Lecture General Chemistry
Winter Term 2024/25

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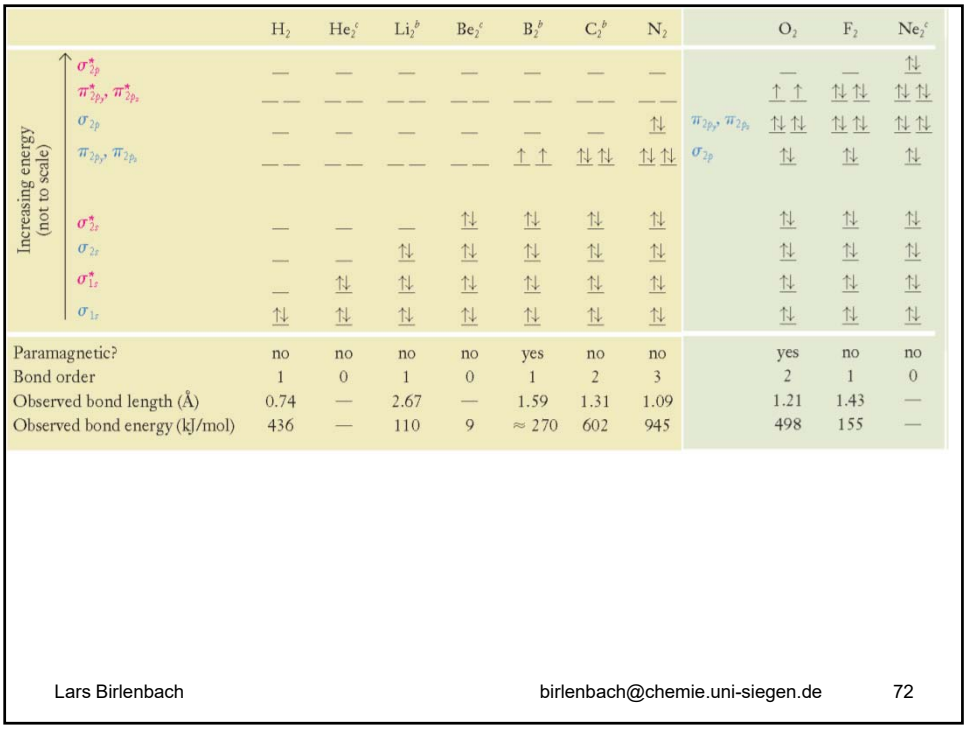
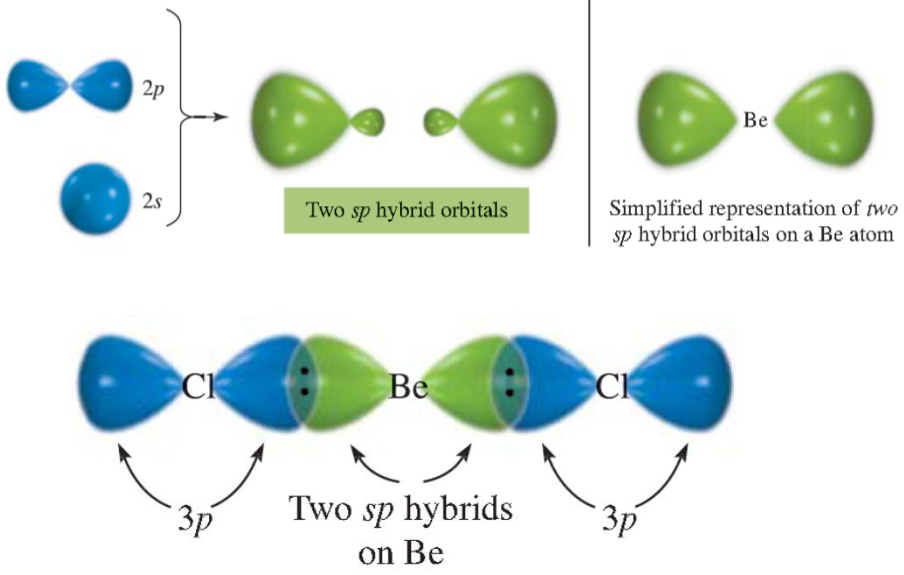
- Website (Slides, Excercises):
- http://www.chemie.uni-siegen.de/pc/lehre/nanoscitec/

Login Data for slides:
User: Ludwig
Password: Boltzmann



	H_2	He_2^c	Li_2^b	Be_2^c	B_2^b	C_2^b	N_2	O_2	F_2	Ne_2^c
Paramagnetic?	no	no	no	no	yes	no	no	yes	no	no
Bond order	1	0	1	0	1	2	3	2	1	0
Observed bond length (Å)	0.74	—	2.67	—	1.59	1.31	1.09	1.21	1.43	—
Observed bond energy (kJ/mol)	436	—	110	9	≈ 270	602	945	498	155	—



Mathematical modeling of hybrid orbitals

$$\psi_{sp} = \frac{1}{\sqrt{2}}(2s \pm 2p_z)$$

aus: McQuarrie, Simon: Physical Chemistry. University Science Books

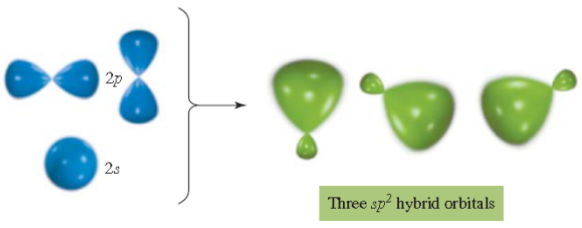
$$\psi_1 = \frac{1}{\sqrt{3}}2s + \sqrt{\frac{2}{3}}2p_z$$

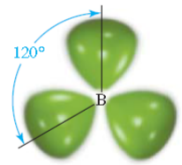
$$\psi_2 = \frac{1}{\sqrt{3}}2s - \frac{1}{\sqrt{6}}2p_z + \frac{1}{\sqrt{2}}2p_x$$

$$\psi_3 = \frac{1}{\sqrt{3}}2s - \frac{1}{\sqrt{6}}2p_z - \frac{1}{\sqrt{2}}2p_x$$

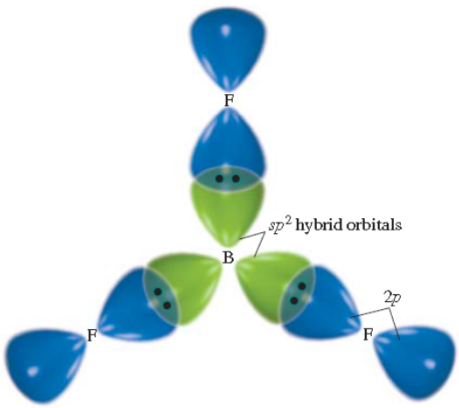
aus: McQuarrie, Simon: Physical Chemistry. University Science Books

Three sp^2 hybrid orbitals point toward the corners of an equilateral triangle:





Simplified representation of *three* sp^2 hybrid orbitals on a B atom



$$\psi_1 = \frac{1}{2}(2s + 2p_x + 2p_y + 2p_z)$$

$$\psi_2 = \frac{1}{2}(2s - 2p_x - 2p_y + 2p_z)$$

$$\psi_3 = \frac{1}{2}(2s + 2p_x - 2p_y - 2p_z)$$

$$\psi_4 = \frac{1}{2}(2s - 2p_x + 2p_y - 2p_z)$$

aus: McQuarrie, Simon: Physical Chemistry. University Science Books

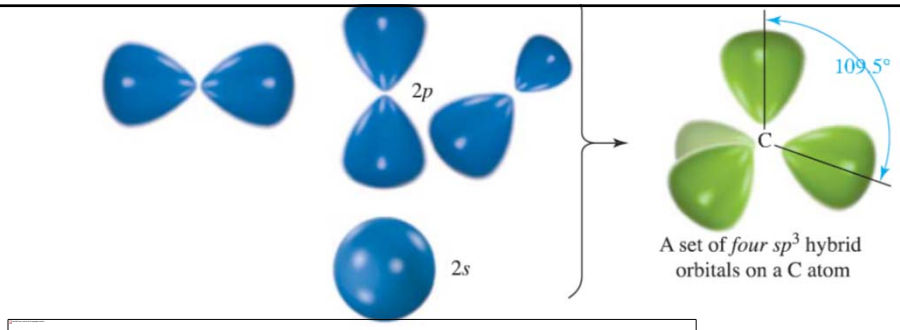


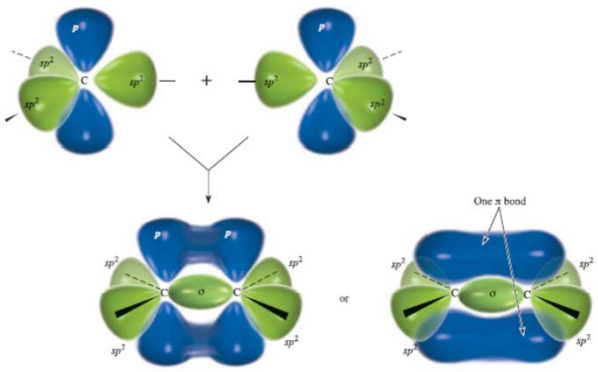
TABLE 6.5

The complete hydrogenlike atomic wave functions for $n = 1$, 2, and 3. The quantity Z is the atomic number of the nucleus, and $\sigma = Zr/a_0$, where a_0 is the Bohr radius.

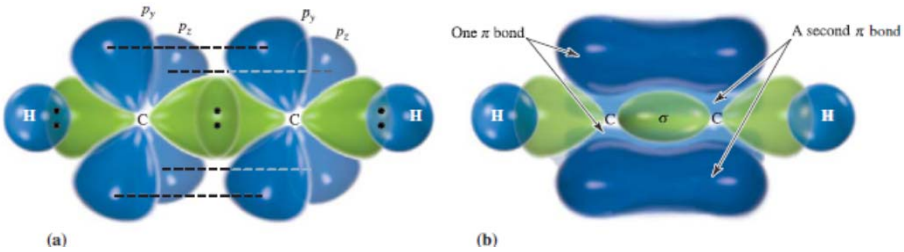
$n = 1,$	$l = 0,$	$m = 0$	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$
$n = 2,$	$l = 0,$	$m = 0$	$\psi_{200} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma)e^{-\sigma/2}$
	$l = 1,$	$m = 0$	$\psi_{210} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\cos\theta$
	$l = 1,$	$m = \pm 1$	$\psi_{21\pm1} = \frac{1}{\sqrt{64\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\sin\theta e^{\pm i\phi}$
$n = 3,$	$l = 0,$	$m = 0$	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (27-18\sigma+2\sigma^2)e^{-\sigma/3}$
	$l = 1,$	$m = 0$	$\psi_{310} = \frac{1}{81}\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\cos\theta$
	$l = 1,$	$m = \pm 1$	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\sin\theta e^{\pm i\phi}$
	$l = 2,$	$m = 0$	$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}(3\cos^2\theta - 1)$
	$l = 2,$	$m = \pm 1$	$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\sin\theta\cos\theta e^{\pm i\phi}$
	$l = 2,$	$m = \pm 2$	$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\sin^2\theta e^{\pm 2i\phi}$

aus: McQuarrie, Simon: Physical Chemistry. University Science Books

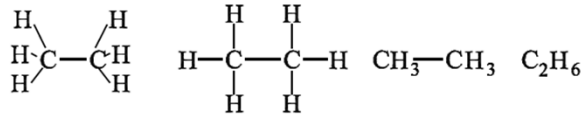
Double bonds

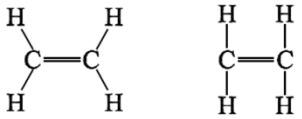


Triple bonds



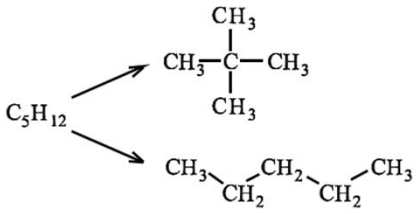
Structural and total formulas

Ethan  $CH_3—CH_3$ C_2H_6

Ethen  $CH_2=CH_2$ C_2H_4

structural formula total formula

Structural and total formulas

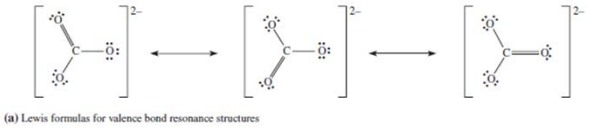


2.2-Dimethyl-propan
(Tetramethyl-methan, Neopentan)

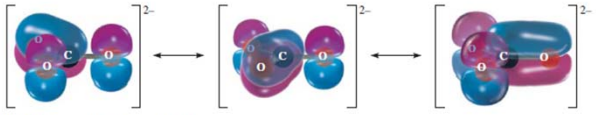
n-Pentan

total formula structural formula

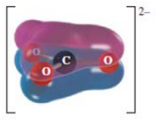
Delocalized bonds: mesomerism



(a) Lewis formulas for valence bond resonance structures



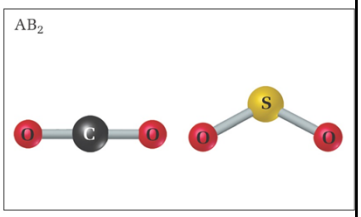
(b) *p*-Orbital overlap in valence bond resonance

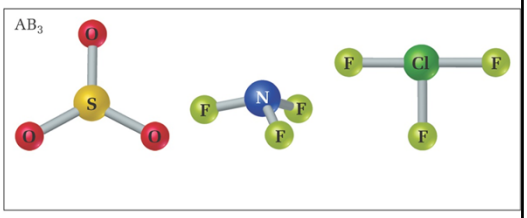


(c) Delocalized MO representation

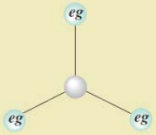
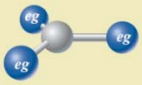
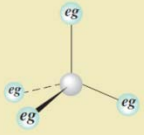
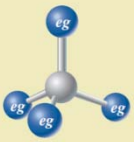
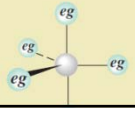
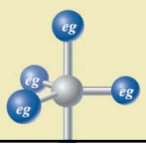
Bonding form and molecular geometry

- Diatomic molecules: always linear
- Three-atom molecules: linear or angled
- More atoms: more complicated shapes





VSEPR-Model

Electron Groups on Central Atom	Electronic Geometry* Orientation of Electron Groups	Description; Angles†	Line Drawing‡	Ball and Stick Model
2		linear; 180°		
3		trigonal planar; 120°		
4		tetrahedral; 109.5°		
5		trigonal bipyramidal; 90°, 120°, 180°		

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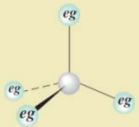
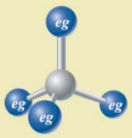
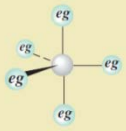
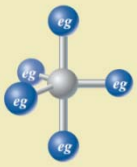
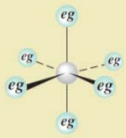
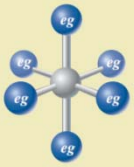
		120°	
4		tetrahedral; 109.5°	 
5		trigonal bipyramidal; 90°, 120°, 180°	 
6		octahedral; 90°, 180°	 

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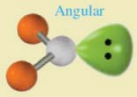
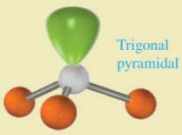
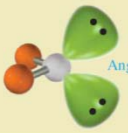
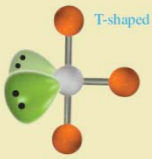
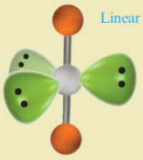
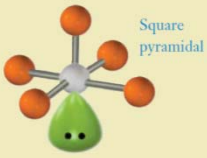
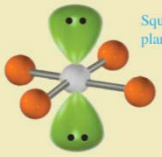
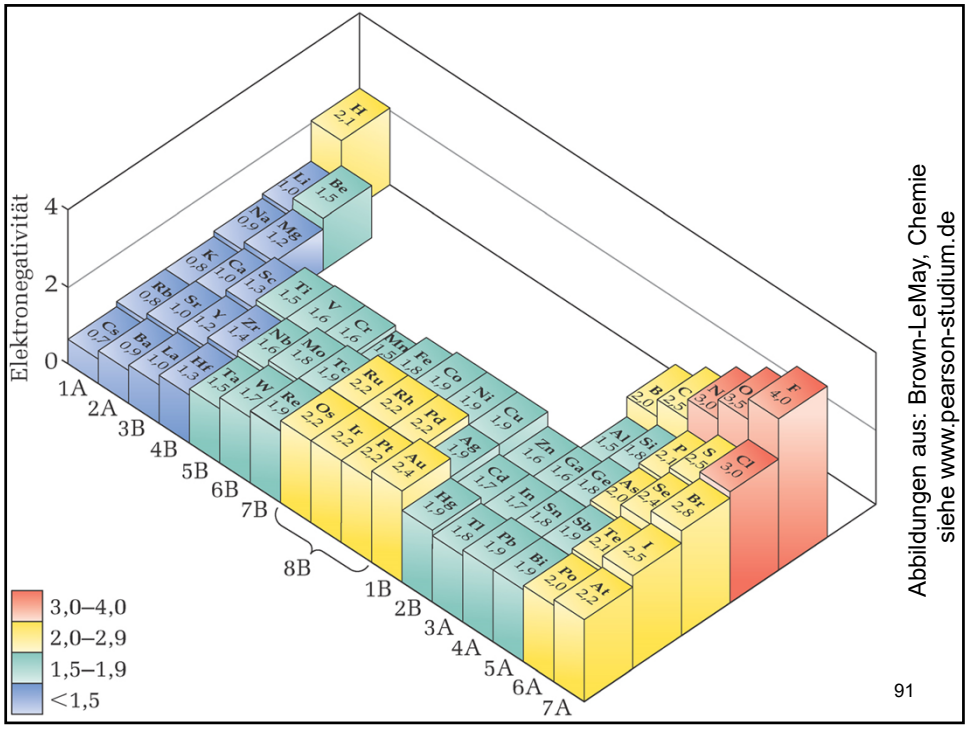
General Formula	Electron Groups[a]	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_2U	3	trigonal planar	sp^2	1		O_3, NO_2^-, SO_2
AB_3U	4	tetrahedral	sp^3	1		NH_3, SO_3^{2-}
AB_2U_2	4	tetrahedral	sp^3	2		H_2O, NH_2^-

General Formula	Electron Groups[a]	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_4U	5	trigonal bipyramidal	sp^3d	1		SF_4
AB_3U_2	5	trigonal bipyramidal	sp^3d	2		ICl_3, ClF_3
AB_2U_3	5	trigonal bipyramidal	sp^3d	3		XeF_2, I_3^-

General Formula	Electron Groups[a]	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_5U	6	octahedral	sp^3d^2	1		IF_5, BrF_5
AB_4U_2	6	octahedral	sp^3d^2	2		XeF_4, IF_4^-



Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

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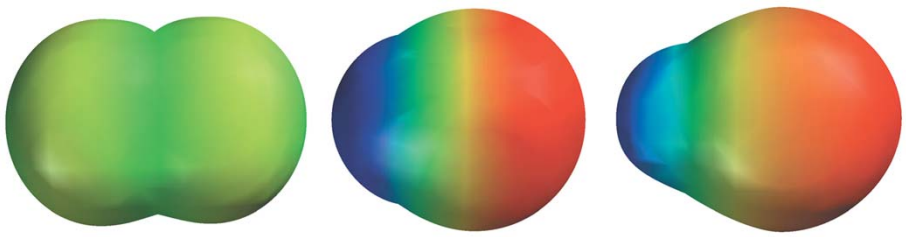
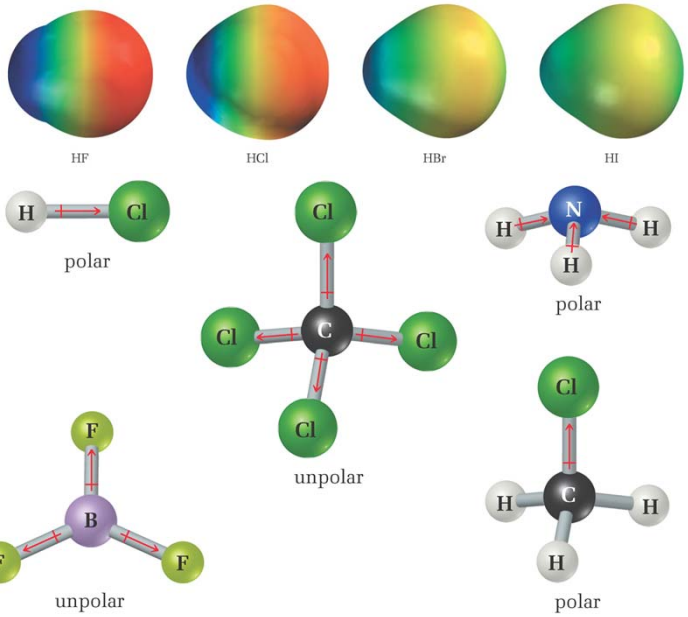
Distribution of electronic density:
Dipol moments

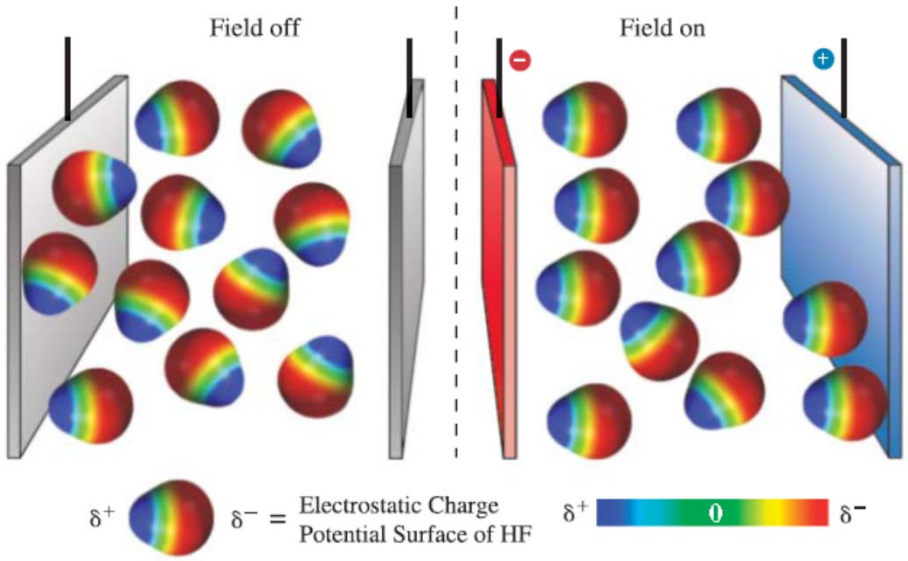


F_2 HF LiF

- Low electronic density: blue
- high electronic density: red
- average electronic density: green



Orientation of dipoles in electrical fields



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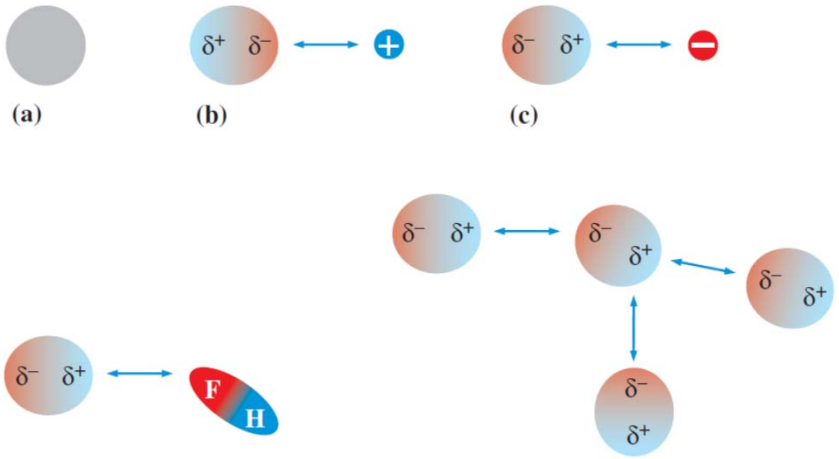
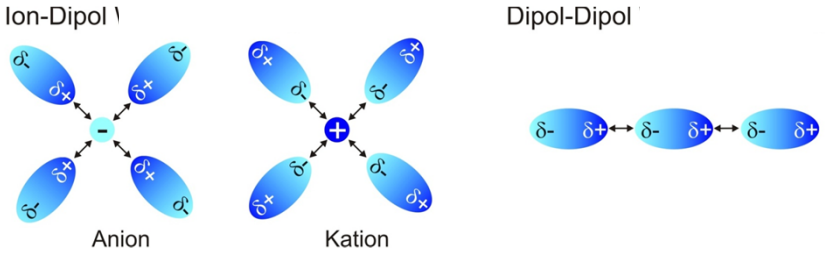
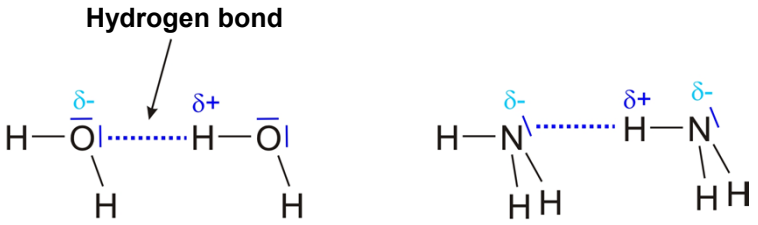
Induced dipol moments



Intermolecular forces



Hydrogen bonds



Possible partners: N,O,F,Cl