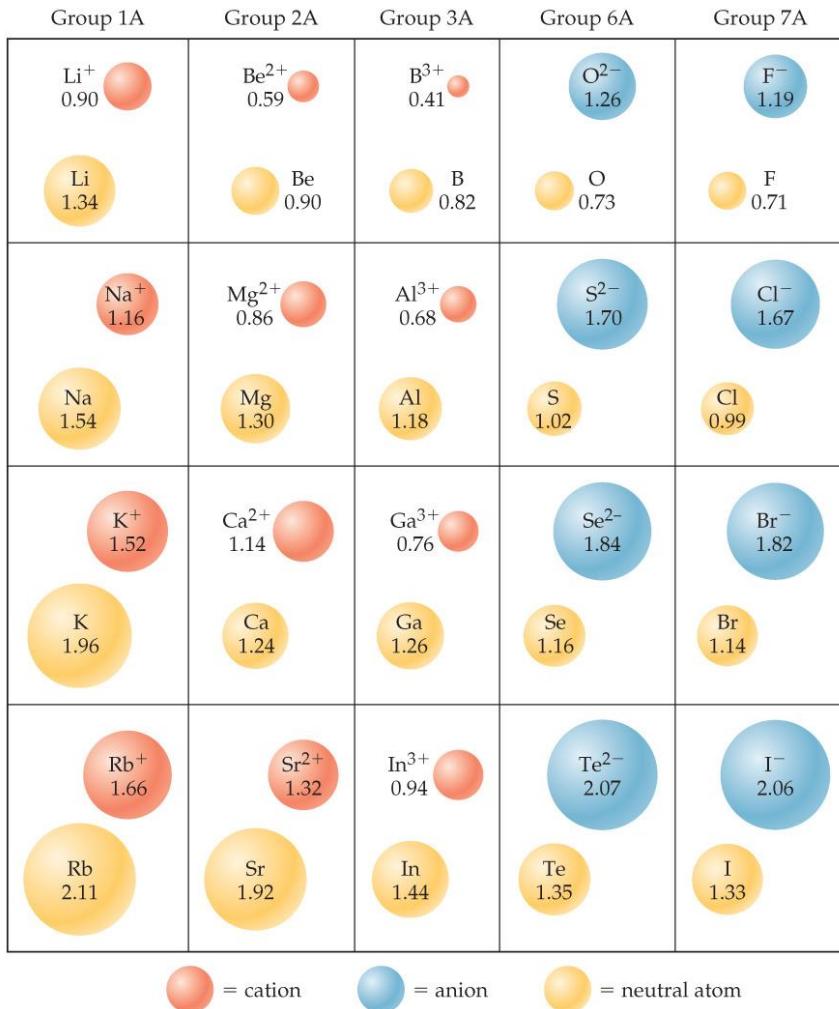
➤ Sizes of Atoms

- The bonding atomic radius tends to decrease from left to right across a row (due to increasing Z_{eff}).
- Increase from top to bottom of a column (due to the increasing value of n).



➤ Sizes of Ions

- Ionic size depends upon
 - The nuclear charge
 - The number of electrons
 - The orbitals in which electrons reside

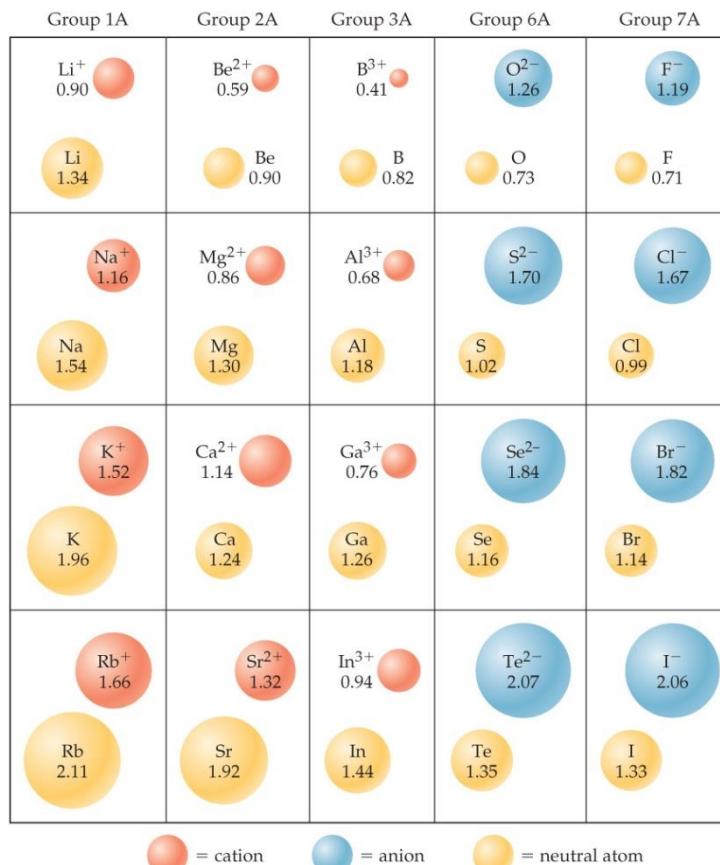


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➤ Sizes of Atoms

- Cations are smaller than their parent atoms:

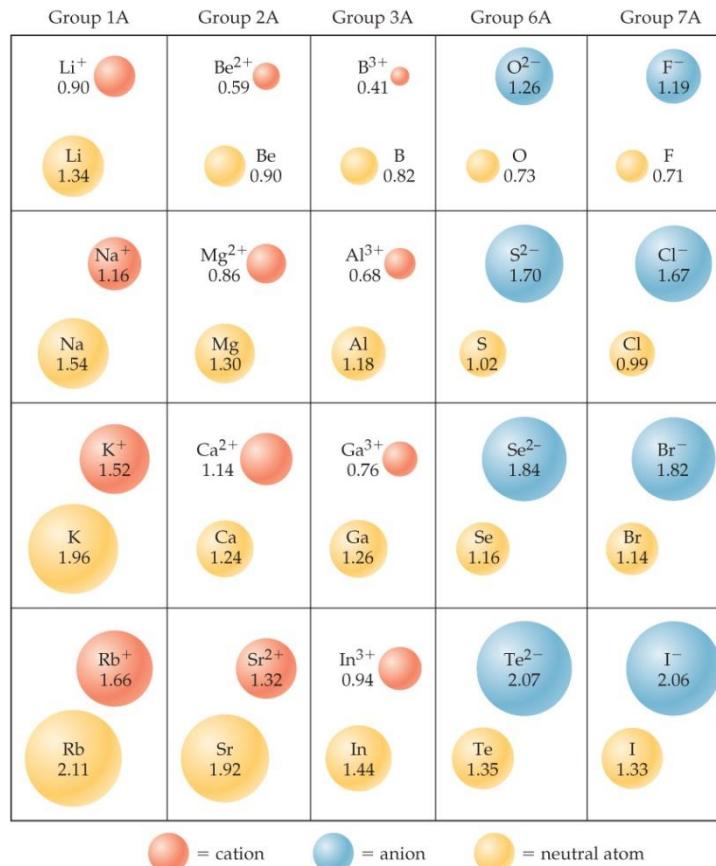
The outermost electron is removed and repulsions between electrons are reduced



➤ Sizes of Atoms

- Anions are larger than their parent atoms":

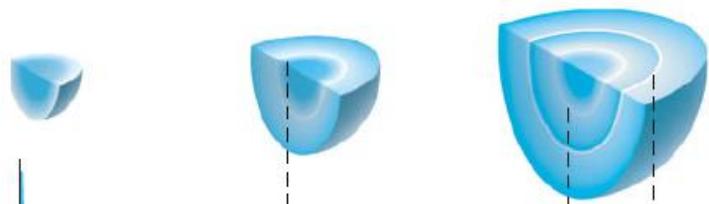
Electrons are added and repulsions between electrons are increased



➤ Sizes of Atoms

- Ions increase in size as you go down a column:

This increase in size is due to the increasing value of n



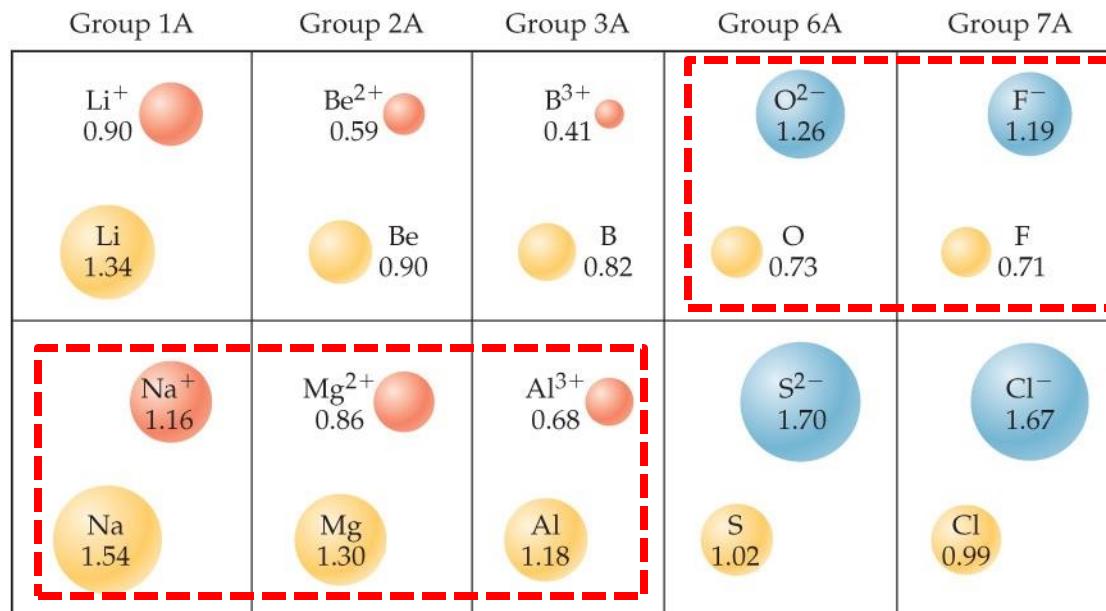
| Group 1A | Group 2A | Group 3A | Group 6A | Group 7A |
|---------------------------|------------------------------|------------------------------|------------------------------|---------------------------|
| Li^+ 0.90 | Be^{2+} 0.59 | B^{3+} 0.41 | O^{2-} 1.26 | F^- 1.19 |
| Na^+ 1.16 | Mg^{2+} 0.86 | Al^{3+} 0.68 | S^{2-} 1.70 | Cl^- 1.67 |
| K^+ 1.52 | Ca^{2+} 1.14 | Ga^{3+} 0.76 | Se^{2-} 1.84 | Br^- 1.82 |
| Rb^+ 1.66 | Sr^{2+} 1.32 | In^{3+} 0.94 | Te^{2-} 2.07 | I^- 2.06 |

= cation = anion = neutral atom

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➤ Sizes of Atoms

- In an **isoelectronic(等电子) series**, ions have the same number of electrons
- Ionic size decreases with an increasing nuclear charge



➤ Ionization Energy(电离能)

- The **ionization energy** is the amount of energy required to remove an electron from the **ground state** of a **gaseous atom or ion**
 - The first ionization energy (I_1) is that energy required to remove the first electron
 - The second ionization energy is that energy required to remove the second electron (I_2), etc



➤ Ionization Energy(电离能)

- It requires more energy to remove each successive electron($I_1 < I_2 < I_3$)
- Sharp increase in ionization energy occurs when an inner-shell electron is removed.

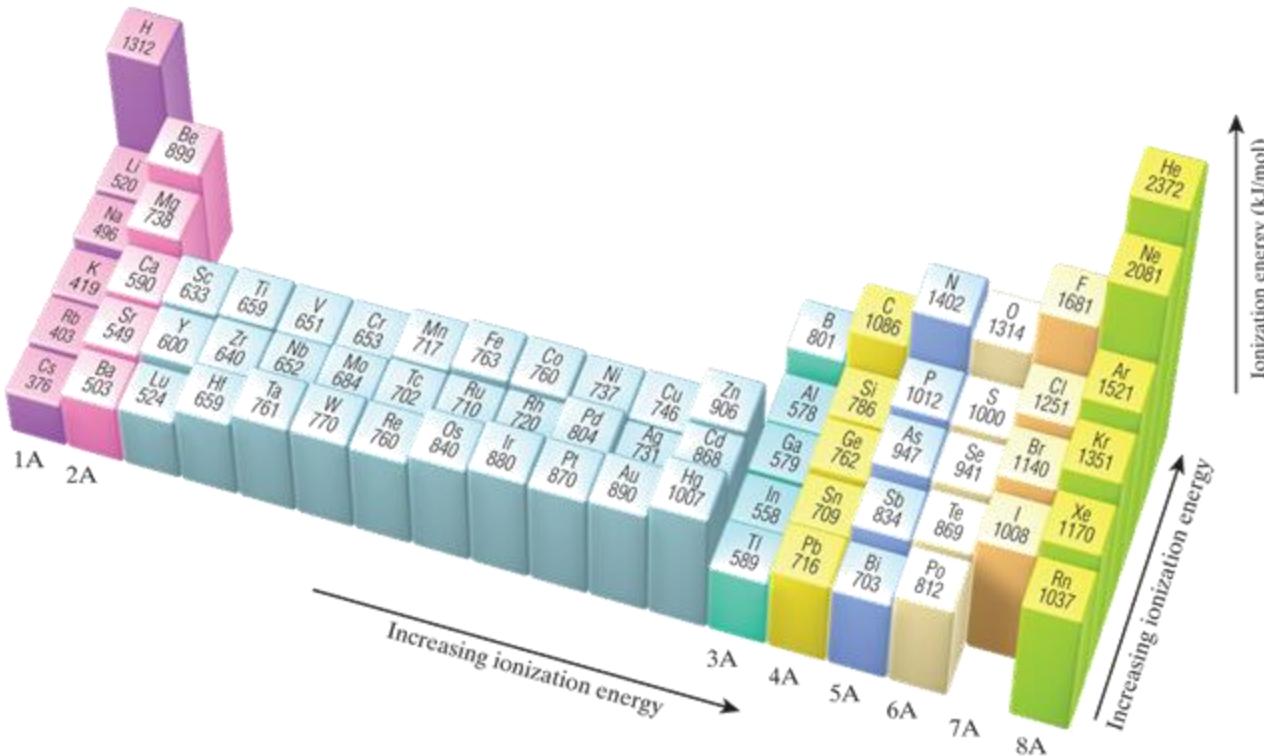
TABLE 7.2 • Successive Values of Ionization Energies, I , for the Elements Sodium through Argon (kJ/mol)

| Element | I_1 | I_2 | I_3 | I_4 | I_5 | I_6 | I_7 |
|---------|-------|-------|-------|--------|--------|--------|--------|
| Na | 496 | 4562 | | | | | |
| Mg | 738 | 1451 | 7733 | | | | |
| Al | 578 | 1817 | 2745 | 11,577 | | | |
| Si | 786 | 1577 | 3232 | 4356 | 16,091 | | |
| P | 1012 | 1907 | 2914 | 4964 | 6274 | 21,267 | |
| S | 1000 | 2252 | 3357 | 4556 | 7004 | 8496 | 27,107 |
| Cl | 1251 | 2298 | 3822 | 5159 | 6542 | 9362 | 11,018 |
| Ar | 1521 | 2666 | 3931 | 5771 | 7238 | 8781 | 11,995 |

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➤ Trends in First Ionization Energies

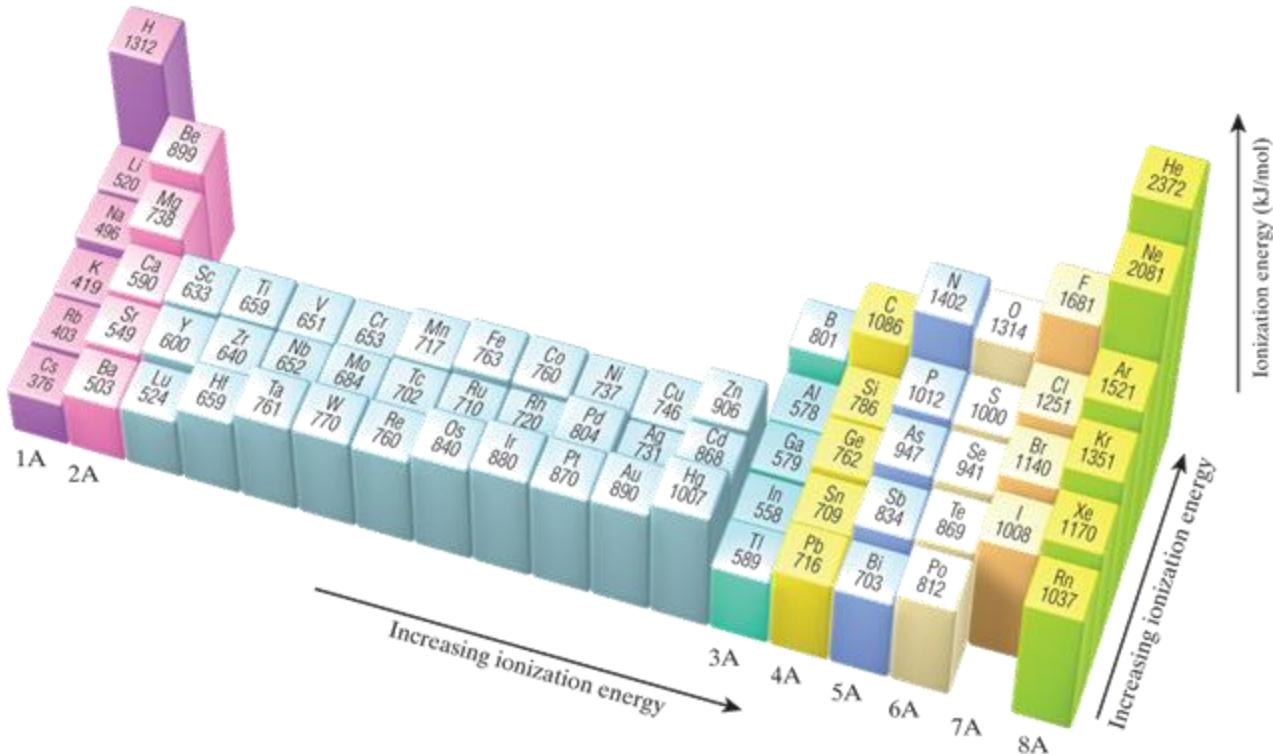
- As one goes down a column, less energy is required to remove the first electron
 - For atoms in the same group, the valence electrons are further from the nucleus



- ◆ Effective nuclear charge
- ◆ Distance of the electron from the nucleus
- ◆ Repulsion of paired electrons

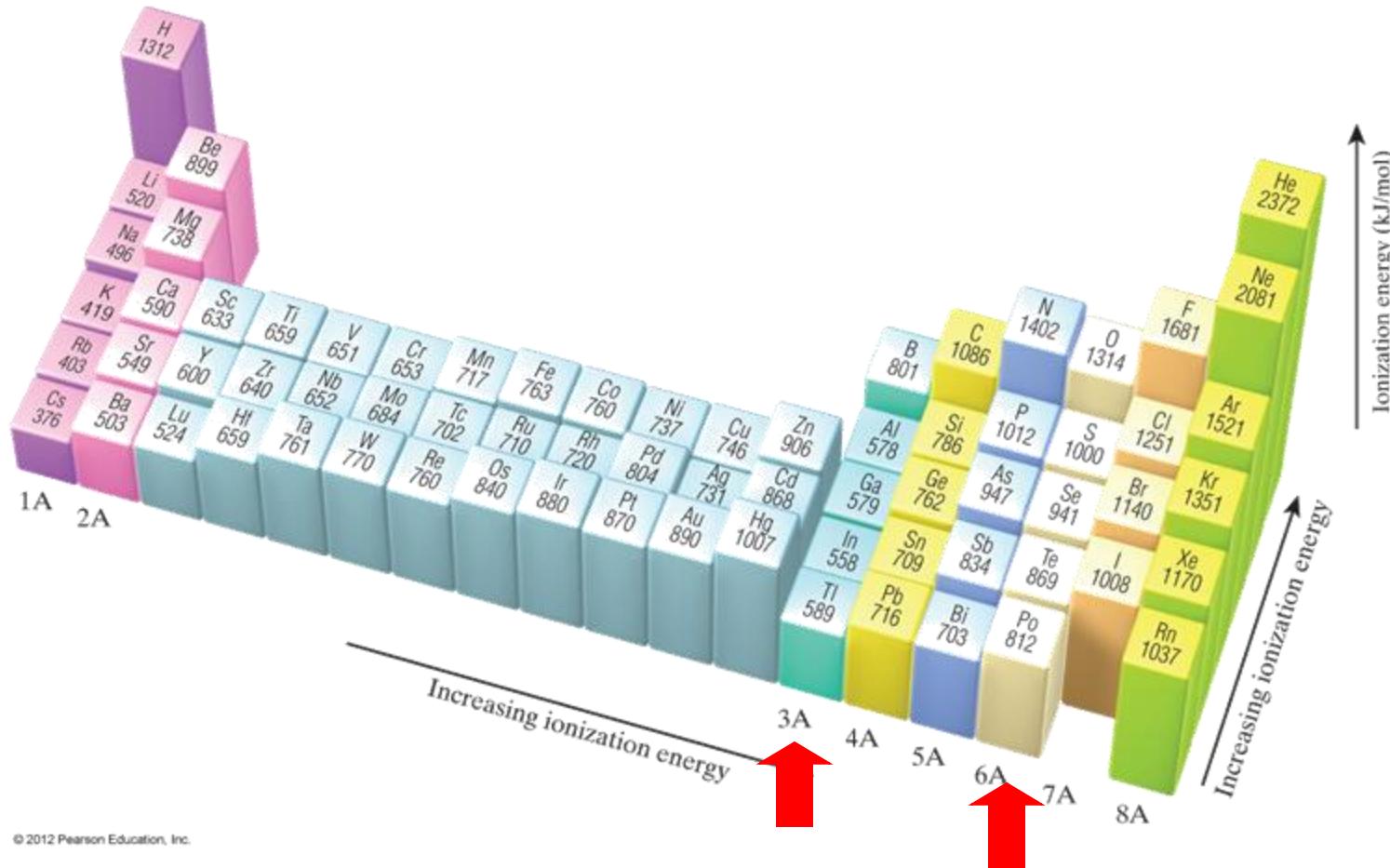
➤ Trends in First Ionization Energies

- Generally, as one goes across a row, it gets harder to remove an electron
 - As you go from left to right, Z_{eff} increases



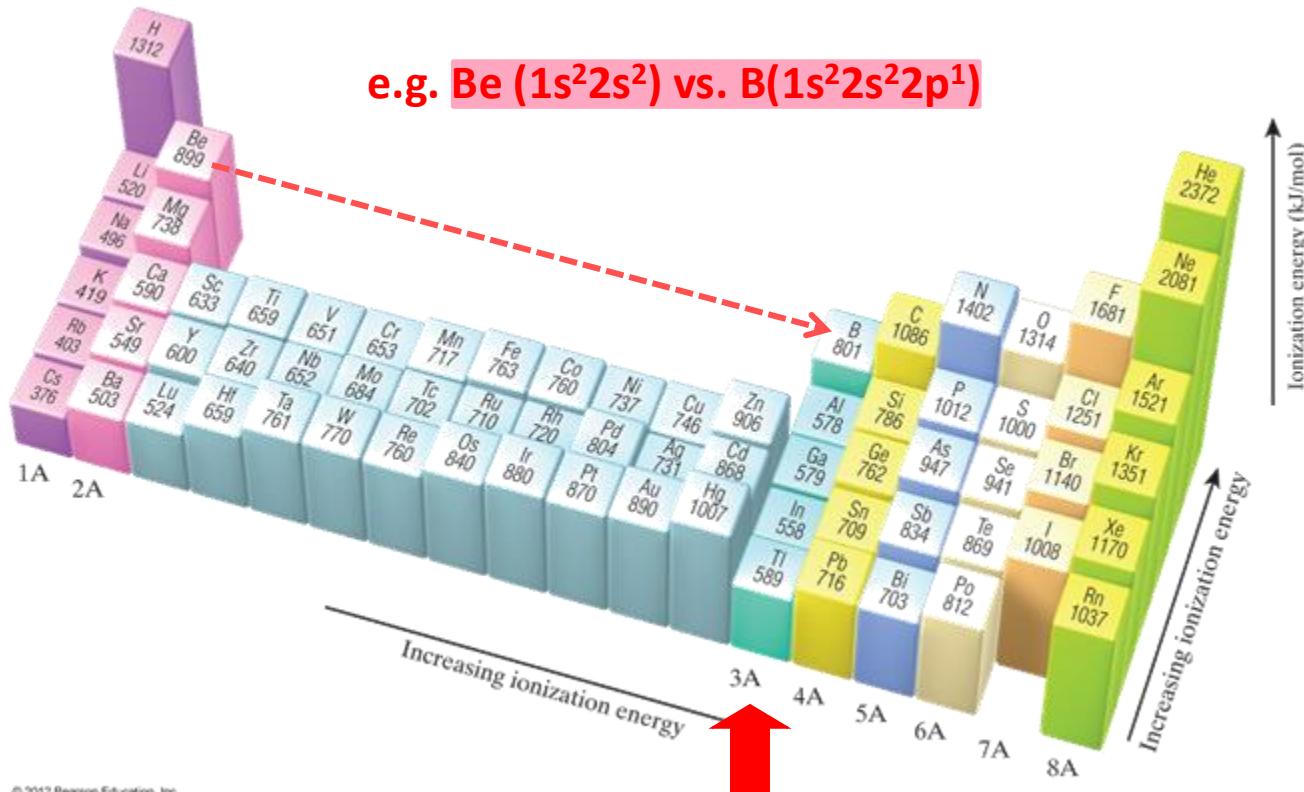
➤ Trends in First Ionization Energies

- However, there are two apparent discontinuities in this trend.



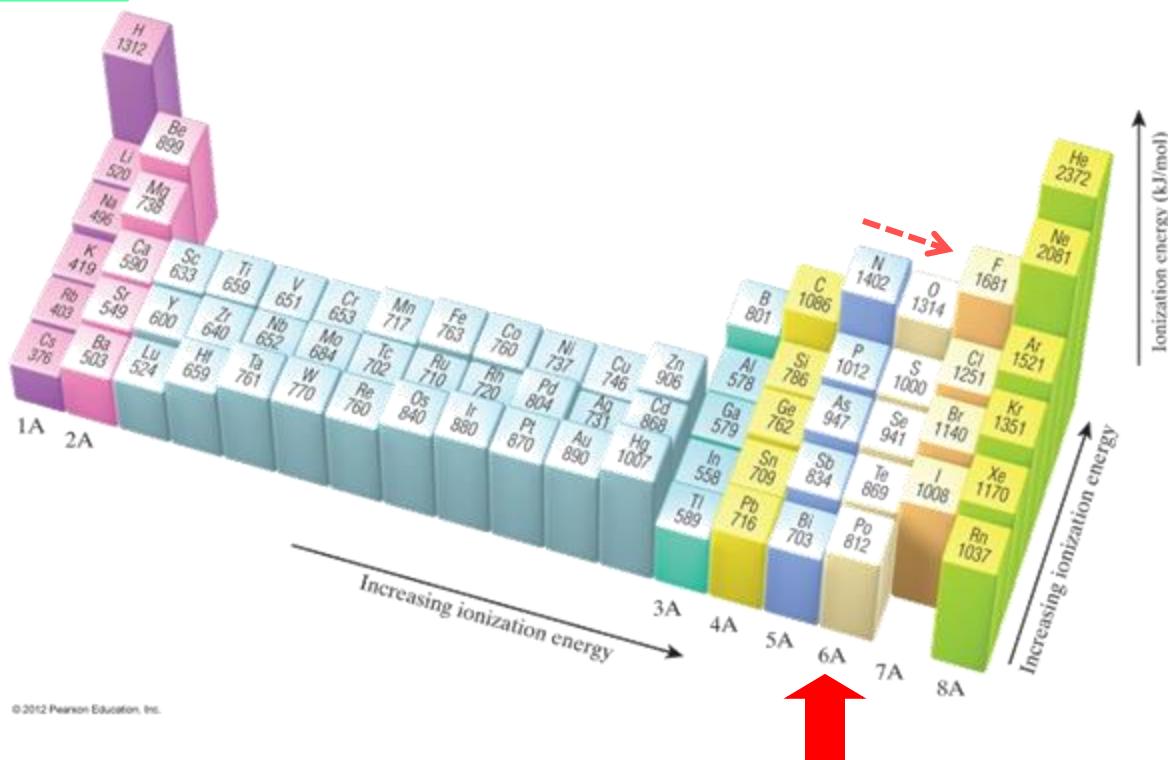
➤ Trends in First Ionization Energies

- The first discontinuity occurs between Groups IIA and IIIA
- In this case the electron is removed from a *p* orbital rather than an *s* orbital
 - The electron removed is farther from the nucleus
 - There is also a small amount of repulsion by the *s* electrons



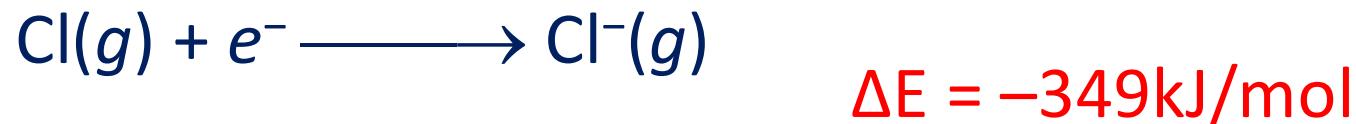
➤ Trends in First Ionization Energies

- The second discontinuity occurs between Groups VA and VIA
 - The electron removed comes from a doubly occupied orbital
 - e.g. N ($1s^2 2s^2 p^3$) vs. O($1s^2 2s^2 p^4$)
 - Repulsion from the other electron in the orbital aids in (helps) its removal.



➤ Electron Affinity(电子亲和能)

- The energy change accompanying the addition of an electron to a gaseous atom:



➤ Trends in Electron Affinity

- In general, electron affinity becomes more exothermic (the product is more stable) as you go from left to right across a row



| 1A | | | | | | | 8A |
|-----------|-----------|-----------|------------|------------|------------|------------|-----------|
| H -73 | 2A | 3A | 4A | 5A | 6A | 7A | He > 0 |
| Li -60 | Be > 0 | B -27 | C -122 | N > 0 | O -141 | F -328 | Ne > 0 |
| Na -53 | Mg > 0 | Al -43 | Si -134 | P -72 | S -200 | Cl -349 | Ar > 0 |
| K -48 | Ca -2 | Ga -30 | Ge -119 | As -78 | Se -195 | Br -325 | Kr > 0 |
| Rb -47 | Sr -5 | In -30 | Sn -107 | Sb -103 | Te -190 | I -295 | Xe > 0 |

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➤ Trends in Electron Affinity

- There are again, however, two discontinuities in this trend

| 1A | | 8A | | | | | |
|-----------|-----------|-----------|------------|------------|------------|------------|-----------|
| H -73 | Be > 0 | B -27 | C -122 | N > 0 | O -141 | F -328 | He > 0 |
| Li -60 | Mg > 0 | Al -43 | Si -134 | P -72 | S -200 | Cl -349 | Ne > 0 |
| Na -53 | Ca -2 | Ga -30 | Ge -119 | As -78 | Se -195 | Br -325 | Ar > 0 |
| K -48 | Sr -5 | In -30 | Sn -107 | Sb -103 | Te -190 | I -295 | Kr > 0 |
| Rb -47 | | | | | | | Xe > 0 |

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➤ Trends in Electron Affinity

□ The first occurs between Groups IA and IIA

- The added electron must go in a *p* orbital, not an *s* orbital
- The electron is farther from the nucleus and feels repulsion from the *s* electrons

| 1A | | 8A | | | | | | |
|-----------|-----------|-----------|------------|------------|------------|------------|-----------|--|
| H -73 | 2A | B -27 | C -122 | N > 0 | O -141 | F -328 | He > 0 | |
| Li -60 | Be > 0 | Al -43 | Si -134 | P -72 | S -200 | Cl -349 | Ar > 0 | |
| Na -53 | Mg > 0 | Ga -30 | Ge -119 | As -78 | Se -195 | Br -325 | Kr > 0 | |
| K -48 | Ca -2 | In -30 | Sn -107 | Sb -103 | Te -190 | I -295 | Xe > 0 | |
| Rb -47 | Sr -5 | | | | | | | |

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➤ Trends in Electron Affinity

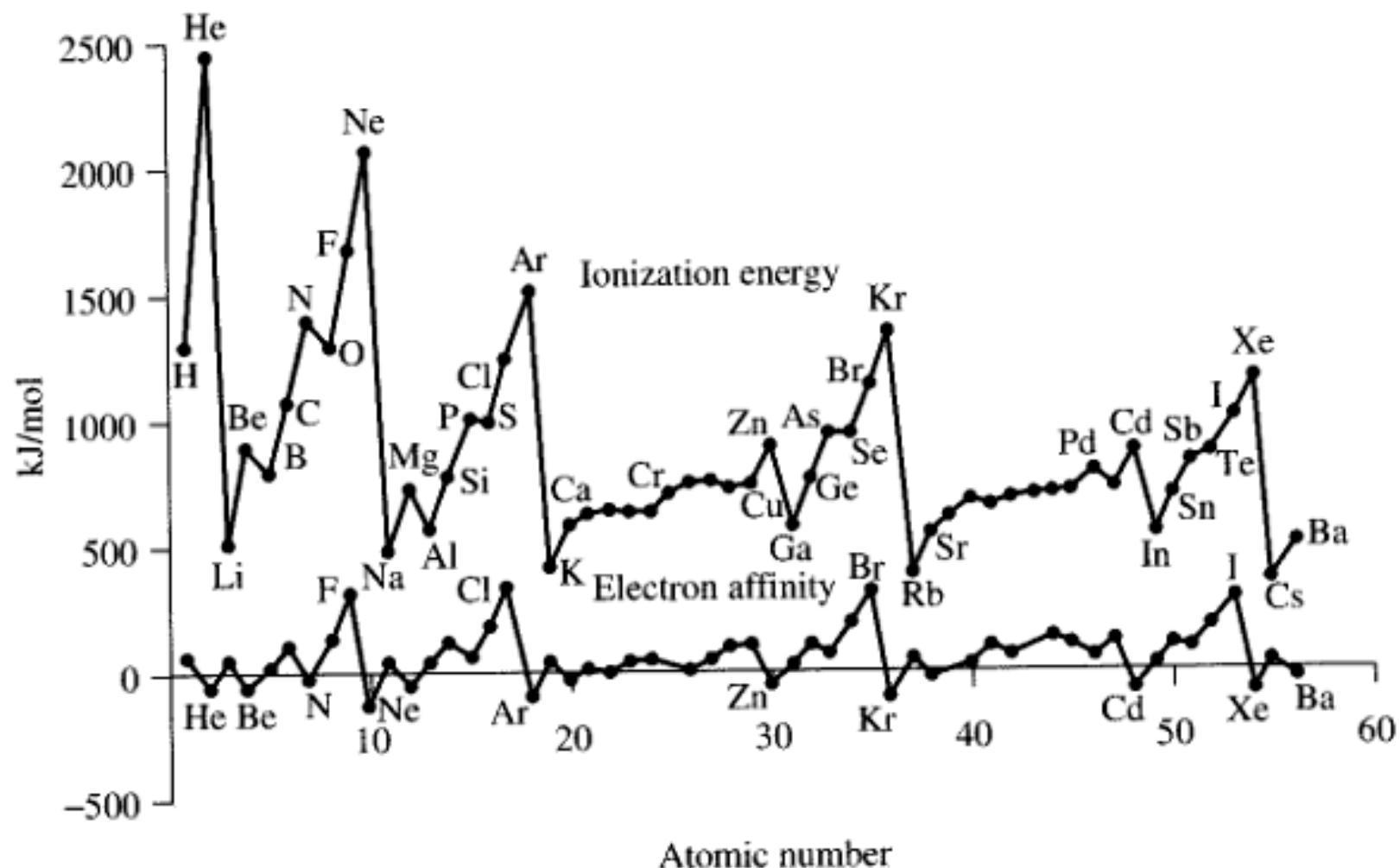
- The second discontinuity occurs between Groups IVA and VA
 - Group VA has no empty orbitals
 - The extra electron must go into an already occupied orbital, creating repulsion 成对电子互斥

| 1A | | | | | | | | 8A | |
|-----------|-----------|-----------|------------|------------|------------|------------|-----------|----|--|
| H -73 | Be > 0 | Li -60 | C -122 | N > 0 | O -141 | F -328 | Ne > 0 | | |
| Na -53 | Mg > 0 | B -27 | | | | | | | |
| K -48 | Ca -2 | Al -43 | Si -134 | P -72 | S -200 | Cl -349 | Ar > 0 | | |
| Rb -47 | Sr -5 | Ga -30 | Ge -119 | As -78 | Se -195 | Br -325 | Kr > 0 | | |
| | | In -30 | Sn -107 | Sb -103 | Te -190 | I -295 | Xe > 0 | | |

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➤ Trends in Ionization Energy & Electron Affinity



► Properties of Metal, Nonmetals, and Metalloids

| Increasing metallic character | | | | | | | | | | | | | | | | | |
|-------------------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|-----------------------|------------------|------------------|------------------|------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 1A 1 H | 2A 2 He | 3A 13 B | 4A 14 C | 5A 15 N | 6A 16 O | 7A 17 F | 8A 18 Ne | | | | | | | | | | |
| 3 Li | 4 Be | 3B 3 Na | 4B 4 Mg | 5B 5 Al | 6B 6 Si | 7B 7 Si | 8B 8 Ge | 9 As | 10 Br | 11 Kr | 12 Ca | 13 Zn | 14 Ge | 15 As | 16 Se | 17 Br | 18 Kr |
| 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 | 71 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 | 103 Lr | 104 Rf | 105 Db | 106 Sg | 107 Bh | 108 Hs | 109 Mt | 110 Ds | 111 Rg | 112 Cp | 113 | 114 | 115 | 116 | 117 | 118 |

| | | | | | | | | | | | | | | |
|------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|------------------|------------------|------------------|
| Metals | 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 |
| Metalloids | 89 As | 90 Se | 91 Br | 92 Rb | 93 Sr | 94 Zr | 95 Hf | 96 Ta | 97 Tl | 98 Pt | 99 Bi | 100 Po | 101 At | 102 Fr |
| Nonmetals | Ac Th | Th Pa | U Np | Pu Am | Am Cm | Bk Cf | Es Es | Fm Md | | | | | | No No |

- **Metals versus Nonmetals**
- Differences between metals and nonmetals tend to revolve (循环) around these properties.

Metals

Have a shiny luster; various colors, although most are silvery

Solids are malleable and ductile **Extensible and flexible**

Good conductors of heat and electricity

Most metal oxides are ionic solids that are basic

Tend to form cations in aqueous solution

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Nonmetals

Do not have a luster; various colors

Solids are usually brittle; some are hard, some are soft

Poor conductors of heat and electricity

Most nonmetal oxides are molecular substances that form acidic solutions

Tend to form anions or oxyanions in aqueous solution

➤ Metals versus Nonmetals

- Metals tend to form cations
- Nonmetals tend to form anions

| 1A | | | | | | | | | | | | | | | | 7A | | 8A | |
|--------|-----------|-------------------|-----------|----------------------|-----------|------------------------|------------------------|------------------------|-----------|---------------------|--------------------------|--|--|--|------------------------|------------------------|-----------|--------|--|
| H^+ | | | | | | | | | | | | | | | | H^- | | | |
| 2A | | | | | | | | | | | | | | | | N^{3-} | O^{2-} | F^- | |
| Li^+ | | | | | | | | | | | | | | | | | | | |
| Na^+ | Mg^{2+} | Transition metals | | | | | | | | | | | | | | Al^{3+} | | | |
| K^+ | Ca^{2+} | Sc^{3+} | Ti^{4+} | V^{5+} V^{4+} | Cr^{3+} | Mn^{2+} Mn^{4+} | Fe^{2+} Fe^{3+} | Co^{2+} Co^{3+} | Ni^{2+} | Cu^+ Cu^{2+} | Zn^{2+} | | | | | | Se^{2-} | Br^- | |
| Rb^+ | Sr^{2+} | | | | | | | | Pd^{2+} | Ag^+ | Cd^{2+} | | | | Sn^{2+} Sn^{4+} | Sb^{3+} Sb^{5+} | Te^{2-} | I^- | |
| Cs^+ | Ba^{2+} | | | | | | | | Pt^{2+} | Au^+ Au^{3+} | Hg_2^{2+} Hg^{2+} | | | | Pb^{2+} Pb^{4+} | Bi^{3+} Bi^{5+} | | | |

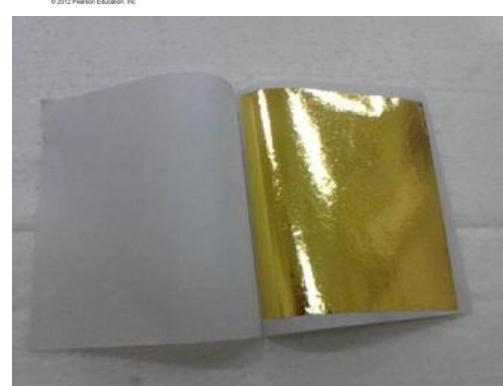
N
O
B
L
E

G
A
S
E
S

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➤ Metals

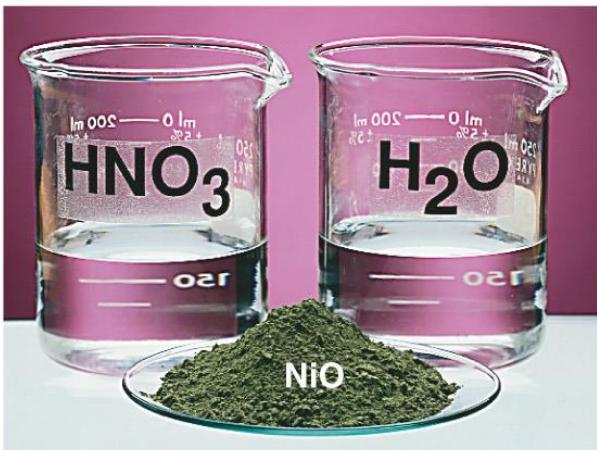
- Metals tend to be lustrous(有光泽的), malleable(可锻), and good conductors of heat and electricity



1克黄金制0.47平米(厚度0.12 um)98金箔)

➤ Metals

- Compounds formed between metals and nonmetals tend to be ionic
- Metal oxides tend to be basic



Nickle oxide (NiO), nitric acid (HNO_3), and water

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NiO is insoluble in water but reacts with HNO_3 to give a green solution of the salt $\text{Ni}(\text{NO}_3)_2$

➤ Nonmetals

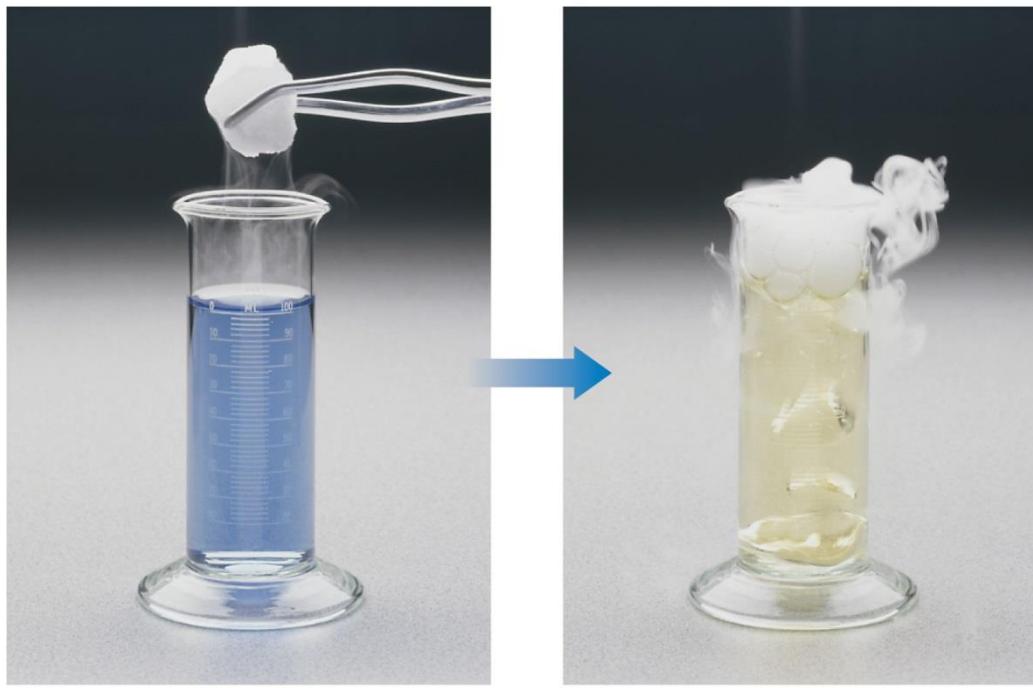
- Nonmetals are dull(暗的), brittle substances that are poor conductors of heat and electricity
- They tend to gain electrons in reactions with metals to acquire a noble-gas configuration



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➤ Nonmetals

- Substances containing only nonmetals are molecular compounds
- Most nonmetal oxides are acidic

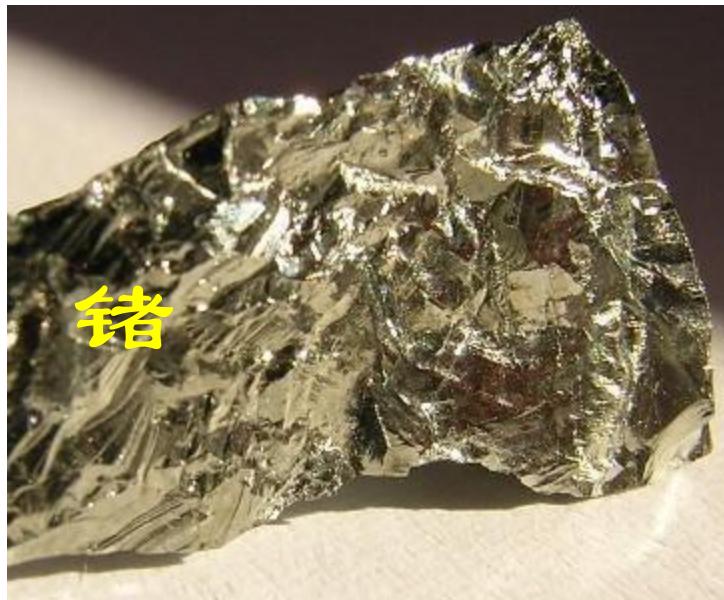


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➤ Metalloids(准金属)

- Metalloids have some characteristics of metals and some of nonmetals
- For instance, silicon looks shiny, but is brittle and a fairly poor conductor



Group Trends

➤ Alkali(碱) Metals

- Alkali metals are soft, metallic solids.
- The name comes from the Arabic word for ashes.



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➤ Alkali(碱) Metals

- They are found only in compounds in nature, not in their elemental forms.
- They have low densities and melting points.
- They also have low ionization energies.

TABLE 7.4 • Some Properties of the Alkali Metals

| Element | Electron Configuration | Melting Point (°C) | Density (g/cm ³) | Atomic Radius (Å) | I_1 (kJ/mol) |
|-----------|------------------------|--------------------|------------------------------|-------------------|----------------|
| Lithium | [He]2s ¹ | 181 | 0.53 | 1.34 | 520 |
| Sodium | [Ne]3s ¹ | 98 | 0.97 | 1.54 | 496 |
| Potassium | [Ar]4s ¹ | 63 | 0.86 | 1.96 | 419 |
| Rubidium | [Kr]5s ¹ | 39 | 1.53 | 2.11 | 403 |
| Cesium | [Xe]6s ¹ | 28 | 1.88 | 2.25 | 376 |

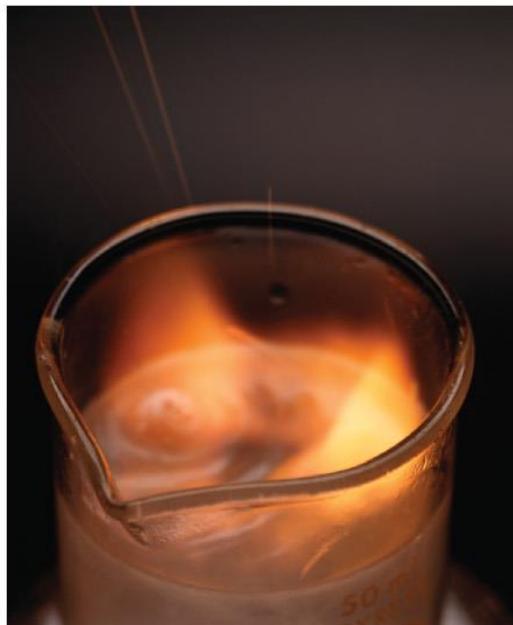
➤ Alkali(碱) Metals

- Their reactions with water are famously exothermic. 放热的



Li

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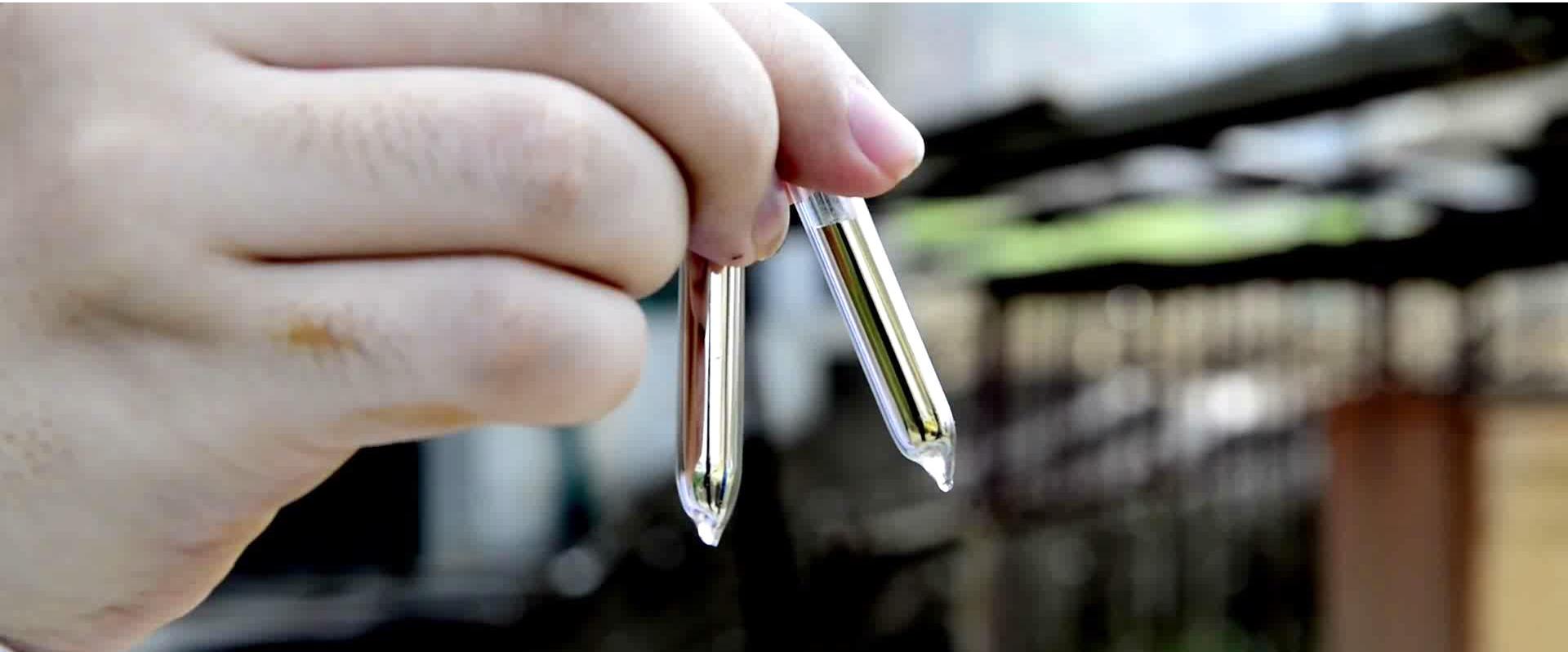


Na



K

➤ Alkali(碱) Metals



Their reactions with water are famously exothermic.

➤ Alkali(碱) Metals

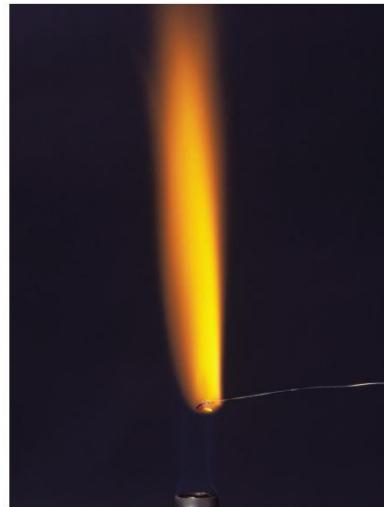
- Alkali metals (except Li) react with oxygen to form peroxides
- K, Rb, and Cs also form superoxides:



- They produce bright colors when placed in a flame



Li



Na



K

➤ Alkaline Earth(碱土) Metals

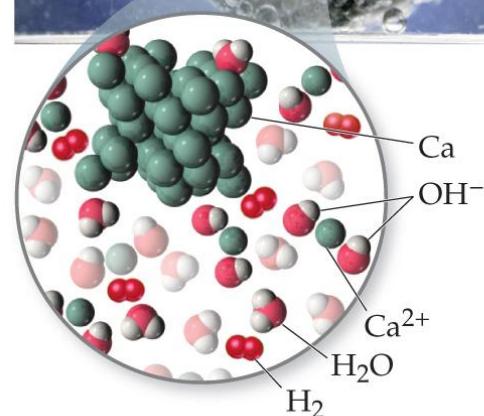
- Alkaline earth metals have higher densities and melting points than alkali metals
- Their ionization energies are low, but not as low as those of alkali metals

TABLE 7.5 • Some Properties of the Alkaline Earth Metals

| Element | Electron Configuration | Melting Point (°C) | Density (g/cm ³) | Atomic Radius (Å) | I_1 (kJ/mol) |
|-----------|------------------------|--------------------|------------------------------|-------------------|----------------|
| Beryllium | [He]2s ² | 1287 | 1.85 | 0.90 | 899 |
| Magnesium | [Ne]3s ² | 650 | 1.74 | 1.30 | 738 |
| Calcium | [Ar]4s ² | 842 | 1.55 | 1.74 | 590 |
| Strontium | [Kr]5s ² | 777 | 2.63 | 1.92 | 549 |
| Barium | [Xe]6s ² | 727 | 3.51 | 1.98 | 503 |

➤ Alkaline Earth(碱土) Metals

- Beryllium does not react with water, and magnesium reacts only with steam, but the other alkaline earth metals react readily with water
- Reactivity tends to increase as you go down the group



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➤ Group 6A

- Oxygen, sulfur, and selenium are nonmetals.
- Tellurium is a metalloid
- The radioactive polonium is a metal

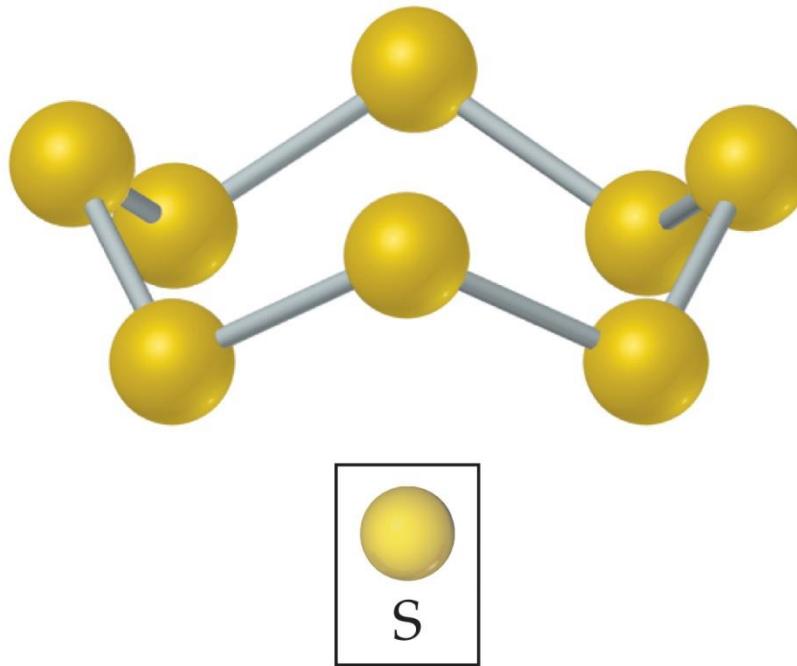
TABLE 7.6 • Some Properties of the Group 6A Elements

| Element | Electron Configuration | Melting Point (°C) | Density | Atomic Radius (Å) | I_1 (kJ/mol) |
|-----------|-------------------------------|--------------------|------------------------|-------------------|----------------|
| Oxygen | [He] $2s^22p^4$ | -218 | 1.43 g/L | 0.73 | 1314 |
| Sulfur | [Ne] $3s^23p^4$ | 115 | 1.96 g/cm ³ | 1.02 | 1000 |
| Selenium | [Ar] $3d^{10}4s^24p^4$ | 221 | 4.82 g/cm ³ | 1.16 | 941 |
| Tellurium | [Kr] $4d^{10}5s^25p^4$ | 450 | 6.24 g/cm ³ | 1.35 | 869 |
| Polonium | [Xe] $4f^{14}5d^{10}6s^26p^4$ | 254 | 9.20 g/cm ³ | — | 812 |

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➤ Sulfur

- Sulfur is a weaker oxidizer than oxygen, i.e. the electron affinity of oxygen > sulfur
- The most stable allotrope is S_8 , a ringed molecule



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➤ Group VIIA: Halogens

卤族元素

- The **halogens** are prototypical nonmetals
- The name comes from the Greek words *halos* and *gennao*: “salt formers”

TABLE 7.7 • Some Properties of the Halogens

| Element | Electron Configuration | Melting Point (°C) | Density | Atomic Radius (Å) | I_1 (kJ/mol) |
|----------|------------------------|--------------------|------------------------|-------------------|----------------|
| Fluorine | [He] $2s^22p^5$ | −220 | 1.69 g/L | 0.71 | 1681 |
| Chlorine | [Ne] $3s^23p^5$ | −102 | 3.12 g/L | 0.99 | 1251 |
| Bromine | [Ar] $3d^{10}4s^24p^5$ | −7.3 | 3.12 g/cm ³ | 1.14 | 1140 |
| Iodine | [Kr] $4d^{10}5s^25p^5$ | 114 | 4.94 g/cm ³ | 1.33 | 1008 |

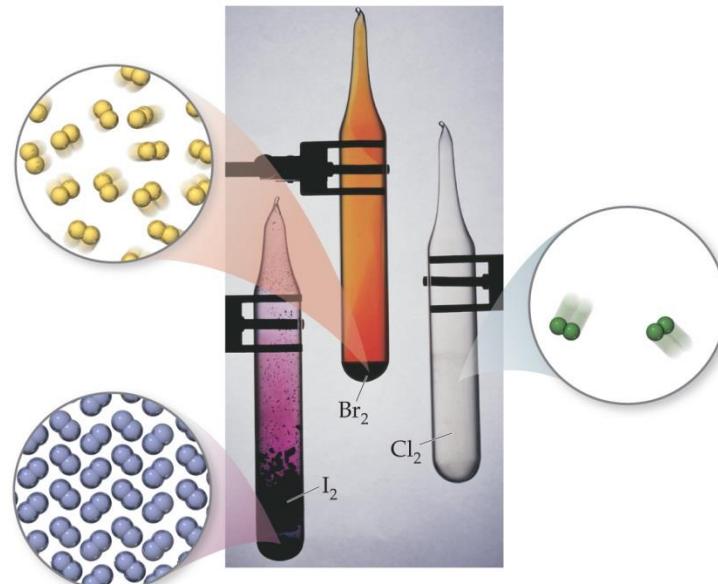
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➤ Group VIIA: Halogens

- They have large, negative electron affinities

Therefore, they tend to oxidize other elements easily

- They react directly with metals to form metal halides(卤化物)
- Chlorine is added to water supplies to serve as a disinfectant(消毒剂)



➤ Group VIIIA: Noble Gases 惰性气体

- The noble gases have astronomical ionization energies
- Their electron affinities are positive

Therefore, they are relatively unreactive
- They are found as monatomic gases

TABLE 7.8 • Some Properties of the Noble Gases

| Element | Electron Configuration | Boiling Point (K) | Density (g/L) | Atomic Radius* (Å) | I_1 (kJ/mol) |
|---------|----------------------------------|-------------------|---------------|--------------------|----------------|
| Helium | $1s^2$ | 4.2 | 0.18 | 0.32 | 2372 |
| Neon | [He] $2s^2 2p^6$ | 27.1 | 0.90 | 0.69 | 2081 |
| Argon | [Ne] $3s^2 3p^6$ | 87.3 | 1.78 | 0.97 | 1521 |
| Krypton | [Ar] $3d^{10} 4s^2 4p^6$ | 120 | 3.75 | 1.10 | 1351 |
| Xenon | [Kr] $4d^{10} 5s^2 5p^6$ | 165 | 5.90 | 1.30 | 1170 |
| Radon | [Xe] $4f^{14} 5d^{10} 6s^2 6p^6$ | 211 | 9.73 | 1.45 | 1037 |

*Only the heaviest of the noble-gas elements form chemical compounds. Thus, the atomic radii for the lighter noble-gas elements are estimated values.

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Xenon was the first noble gas to be made into a compound (xenon hexafluoroplatinate) by Neil Bartlett in 1962, disproving the long-held belief that noble gases were completely inert.