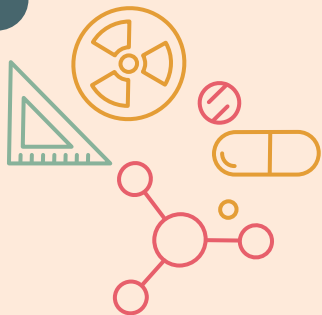


# University Chemistry Review 2





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# Topic 5

Atomic energy





# Types of orbitals



## Quantum # rules

$$n \geq 1$$

$$0 \leq l \leq n-1$$

$$-l \leq m_l \leq l$$

$$m_s = +1/2 \text{ or } -1/2$$

## Kinds of orbitals

1 type of s orbital

3 types of p orbital

5 types of d orbital

7 types of f orbital

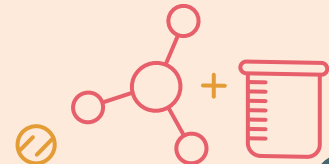
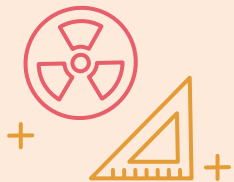
## Maximum number of e<sup>-</sup>

2e<sup>-</sup> in an s orbital

6e<sup>-</sup> in an p orbital

10e<sup>-</sup> in an d orbital

14e<sup>-</sup> in an f orbital





# Types of orbitals

- Pauli exclusion principle:
  - ◆ No 2 e- in an atom can have the same 4 quantum numbers
- Aufbau principle:
  - ◆ E- fill lower energy levels first before filling higher ones
    - E.g., 1S is filled before 2S
  - ◆ Helps determine the configurations of e-
  - ◆ Sometimes not the case! E.g., e- configuration of Silver [Ag]
- Hund's rule
  - ◆ Each orbital must be occupied with one e- before it can be occupied by 2 e-
  - ◆ All single e- that occupy orbitals in a subshell have the same spin
  - ◆ No two e- occupying the same orbital can have the same spin

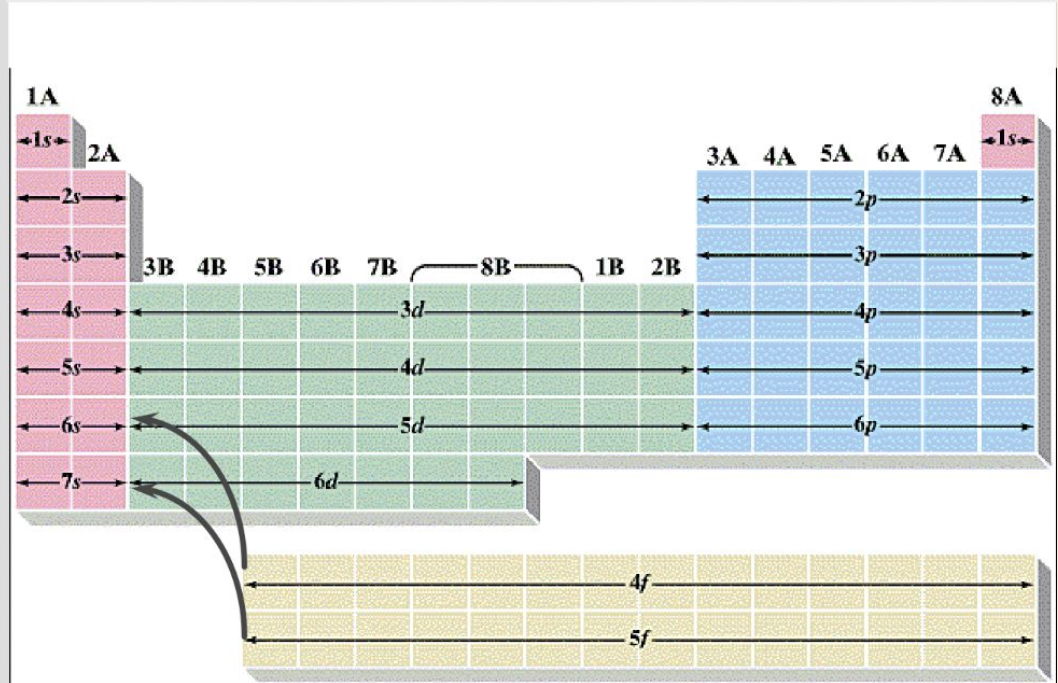




# Orbital filling order



~~1s~~  
~~2s 2p~~  
~~3s 3p 3d~~  
~~4s 4p 4d 4f~~  
~~5s 5p 5d 5f~~  
~~6s 6p 6d~~



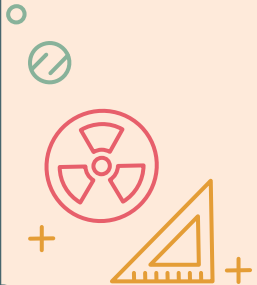


# Periodicity

- What is periodicity?
  - ◆ Predictable changes of physical properties of atoms going across a period or down a group
- E.g., atomic radius

 **Increases** going **down** a group 

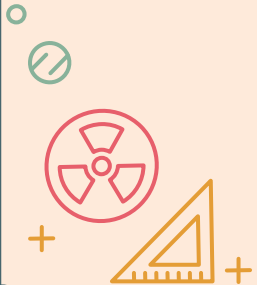
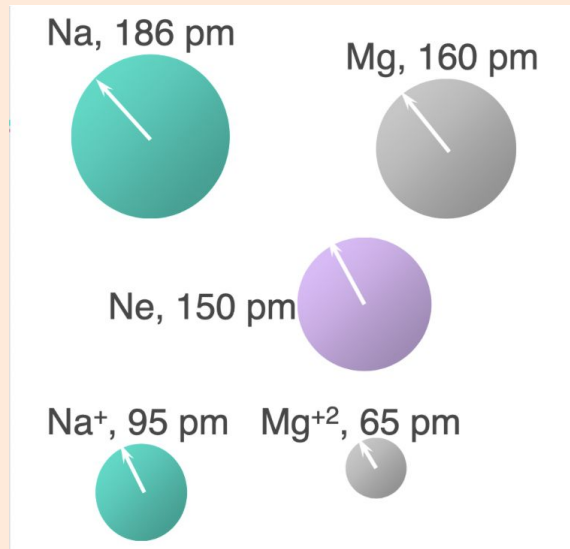
 **Decreases** going **L to R** across a  period





# Ionic radii

- Anions are larger than electrically neutral atoms
  - ◆ Adding  $e^-$  to the same shell
- Cations are smaller than electrically neutral atoms
  - ◆ Loss of  $e^-$

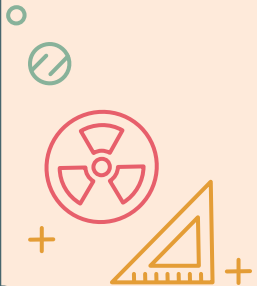
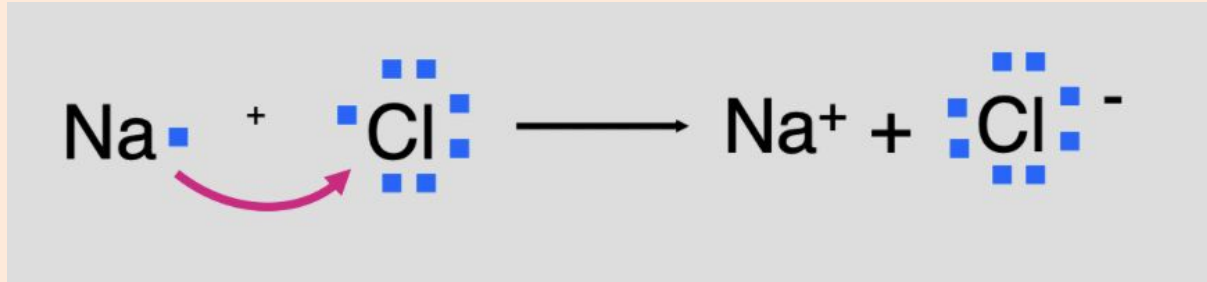






# Ionic compounds

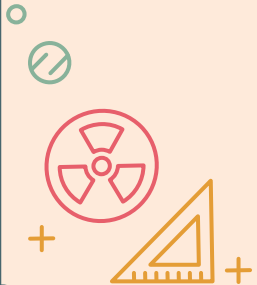
- Formed from a metallic cation and a non-metallic anion
  - ◆ E.g.,  $\text{Na} + \text{Cl} \rightarrow \text{Na}^+(\text{aq}) + \text{Cl}^-(\text{aq})$
  - ◆  $\text{NaCl} \rightarrow \text{Na}$  loses an  $e^-$  to  $\text{Cl}$
- Lewis dot structure:
  - ◆ E.g.,  $\text{NaCl}$





# Lattice energy

- Lattice energy (U) is the energy that is required for salt existing in a solid state to transition into an ionic gas
  - ◆ E.g.,  $\text{NaCl (s)} \rightarrow \text{Na}^+(\text{g}) + \text{Cl}^-(\text{g})$ 
    - $U = +786 \text{ kJ/mol}$
- Properties of ionic solids
  - ◆ High lattice energy = high melting temperature
    - Strong interactions between atoms in solid





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# Topic 6

Overview of bonding





# Bonding

## → Ionization energy

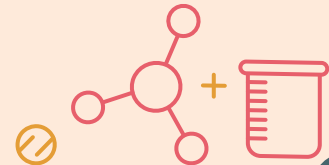
- ◆ The minimum amount of energy that is needed to remove the most weakly bonded  $e^-$  in an outer orbital
  - E.g.,  $\text{Na} \rightarrow \text{Na}^+ + e^-$

## → E- affinity

- ◆ The amount of energy that is released when a neutral molecule gains an  $e^-$  and becomes an anion
- ◆  $\text{Cl} + e^- \rightarrow \text{Cl}^-$

## → Electronegativity (x)

- ◆ Refers to the capability of an element to attract bonded  $e^-$
- ◆ Differences in electronegativity can cause unequal sharing of  $e^-$ 
  - E.g., HF (fluorine is the most electronegative atom and therefore commands the attraction of Hydrogen's  $e^-$ )





# Electronegativity



1A												3A	4A	5A	6A	7A
H												B	C	N	O	F
2.1	2A											2.0	2.5	3.0	3.5	4.0
Li	Be											Al	Si	P	S	Cl
1.0	1.5											1.5	1.8	2.1	2.2	3.0
Na	Mg	3B	4B	5B	6B	7B	8B			1B	2B					
0.9	1.2															
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.7	1.6	1.8	2.0	2.4	2.8
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5
Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
0.7	0.9	1.1	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2
Fr	Ra	Ac†														
0.7	0.9	1.1														

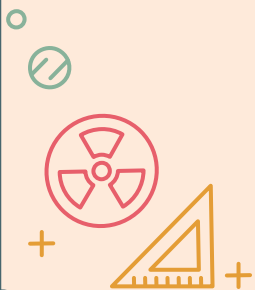
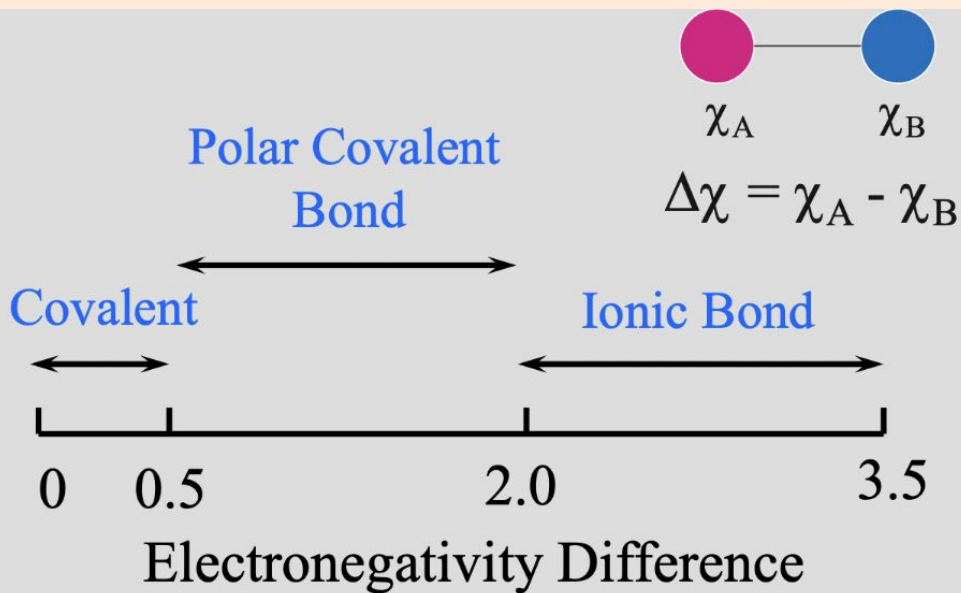
\*Lanthanides: 1.1–1.3  
†Actinides: 1.3–1.5



# Bonding

→ Electronegativity ( $\chi$ )

◆  $\Delta\chi$  determines the type of bond shared between atoms



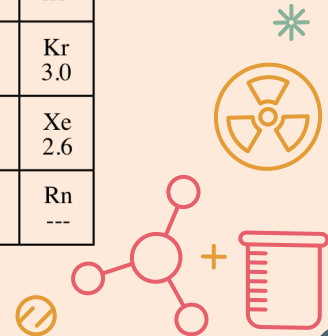
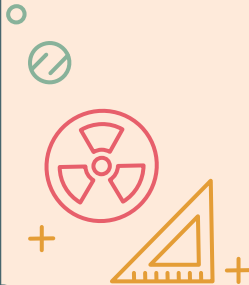


# Electronegativity

→ E.g., Determine  $\Delta X$  for the following molecules and list the type of bond :

- ◆ HCl
- ◆ NaCl
- ◆ N<sub>2</sub>

H 2.1																		He ---
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne ---	
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.2	S 2.5	Cl 3.0	Ar ---	
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr 3.0	
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe 2.6	
Cs 0.7	Ba 0.9	La-Lu 1.1-1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn ---	
Fr 0.7	Ra 0.9	Ac-No 1.1-1.7																





# Electronegativity



→ E.g., Determine  $\Delta X$  for the following molecules and list the type of bond :

◆ HCl

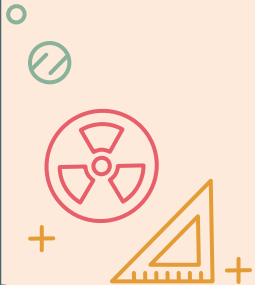
- $\Delta X = 3.0 - 2.1 = 0.9$
- Polar covalent

◆ NaCl

- $\Delta X = 3.0 - 0.9 = 2.1$
- Ionic

◆ N<sub>2</sub>

- $\Delta X = 3.0 - 3.0 = 0.0$
- Covalent



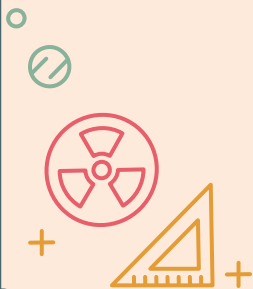




# Drawing lewis diagrams



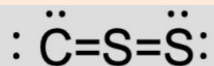
- Determine the # of valence e-
  - ◆  $\text{CCl}_4 \rightarrow (4 \times 7) + 4 = 32 \text{ e}^-$
- Write out skeletal structure
  - ◆ Least electronegative atom in the centre
- Complete octets for each terminal atom
- Assign any additional e- as lone pairs on central atom
- Make multiple bonds where necessary to complete octets



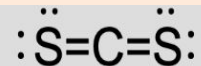


# Formal charge

- Formal charge = (# of valence e<sup>-</sup> in neutral atom) - (# assigned to lewis struct.)
  - ◆ Organization matters
- E.g.,



	C	S	S
Valence electrons	4	6	6
Electrons assigned	6	4	6
Formal Charge	-2	-2	0



	S	C	S
Valence electrons	6	4	6
Electrons assigned	6	4	6
Formal Charge	0	0	0





# VSEPR

## → VSEPR theory

### ◆ Valence Shell Electron Pair Repulsion

- E- clouds repel
- Follow guidelines of predictable geometry rules
- “Terminal atoms move as far apart as possible”

## → Building a VSEPR diagram

### ◆ Count # of e- clouds around central atom

- Bonding pairs (2 e-)
- Double bonds (4 e-)
- Triple bonds (6 e-)
- Lone pairs (2 e-)
- Lone e- (1 e-)

### ◆ Predict molecular shape (e.g., linear, tetrahedral, trigonal planar, etc)




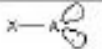






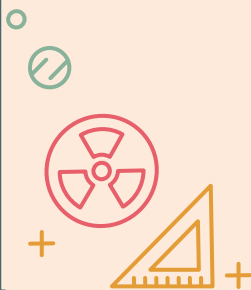


# VSEPR Theory (Molecular Shapes)

A = the central atom, X = an atom bonded to A, E = a lone pair on A

Note: There are lone pairs on X or other atoms, but we don't care. We are interested in only the electron densities or domains around atom A.

Total Domains	Generic Formula	Picture	Bonded Atoms	Lone Pairs	Molecular Shape	Electron Geometry	Example	Hybridization	Bond Angles
1	AX	A—X	1	0	Linear	Linear	H <sub>2</sub>	s	180
2	AX <sub>2</sub>	X—A—X	2	0	Linear	Linear	CO <sub>2</sub>	sp	180
	AXE	 A—X	1	1	Linear	Linear	CN		
3	AX <sub>3</sub>		3	0	Trigonal planar	Trigonal planar	AlBr <sub>3</sub>	sp <sup>2</sup>	120
	AX <sub>2</sub> E		2	1	Bent	Trigonal planar	SnCl <sub>2</sub>		
	AXE <sub>2</sub>		1	2	Linear	Trigonal planar	O <sub>3</sub>		
4	AX <sub>4</sub>		4	0	Tetrahedral	Tetrahedral	SiCl <sub>4</sub>	sp <sup>3</sup>	109.5
	AX <sub>3</sub> E		3	1	Trigonal pyramid	Tetrahedral	PH <sub>3</sub>		
	AX <sub>2</sub> E <sub>2</sub>		2	2	Bent	Tetrahedral	SeBr <sub>2</sub>		
	AXE <sub>3</sub>		1	3	Linear	Tetrahedral	Cl <sub>2</sub>		

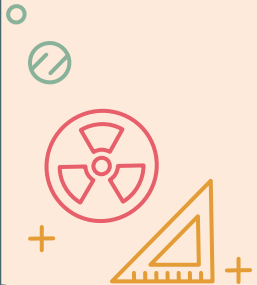




# VSEPR



→ E.g., What is the molecular shape of CH<sub>4</sub> (including bond angles)?



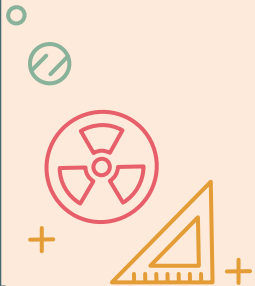
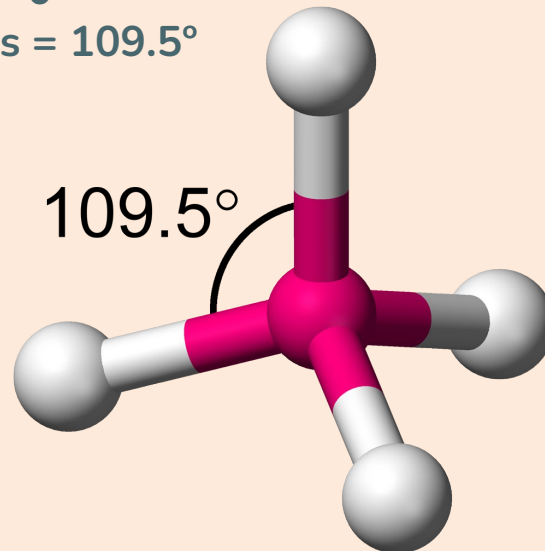


# VSEPR

→ E.g., What is the molecular shape of CH<sub>4</sub> (including bond angles)?

◆ Molecular shape = tetrahedral

- Bonded atoms = 4
- Lone pairs = 0
- Bond angles = 109.5°





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# Topic 7

Theories of chemical bonding





# Dipole moment



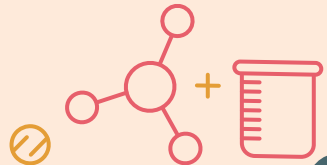
- What is a dipole moment?
  - ◆ Net polarity of a molecule that results from polar bonds
  - ◆ A larger  $\Delta X$  value = larger the dipole
  - ◆ Molecular shape +  $\Delta X$  = polarity
  - ◆ Measured in units of debye
- E.g., N<sub>2</sub>
  - ◆  $\Delta X = 3.0 - 3.0 = 0$
  - ◆ Therefore  $\mu = 0$  and there is not a dipole moment



+



+







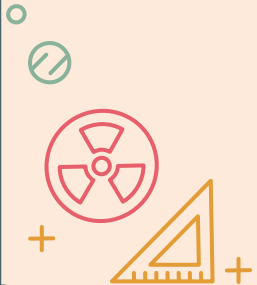
# Dipole moment



→ E.g., Calculate  $\Delta X$  for the following molecules and determine if there is a dipole moment:

◆ SO<sub>2</sub>

◆ CH<sub>4</sub>





# Dipole moment

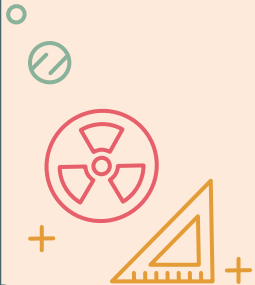
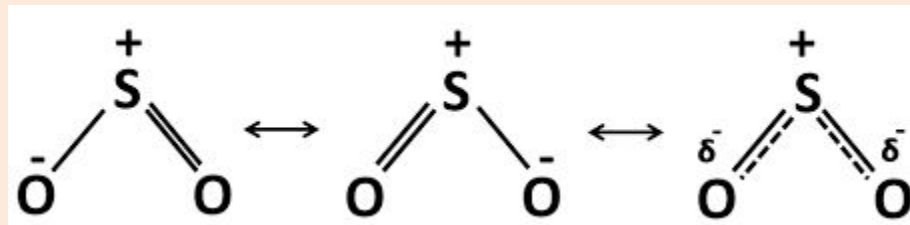


→ E.g., Calculate  $\Delta X$  for the following molecules and determine if there is a dipole moment

◆ SO<sub>2</sub>

- Bent molecular shape
- $X(S) = 2.5$  &  $X(O) = 3.5 \rightarrow \Delta X = 4.5$



◆ Molecular shape and  $\Delta X$  indicate that there is a dipole moment





# Thanks!

Please email me if you need anything!



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