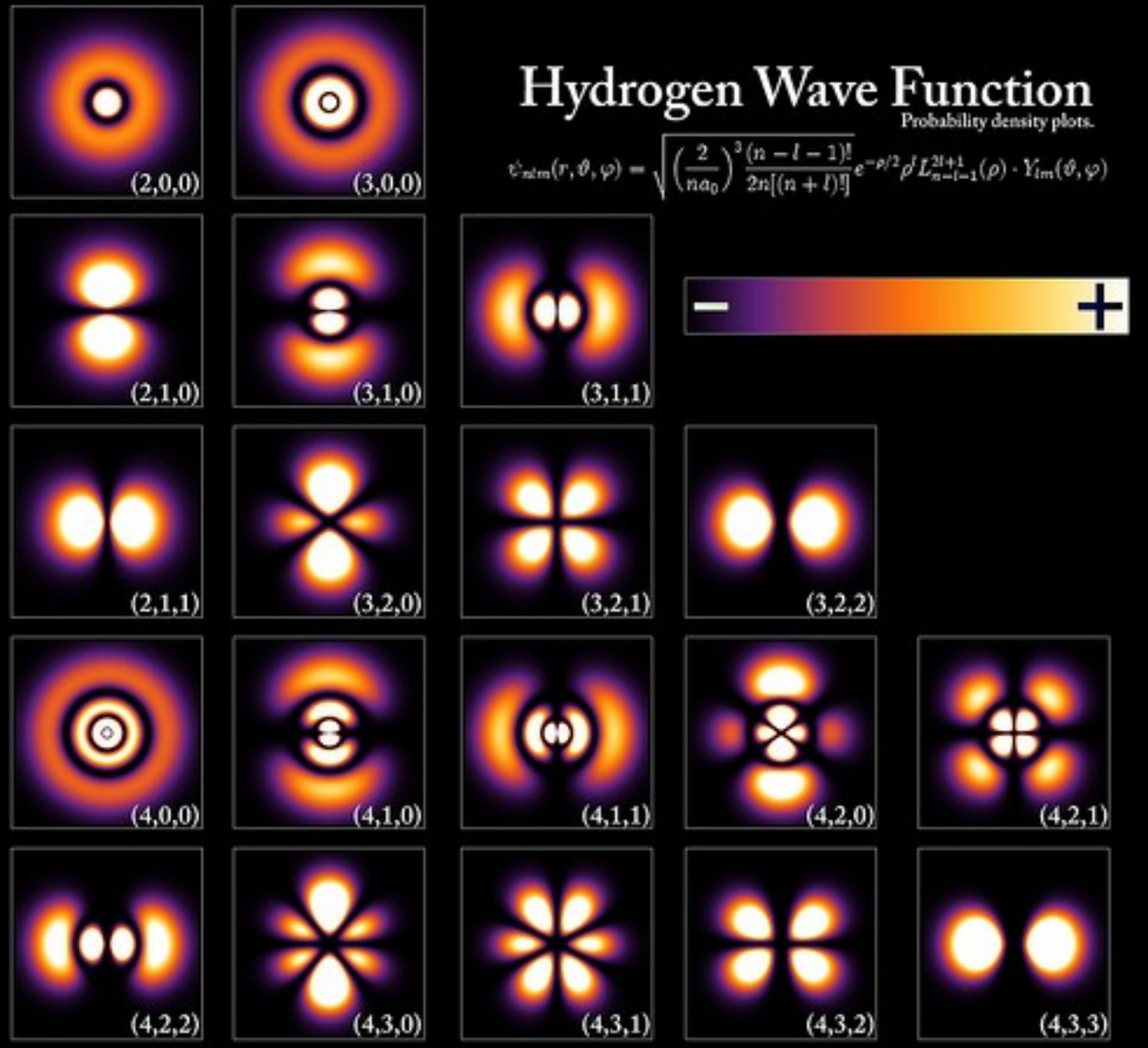
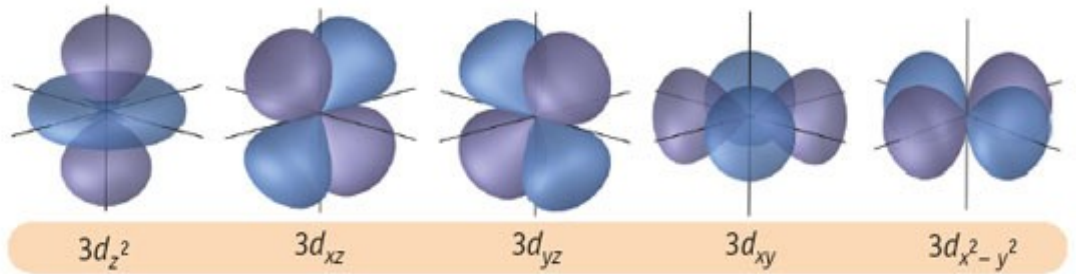
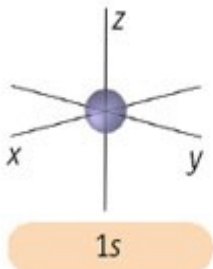
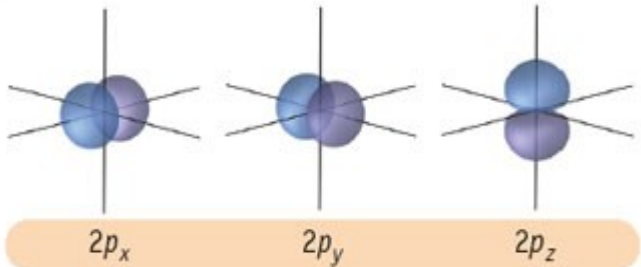
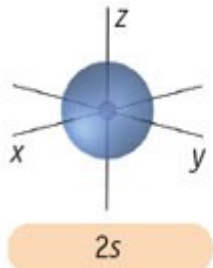
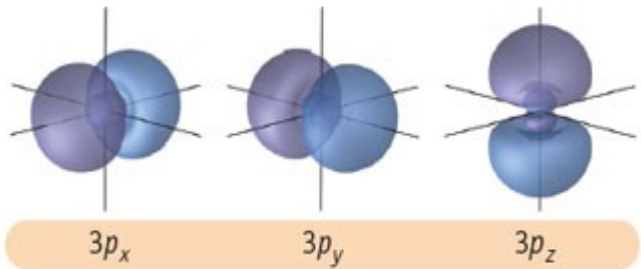
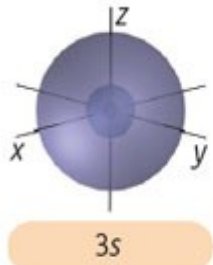


# Hydrogen Wave Function

Probability density plots.

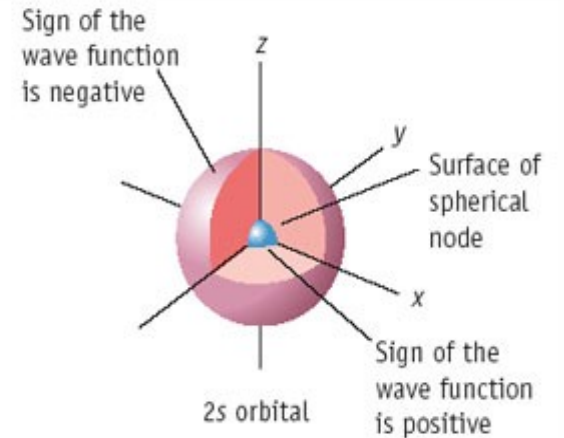
$$\psi_{nlm}(r, \theta, \varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}} e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) \cdot Y_{lm}(\theta, \varphi)$$

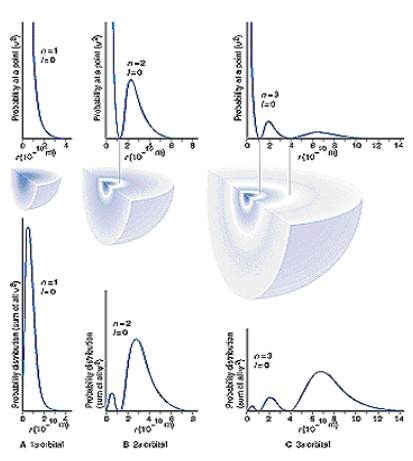
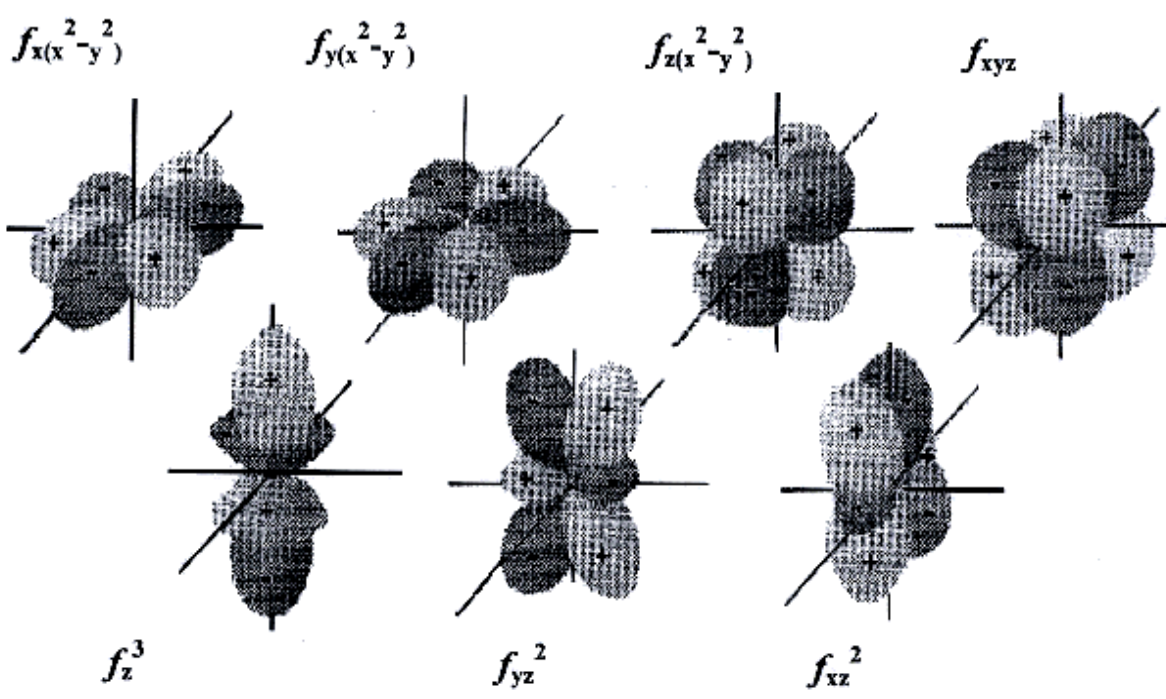
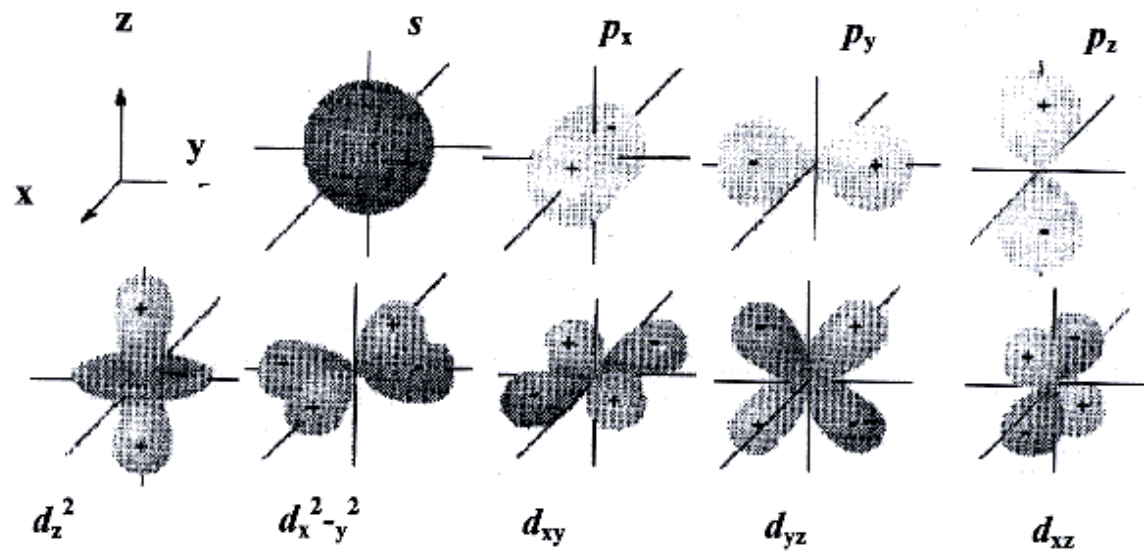




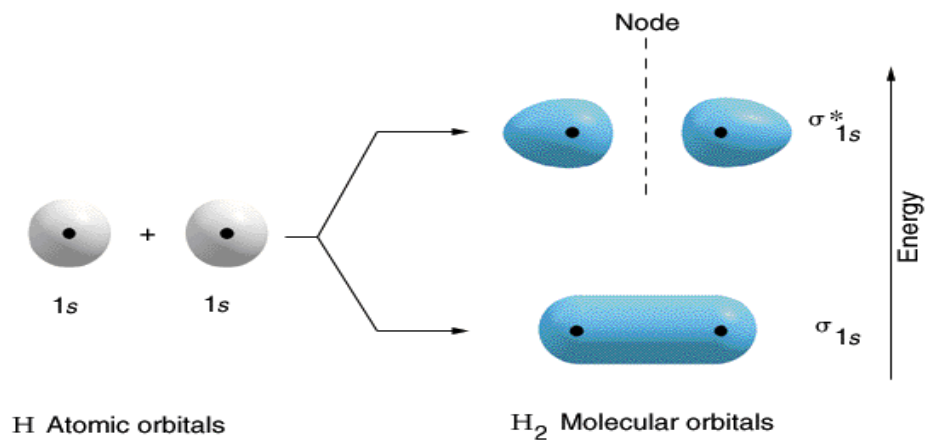
### Spherical Nodes

The drawings of the 2s and 3s orbitals show that they consist of nested spheres because these orbitals (as well as *p* orbitals with  $n > 2$  and *d* orbitals with  $n > 3$ ) have spherical nodes. For a 2s orbital the wave function has a positive value close to the nucleus, but it has a negative value at greater distances. That is, the wave function has a zero value, a node, at this point. The node occurs at the same distance from the nucleus regardless of direction so the node occurs on a spherical surface. The number of spherical nodes for any orbital is  $n - \ell - 1$ .

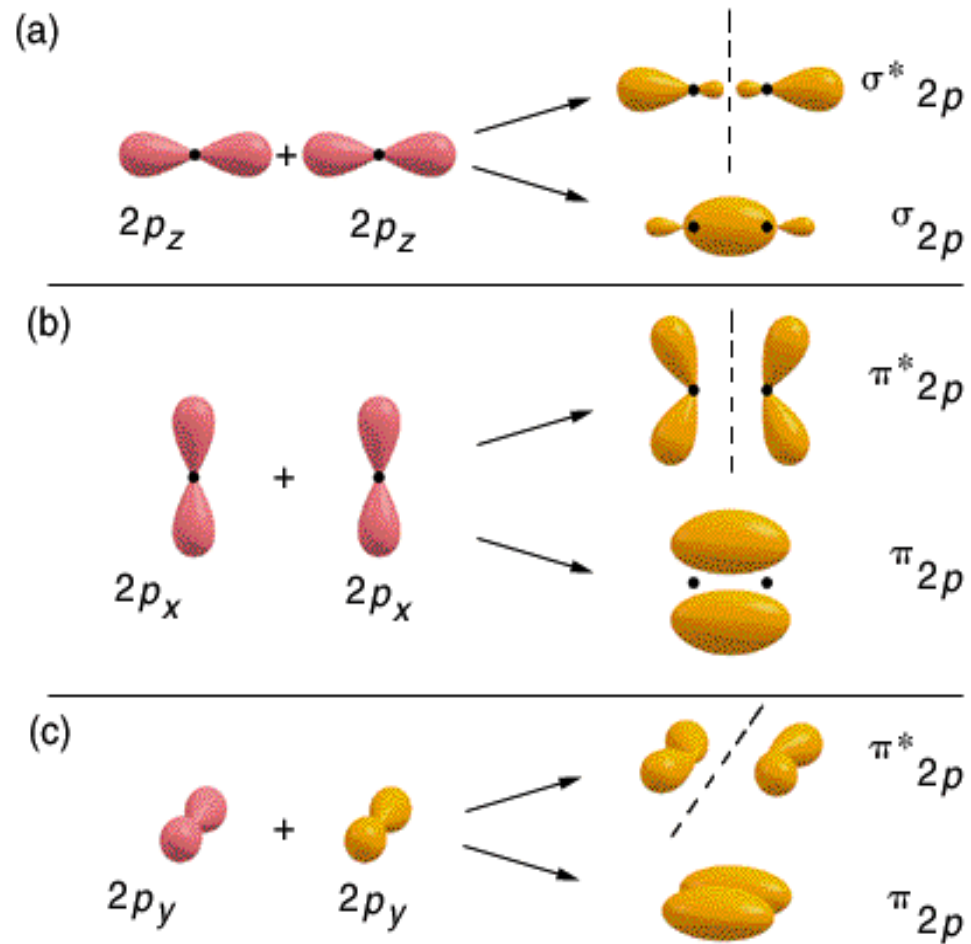




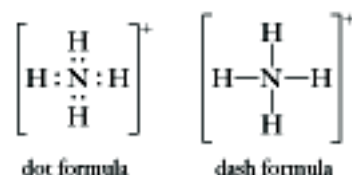
# Molekulové orbitály



# Molekulové orbitály

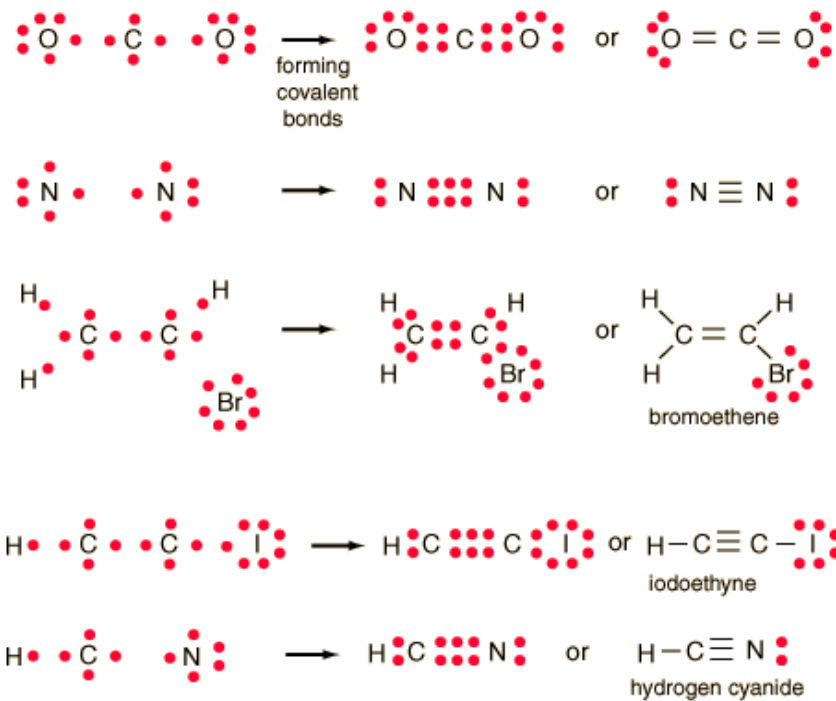
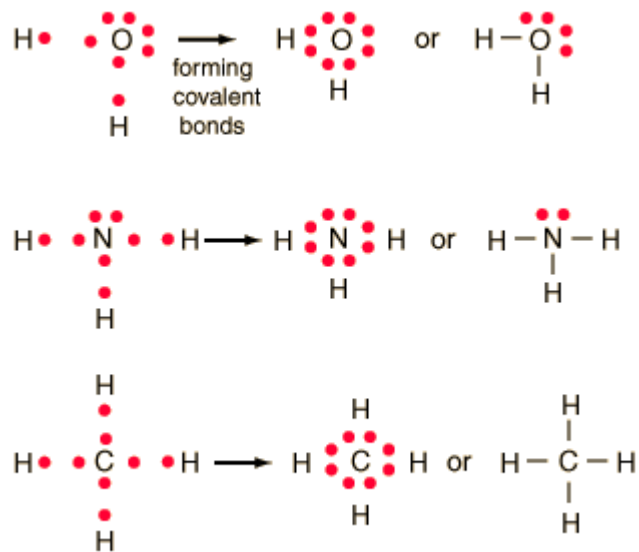
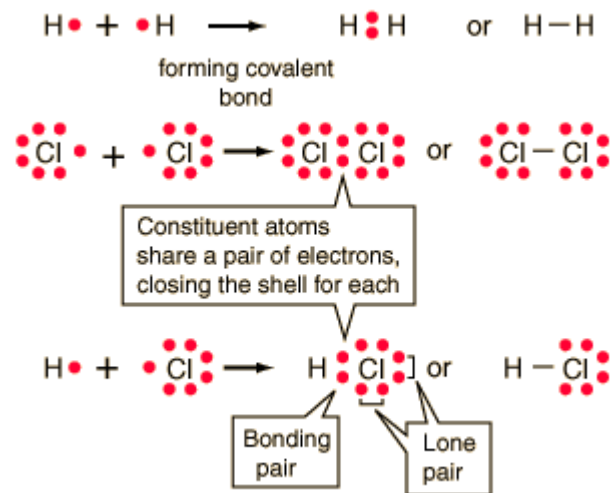
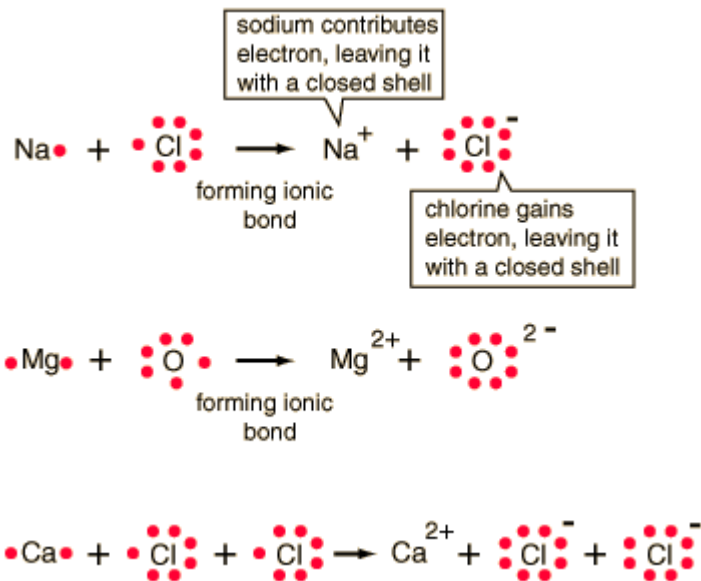


# Lewisový struktury



**TABLE 7-1** *Lewis Dot Formulas for Representative Elements*

Group	IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA
<i>Number of electrons in valence shell</i>	1	2	3	4	5	6	7	8 (except He)
Period 1	H ·							He :
Period 2	Li ·	Be :	·B·	·C·	·N·	·O:	·F:	:Ne:
Period 3	Na ·	Mg :	·Al·	·Si·	·P·	·S:	·Cl:	:Ar:
Period 4	K ·	Ca :	·Ga·	·Ge·	·As·	·Se:	·Br:	:Kr:
Period 5	Rb ·	Sr :	·In·	·Sn·	·Sb·	·Te:	·I:	:Xe:
Period 6	Cs ·	Ba :	·Tl·	·Pb·	·Bi·	·Po:	·At:	:Rn:
Period 7	Fr ·	Ra :						



# Oktetové pravidlo

Ve většině sloučenin zauímají prvky stabilní konfiguraci vzácného plynu. Týká se pouze prvků 2. a 3. periody.



# Formální náboj

$$FC = (\text{č. skupiny}) - [(\text{počet vazeb}) - (\text{počet nevazeb. el})]$$



For Cl,  $FC = 7 - (2 + 4) = +1$

For N,  $FC = 5 - (3 + 2) = 0$

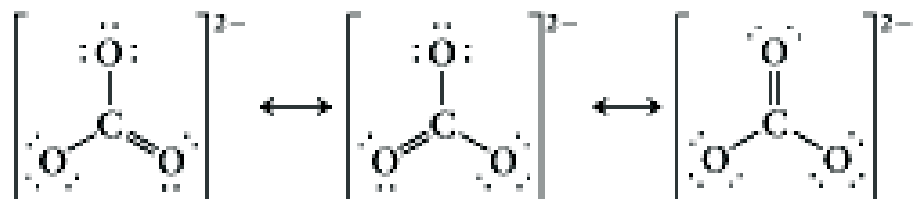
For O,  $FC = 6 - (1 + 6) = -1$



For Cl,  $FC = 7 - (1 + 6) = 0$

For N,  $FC = 5 - (3 + 2) = 0$

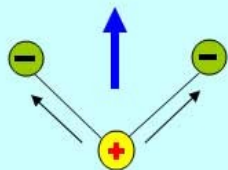
For O,  $FC = 6 - (2 + 4) = 0$



# VSEPR

Bond angles	Spatial geometry	Electron pair geometry	Lone pair substitutions			
180°	 Linear	 ( <i>sp</i> )	...			
120°	 Trigonal planar	 ( <i>sp</i> <sup>2</sup> )	 Bent			
109.5°	 Tetrahedral	 ( <i>sp</i> <sup>3</sup> )	 Trigonal pyramidal	 Bent		
90°, 120°	 Trigonal bipyramidal	 ( <i>dsp</i> <sup>3</sup> )	 "Sawhorse"	 T-shaped	 Linear	
90°	 Octahedral	 ( <i>d</i> <sup>2</sup> <i>sp</i> <sup>3</sup> )	 Square pyramidal	 Square planar	 T-shaped	 Linear

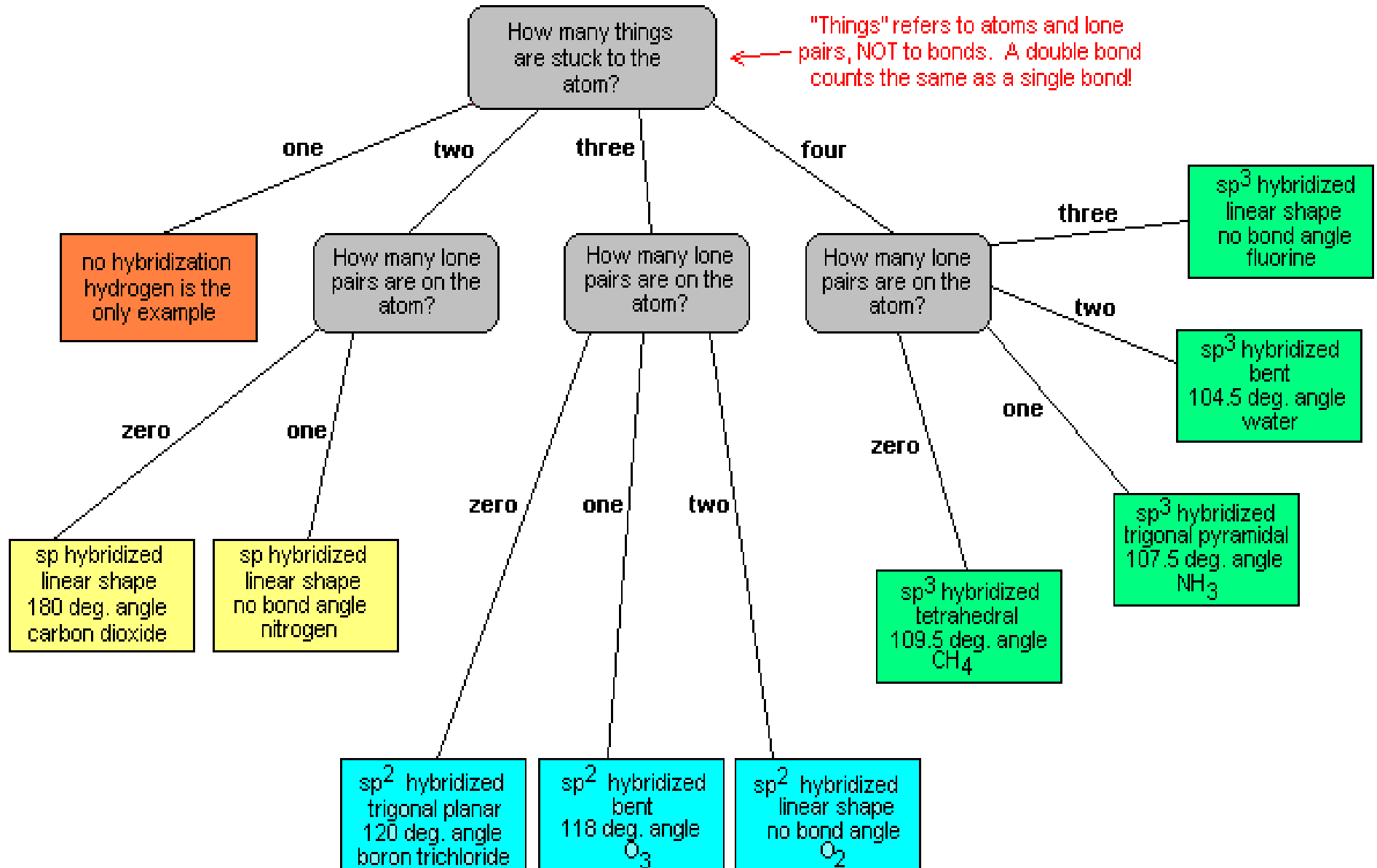
Black Arrows = Dipoles  
Blue Arrow = Generated Dipole Moment



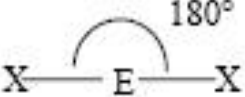
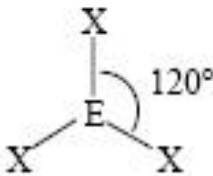
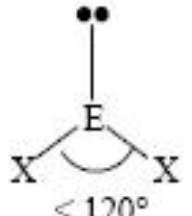
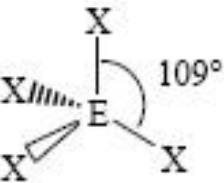
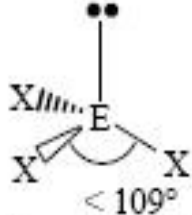

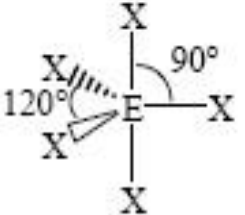
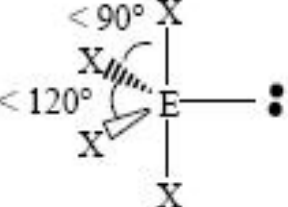
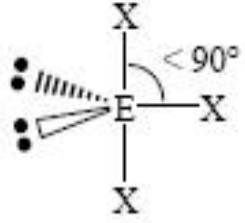
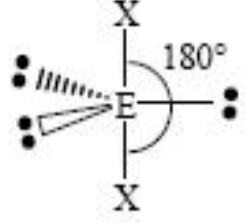
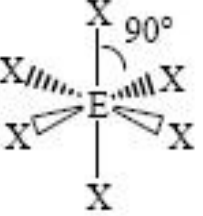
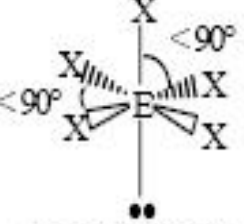
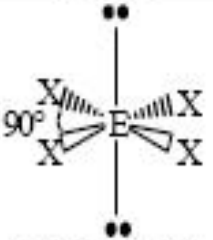
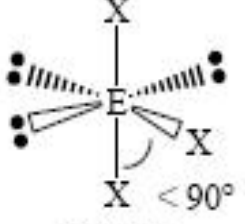
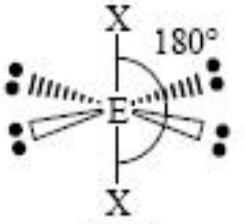
Black Arrows = Dipoles  
Dipoles Cancel Each Other Out  
Dipole Moment = Zero



# VSEPR



## VSEPR Geometries

Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 <p style="text-align: center;">Linear</p>				
3	 <p style="text-align: center;">Trigonal Planar</p>	 <p style="text-align: center;">Bent or Angular</p>			
4	 <p style="text-align: center;">Tetrahedral</p>	 <p style="text-align: center;">Trigonal Pyramid</p>	 <p style="text-align: center;">Bent or Angular</p>		
5	 <p style="text-align: center;">Trigonal Bipyramid</p>	 <p style="text-align: center;">Sawhorse or Seesaw</p>	 <p style="text-align: center;">T-shape</p>	 <p style="text-align: center;">Linear</p>	
6	 <p style="text-align: center;">Octahedral</p>	 <p style="text-align: center;">Square Pyramid</p>	 <p style="text-align: center;">Square Planar</p>	 <p style="text-align: center;">T-shape</p>	 <p style="text-align: center;">Linear</p>

# Hybridizace

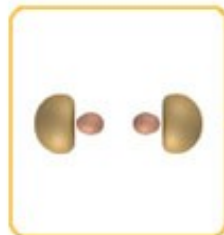
**TABLE 8-2** *Relation Between Electronic Geometries and Hybridization*

Regions of High Electron Density	Electronic Geometry	Atomic Orbitals Mixed from Valence Shell of Central Atom	Hybridization
2	linear	one <i>s</i> , one <i>p</i>	$sp$
3	trigonal planar	one <i>s</i> , two <i>p</i> 's	$sp^2$
4	tetrahedral	one <i>s</i> , three <i>p</i> 's	$sp^3$
5	trigonal bipyramidal	one <i>s</i> , three <i>p</i> 's, one <i>d</i>	$sp^3d$
6	octahedral	one <i>s</i> , three <i>p</i> 's, two <i>d</i> 's	$sp^3d^2$

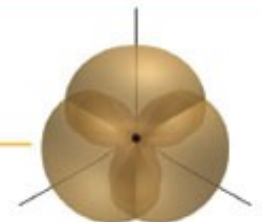
## Arrangement of Hybrid Orbitals

## Geometric figure

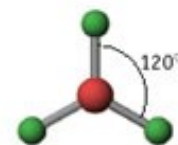
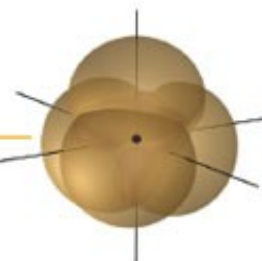
## Example

Two electron pairs  
 $sp$ 

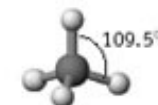
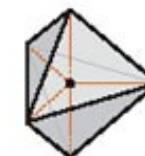
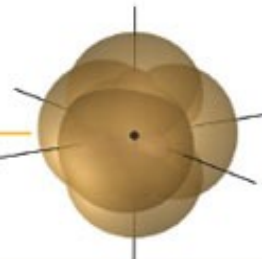
Linear

 $\text{BeCl}_2$ Three electron pairs  
 $sp^2$ 

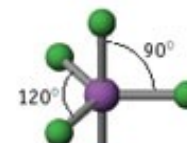
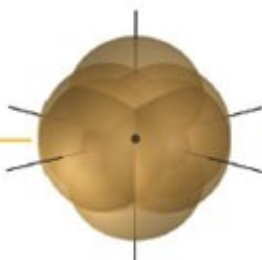
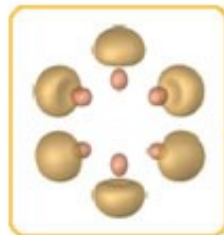
Trigonal-planar

 $\text{BF}_3$ Four electron pairs  
 $sp^3$ 

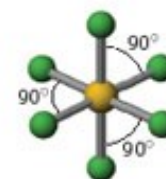
Tetrahedral

 $\text{CH}_4$ Five electron pairs  
 $sp^3d$ 

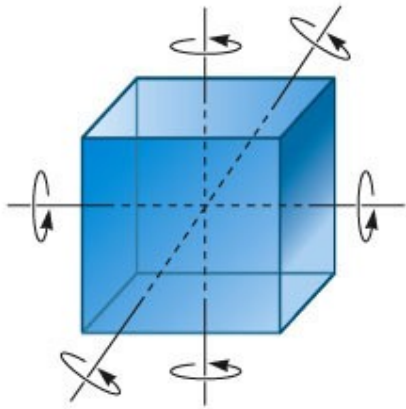
Trigonal-bipyramidal

 $\text{PF}_5$ Six electron pairs  
 $sp^3d^2$ 

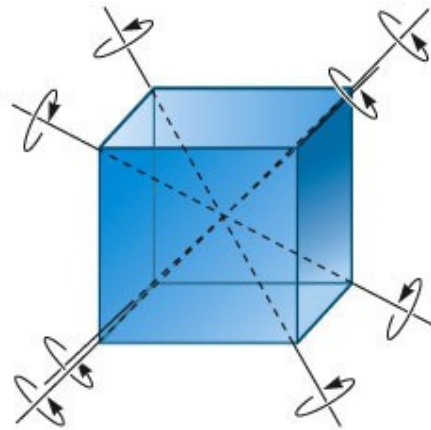
Octahedral

 $\text{SF}_6$

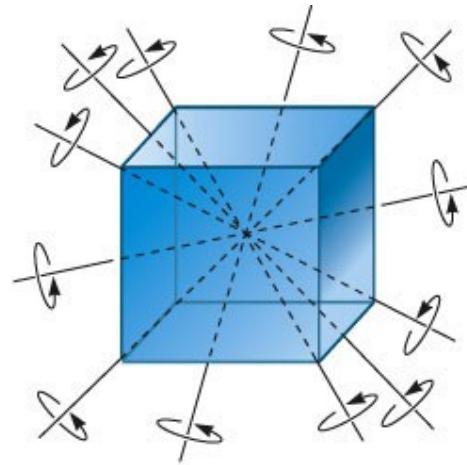
# Symetrie



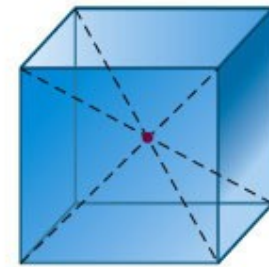
Three 4-fold axes



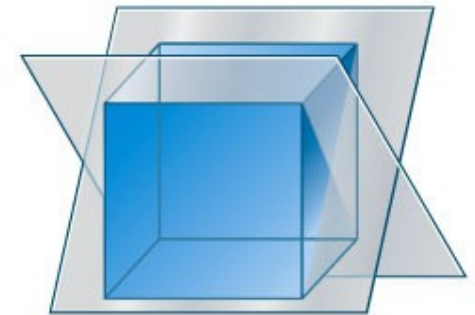
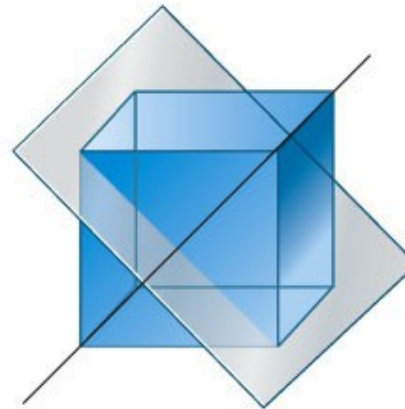
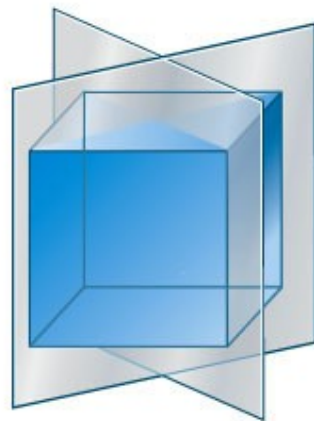
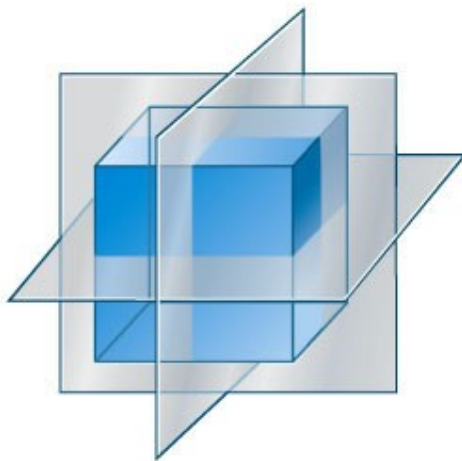
Four 3-fold axes



Six 2-fold axes

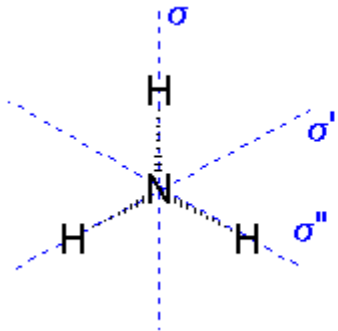


Center of inversion

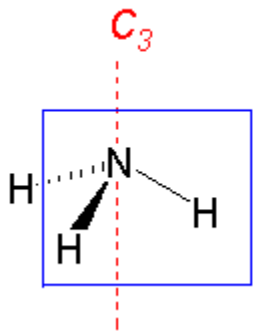


Nine mirror planes

# Symetrie



Top view, there is a plane of symmetry along each NH bond as shown by the blue broken lines



Side view, showing the  $C_3$  axis (broken red line) and one of the three planes of symmetry (blue box)

