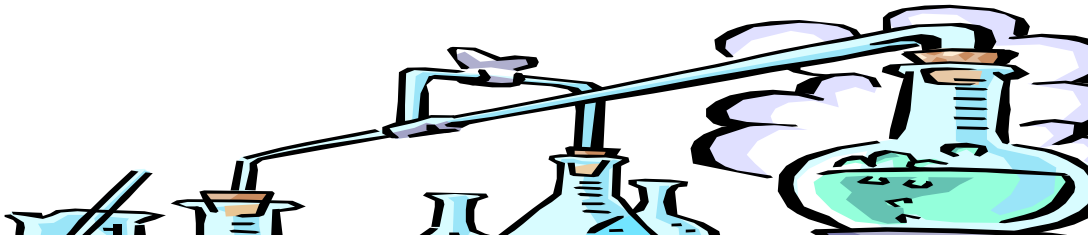
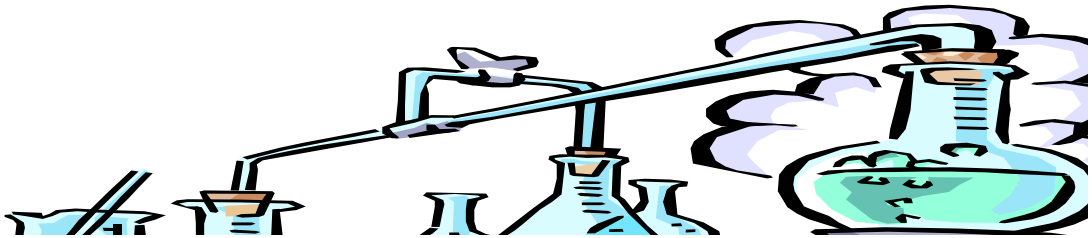
Atom- och molekylorbitaler

När två blir en...

Chang, kapitel 9.1, 9.4, 10.1, 10.3 – 10.7



Lite repetition

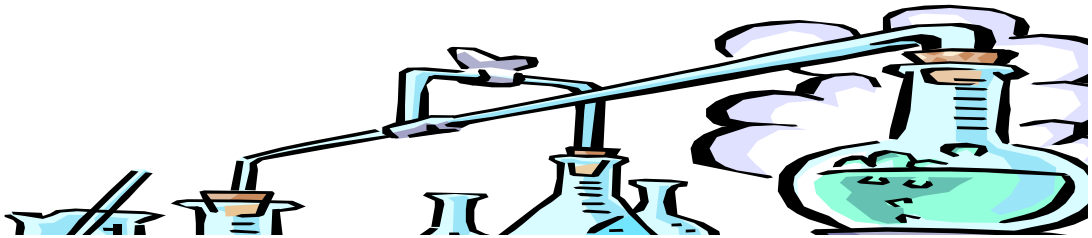


Orbitalteori / Bohrs atommodell

- **Bohrs atommodell:**

K	**2 e^-**	**1s**
L	**8 e^-**	**2s, $2p_x$, $2p_y$, $2p_z$**
M	**18 e^-**	**3s, $3p_x$, $3p_y$, $3p_z$, $3d_{xy}$, $3d_{yz}$, $3d_{xz}$, $3d_{x^2-y^2}$, $3d_{z^2}$**

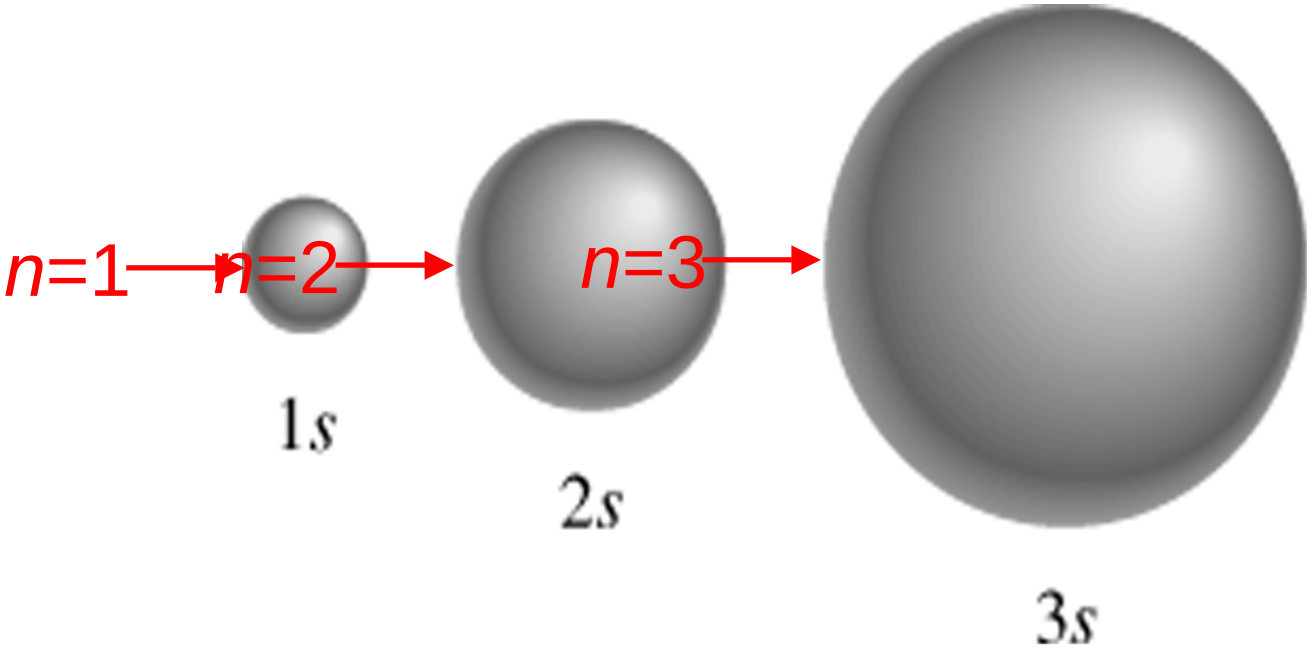
⇨ **2 elektroner i varje orbital!**

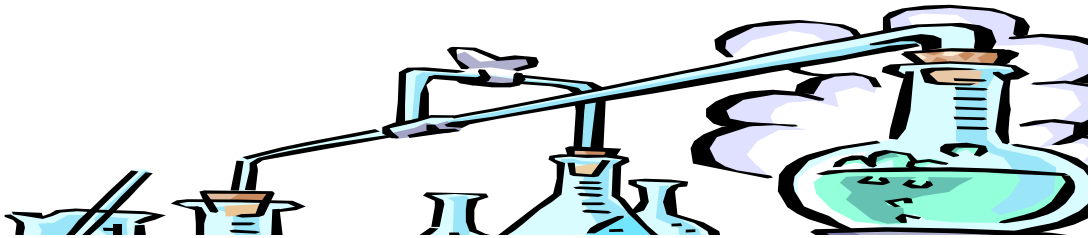


Samband mellan kvanttalen

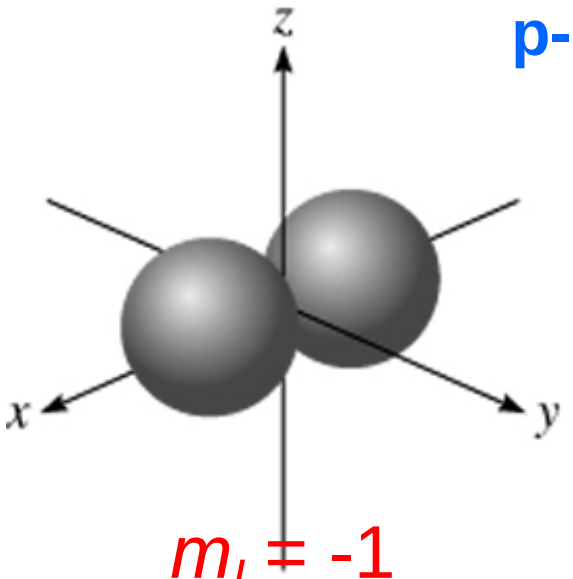
n	l	m_l	orbital
1	0	0	1s
2	0	0	2s
	1	-1, 0, +1	$2p_x$, $2p_y$, $2p_z$
3	0	0	3s
	1	-1, 0, +1	$3p_x$,$3p_y$, $3p_z$
	2	-2, -1, 0, +1, +2	$3d_{xy}$, $3d_{yz}$, $3d_{xz}$,$3d_{x^2-y^2}$, $3d_{z^2}$
4	0	0	4s
	1		
	2	och så vidare...	
	3		

Huvudkvanttalet, *n*



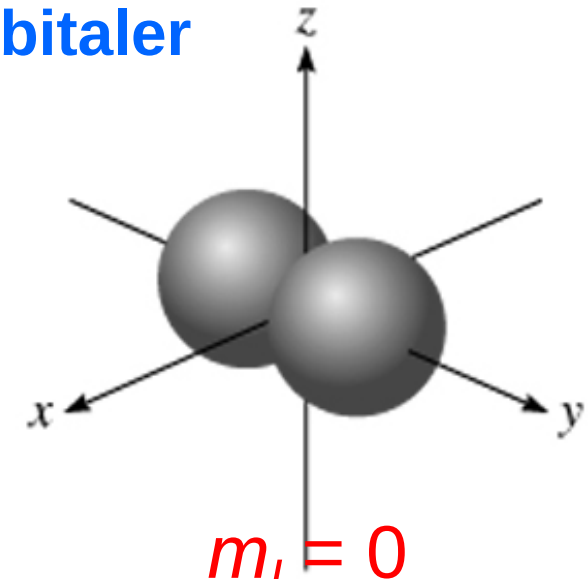


p-orbitaler



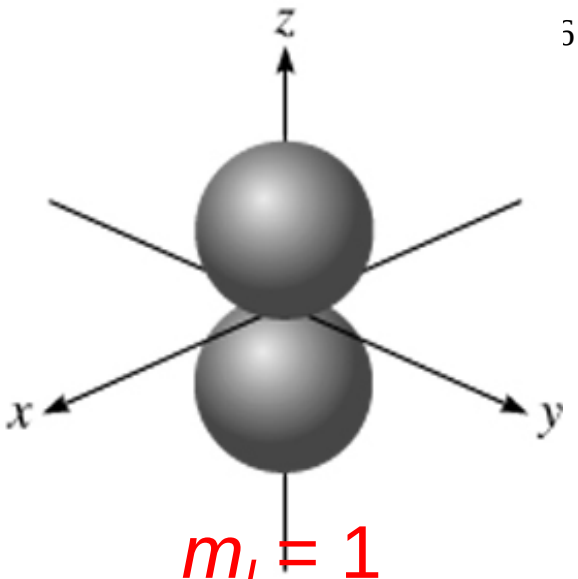
$m_l = -1$

$2p_x$



$m_l = 0$

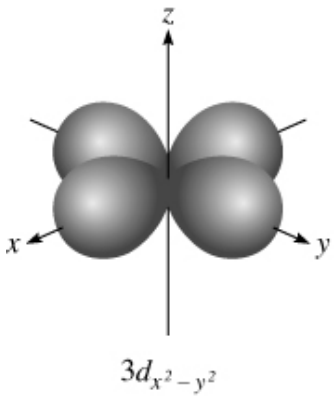
$2p_y$



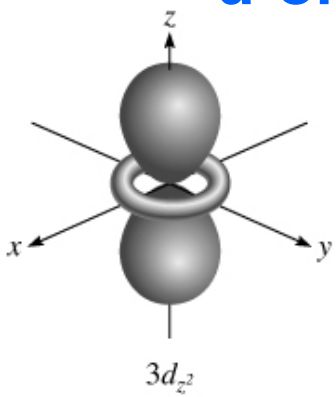
$m_l = 1$

$2p_z$

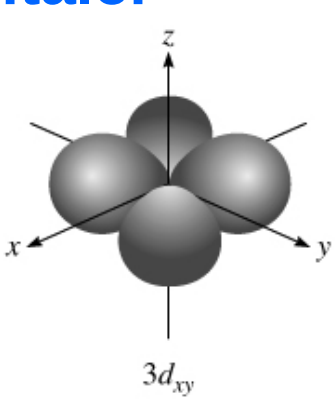
d-orbitaler



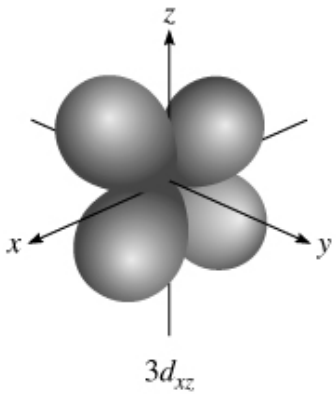
$3d_{x^2-y^2}$



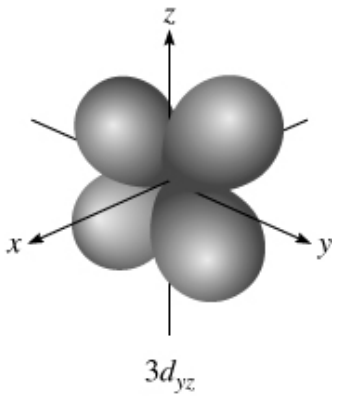
$3d_{z^2}$



$3d_{xy}$

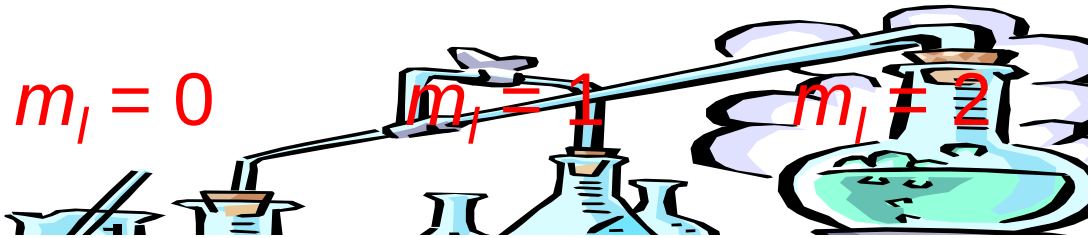


$3d_{xz}$



$3d_{yz}$

$m_l = -2$ $m_l = -1$ $m_l = 0$ $m_l = 1$ $m_l = 2$



Elektronkonfiguration

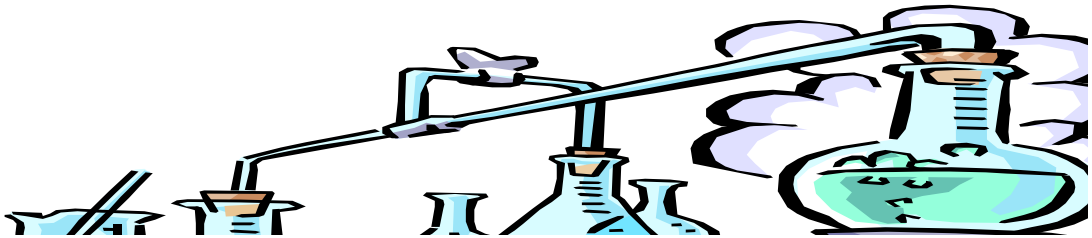
- **Aufbau-processen: elektronkonfigurationen byggs upp stegvis...**

C

$1s^2$ $2s^2$ $2p^2$

O

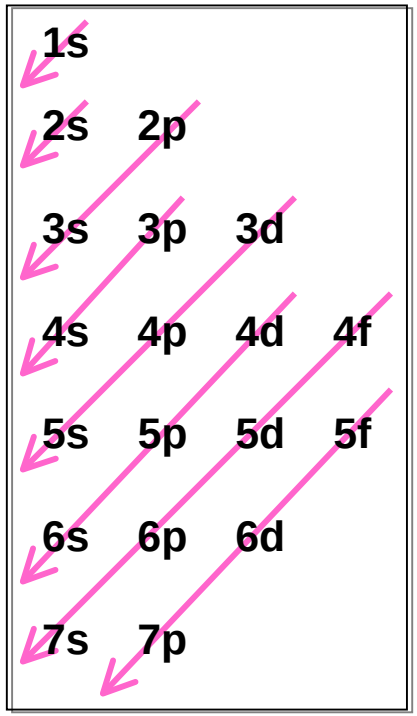
$1s^2$ $2s^2$ $2p^4$

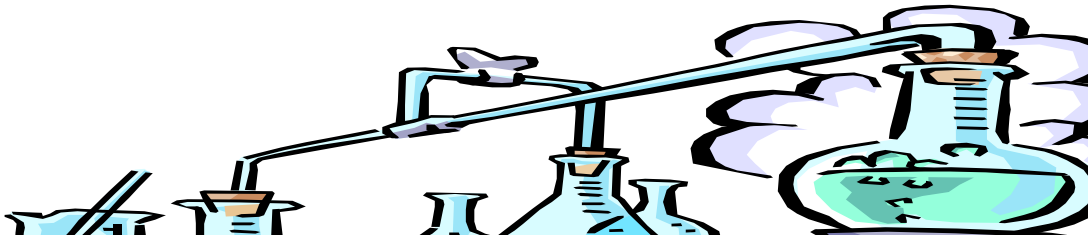


Orbitalernas energi

- **MEN för flerelektronatomer beror energin hos orbitalen både på *n* och *l:***

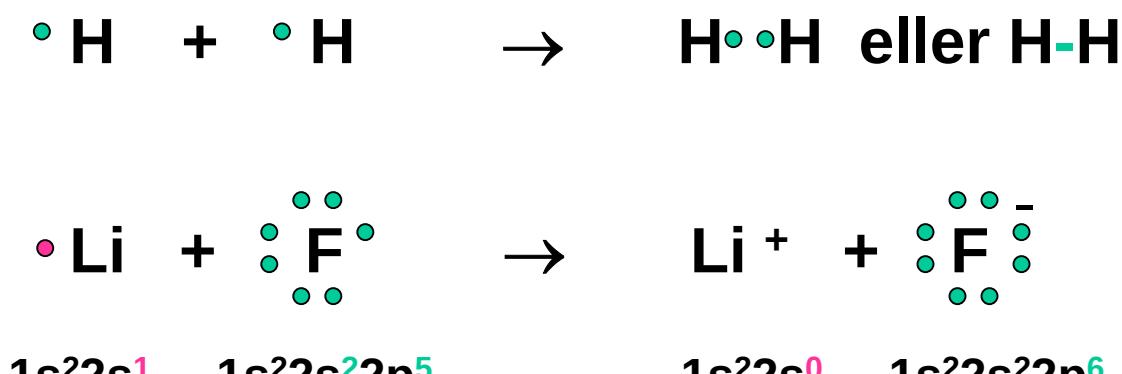
1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d <…

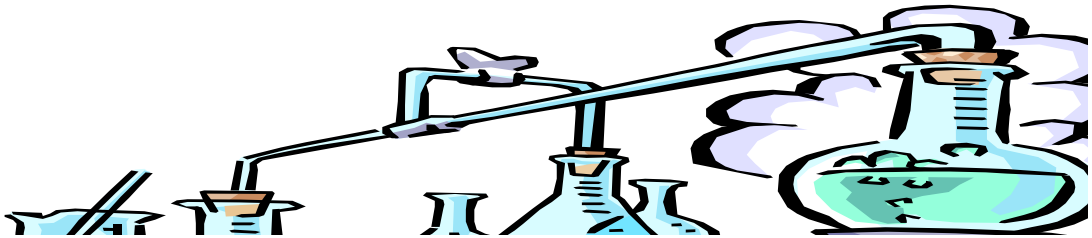




Lewisstrukturer

- **Ett sätt att rita atomer är med hjälp av Lewisstrukturer. Varje valenselektron illustreras med en prick.**

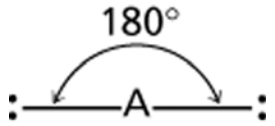


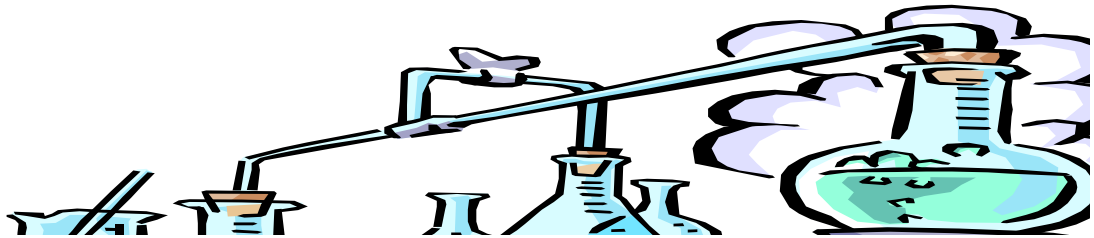


Valence shell electron pair repulsion (VSEPR) model:

Förutsäger geometrin av en molekyl utifrån den elektrostatiska repulsionen mellan elektronpar (bindande resp. fria)

Klass	# atomer bundna till centralatomen	# fria elektronpar på central-atomen	Arrangemang av elektronpar	Geometri
AB_2	2	0	linjär	linjär





Det periodiska systemet

1 1A												13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 **H**	2 2A																2 **He**
3 **Li**	4 **Be**											5 **B**	6 **C**	7 **N**	8 **O**	9 **F**	10 **Ne**
11 **Na**	12 **Mg**	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**
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**	57 **La**	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**	89 **Ac**	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110	111	112	(113)	114	(115)	116	(117)	118

Representative elements

Noble gases

Transition metals

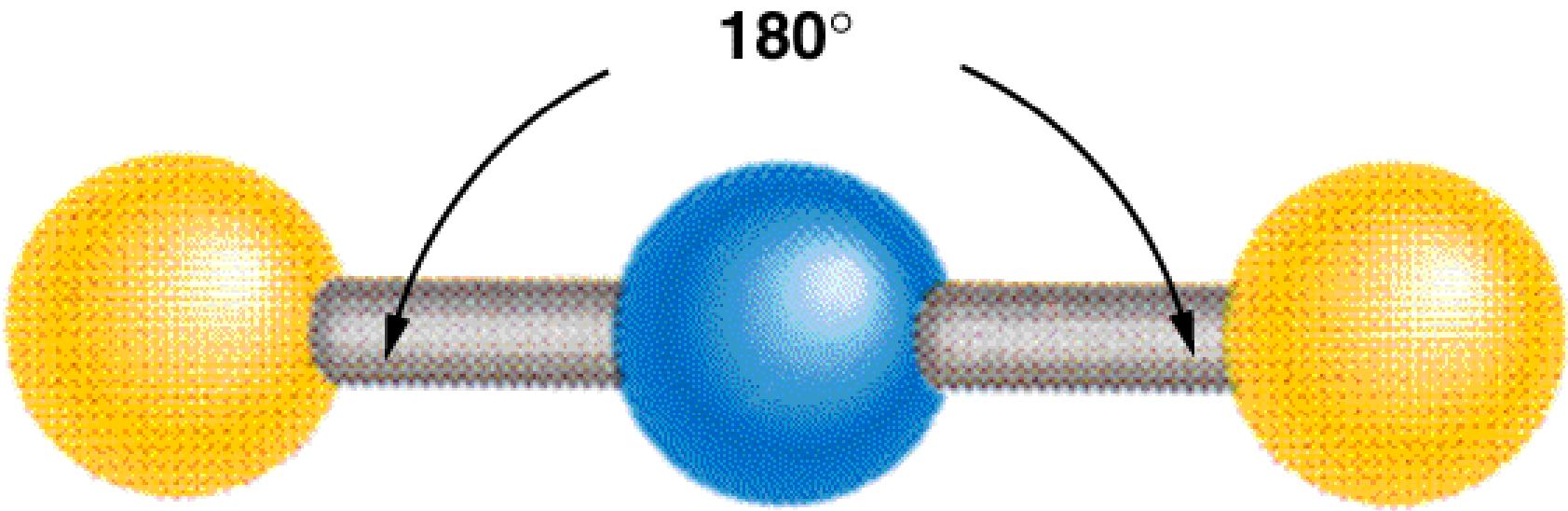
Zinc
Cadium
Mercury

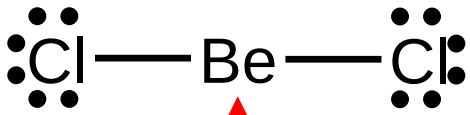
Lanthanides

Actinides

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**	71 **Lu**
90 **Th**	91 **Pa**	92 **U**	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**	103 **Lr**

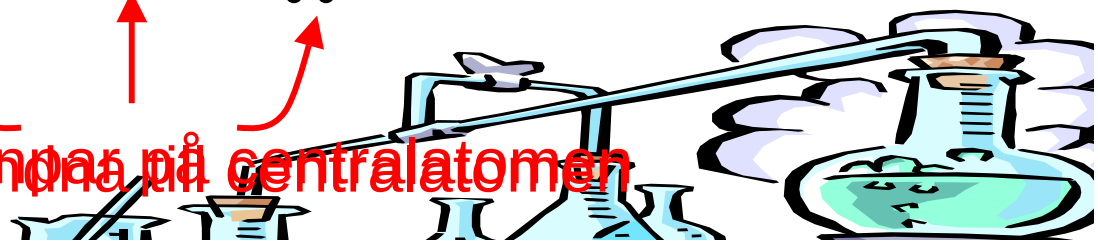
Beryllium Chloride



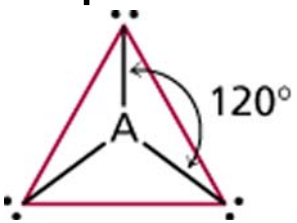
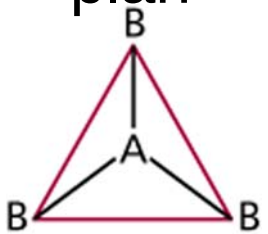


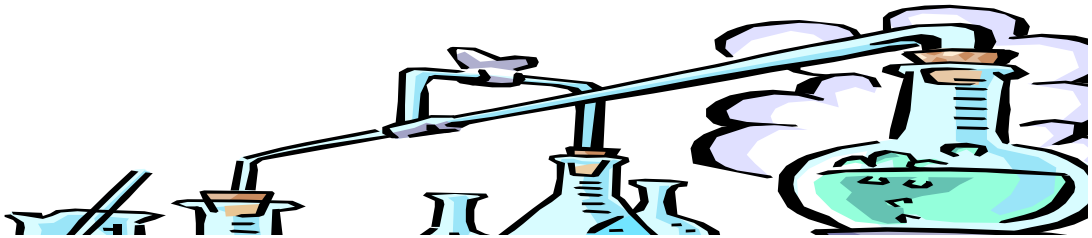
2 fria elektronpar på centralatomen

2 atomer bundna till centralatomen



VSEPR

Class	# atomer bundna till centralatomen	# fria elektronpar på central-atomen	Arrangemang av elektronpar	Geometri
AB_2	2	0	linjär	linjär
AB_3	3	0	trigonalt plan 	trigonalt plan 



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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**	57 **La**	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**	89 **Ac**	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110	111	112	(113)	114	(115)	116	(117)	118

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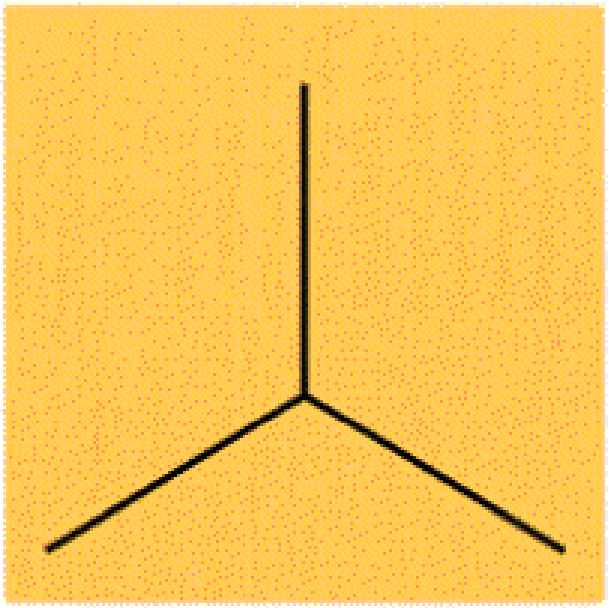
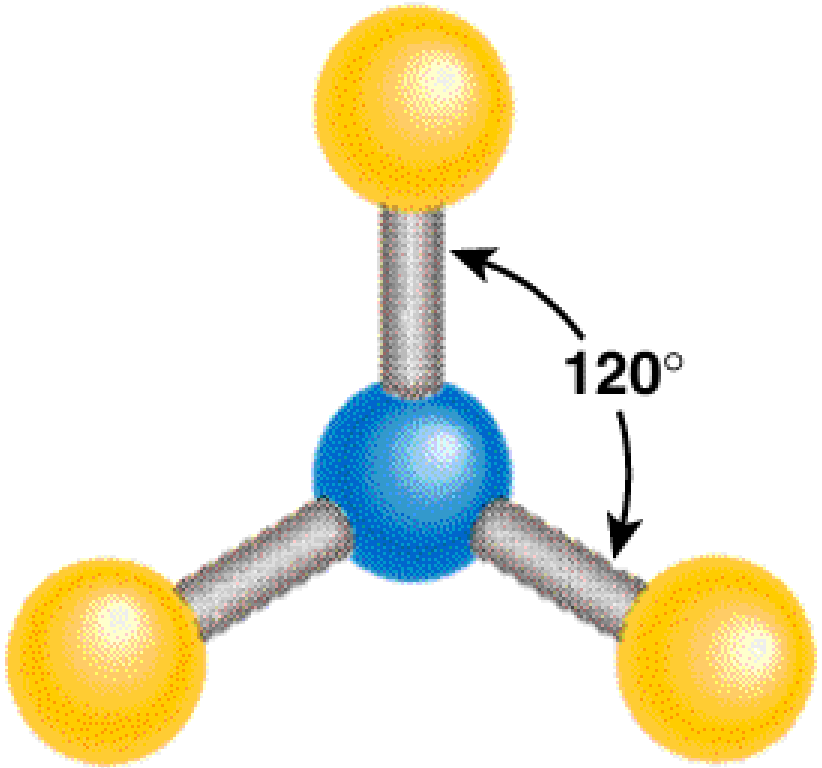
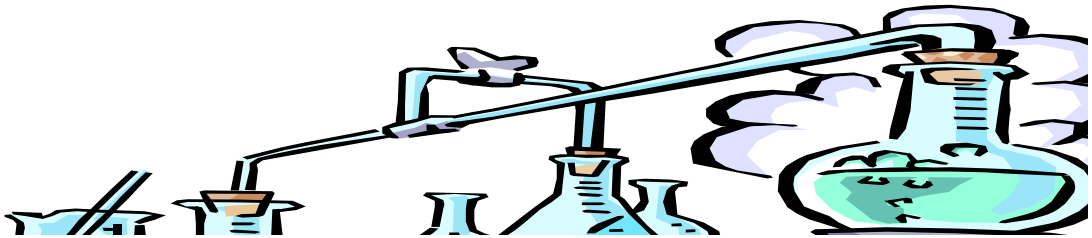
90 **Th**	91 **Pa**	92 **U**	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**	103 **Lr**

Boron Trifluoride



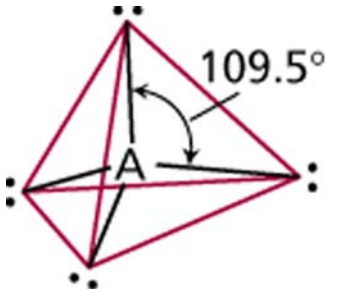
Planar

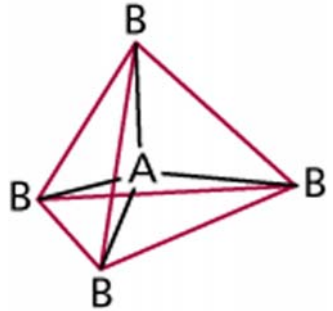




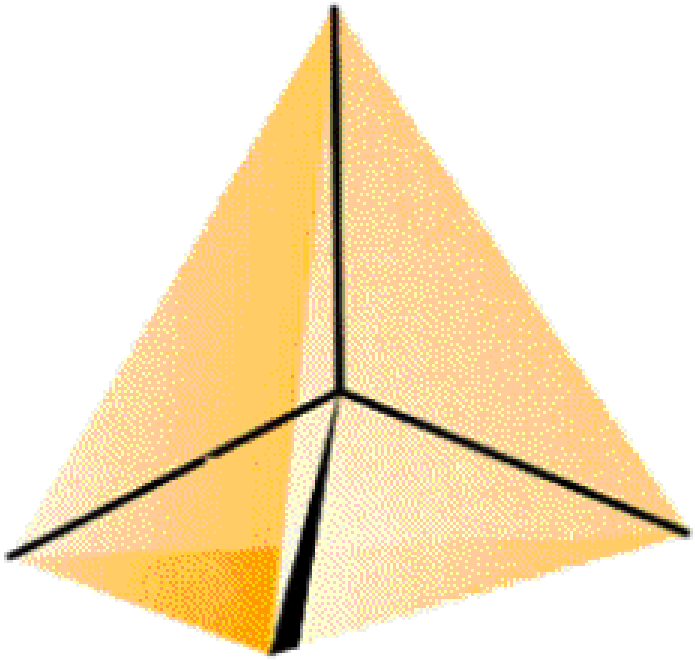
VSEPR

Class	# atomer bundna till centralatomen	# fria elektronpar på central-atomen	Arrangemang av elektronpar	Geometri
AB_2	2	0	linjär	linjär
AB_3	3	0	trigonalt plan	trigonalt plan
AB_4	4	0	tetrahedrisk	tetrahedrisk

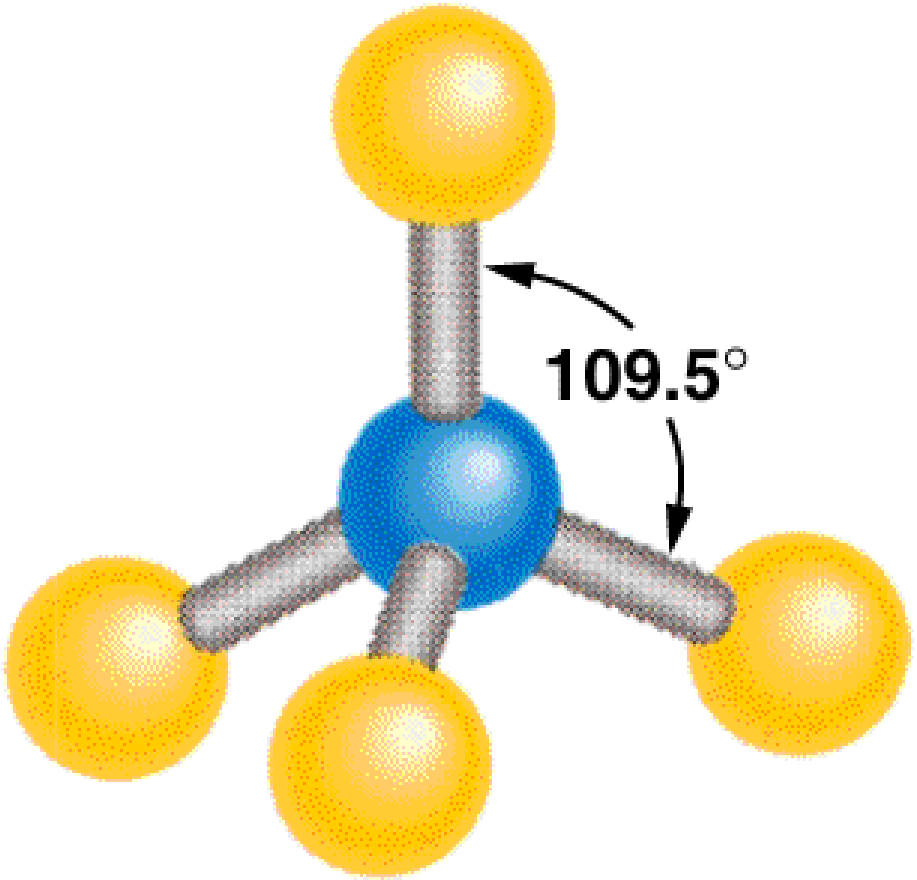


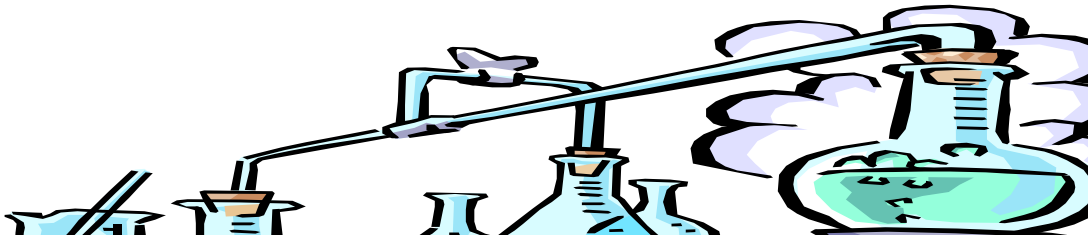


Methane



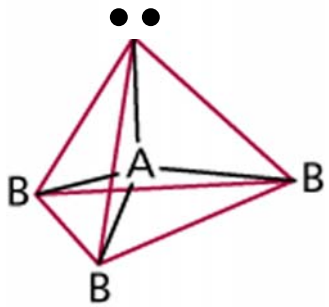
Tetrahedral

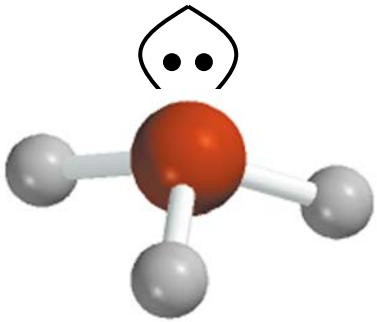


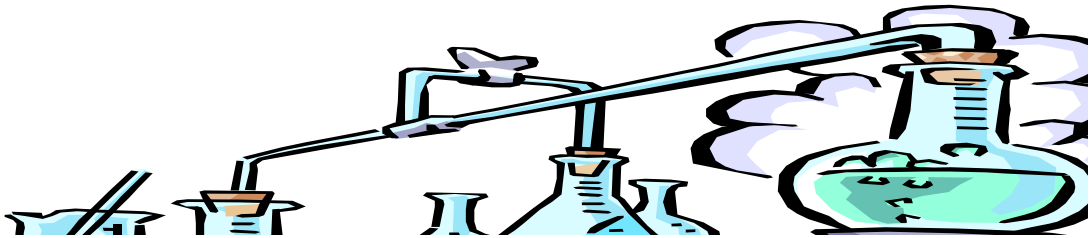


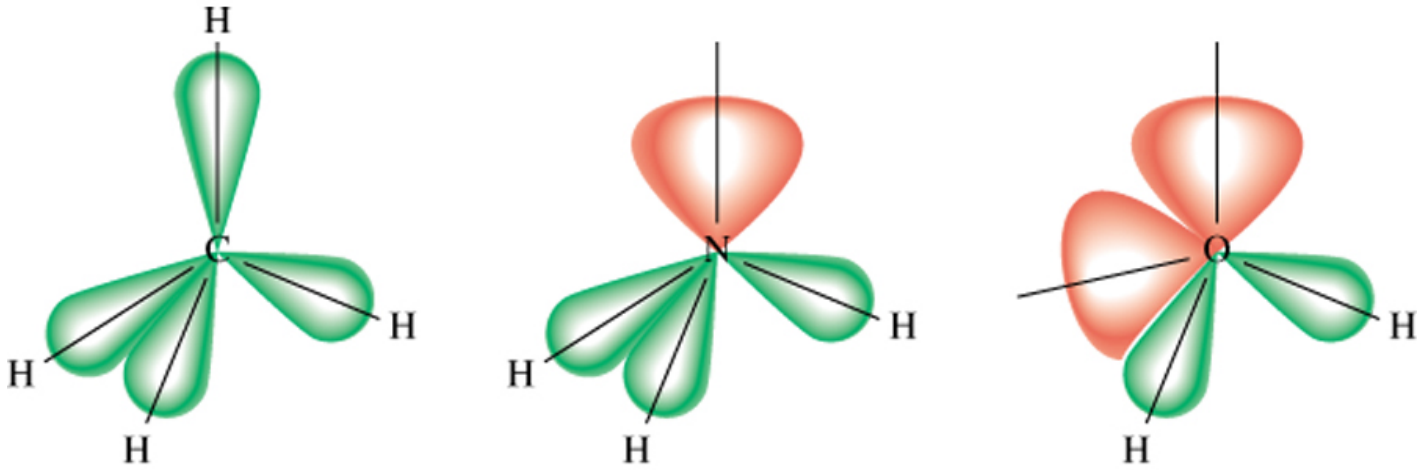
VSEPR

Class	# atomer bundna till centralatomen	# fria elektronpar på central-atomen	Arrangemang av elektronpar	Geometri
AB_4	4	0	tetrahedrisk	tetrahedrisk
AB_3E	3	1	tetrahedrisk	trigonalt pyramidal

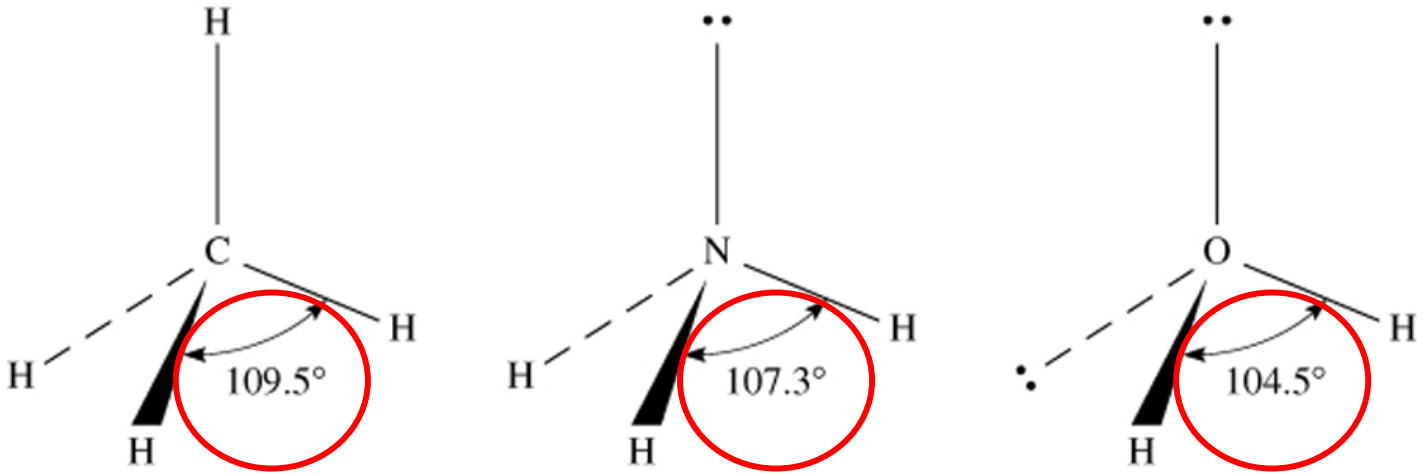








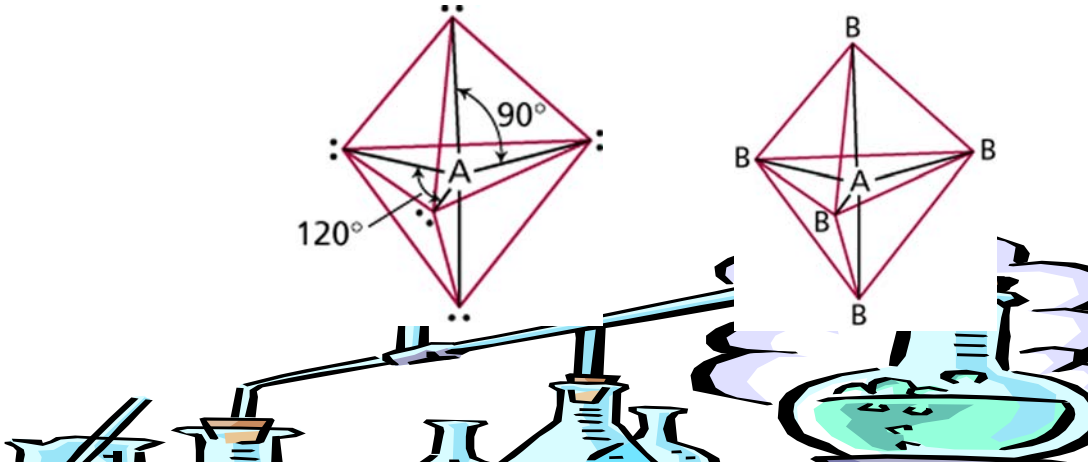
(a)



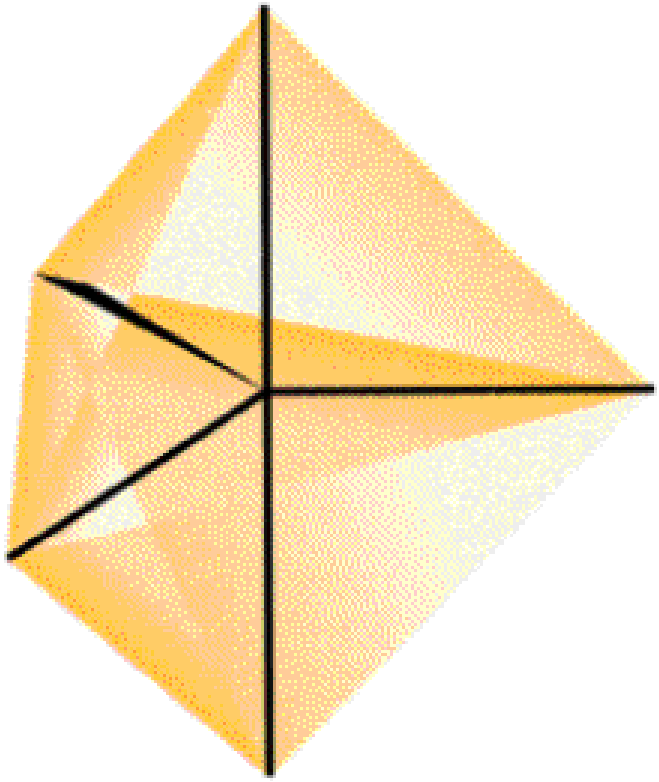
bindande e-par vs. bindande e-par < fritt e-par vs. bindande e-par < fritt e-par vs. fritt e-par

VSEPR

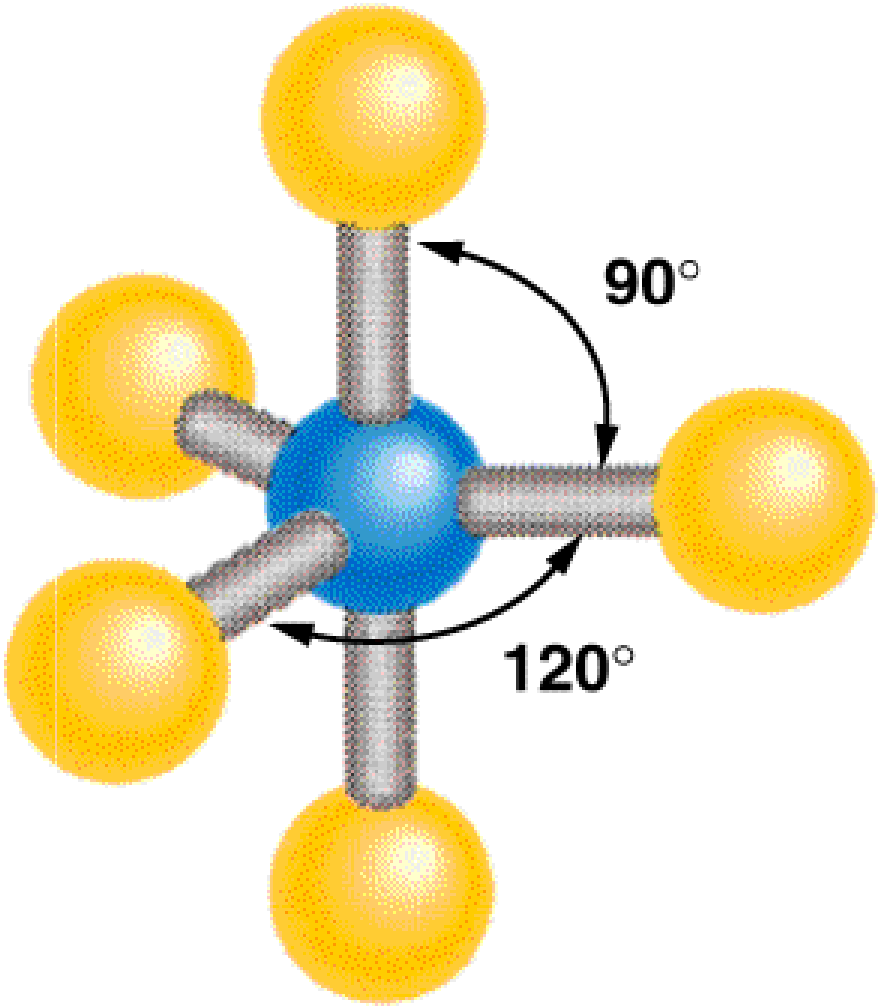
Class	# atomer bundna till centralatomen	# fria elektronpar på central-atomen	Arrangemang av elektronpar	Geometri
AB_2	2	0	linjär	linjär
AB_3	3	0	trigonalt plan	trigonalt plan
AB_4	4	0	tetrahedrisk	tetrahedrisk
AB_5	5	0	trigonalt bipyramidal	trigonalt bipyramidal



Phosphorus Pentachloride

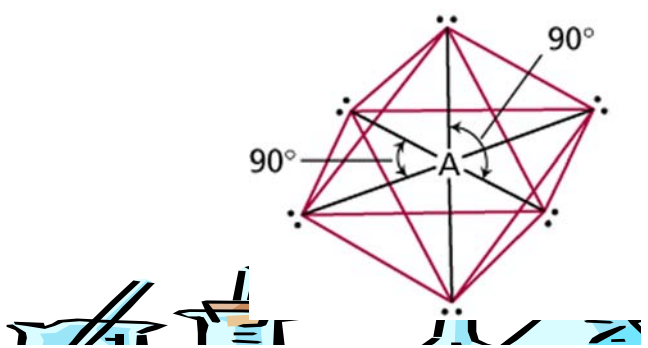


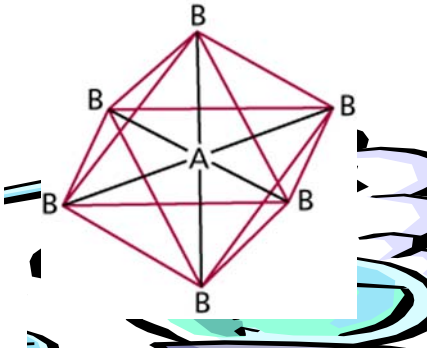
Trigonal bipyramidal



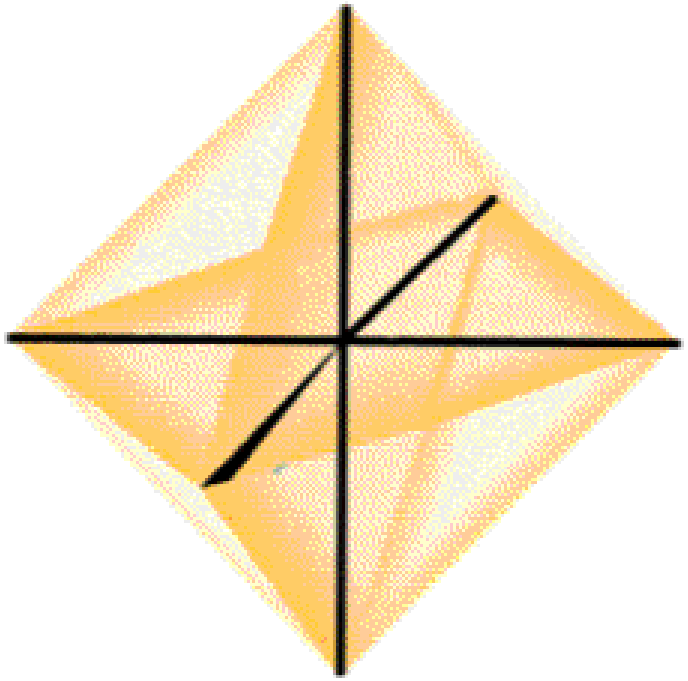
VSEPR

Class	# atomer bundna till centralatomen	# fria elektronpar på central-atomen	Arrangemang av elektronpar	Geometri
AB_2	2	0	linjär	linjär
AB_3	3	0	trigonalt plan	trigonalt plan
AB_4	4	0	tetrahedrisk	tetrahedrisk
AB_5	5	0	trigonalt bipyramidal	trigonalt bipyramidal
AB_6	6	0	oktahedrisk	oktahedrisk

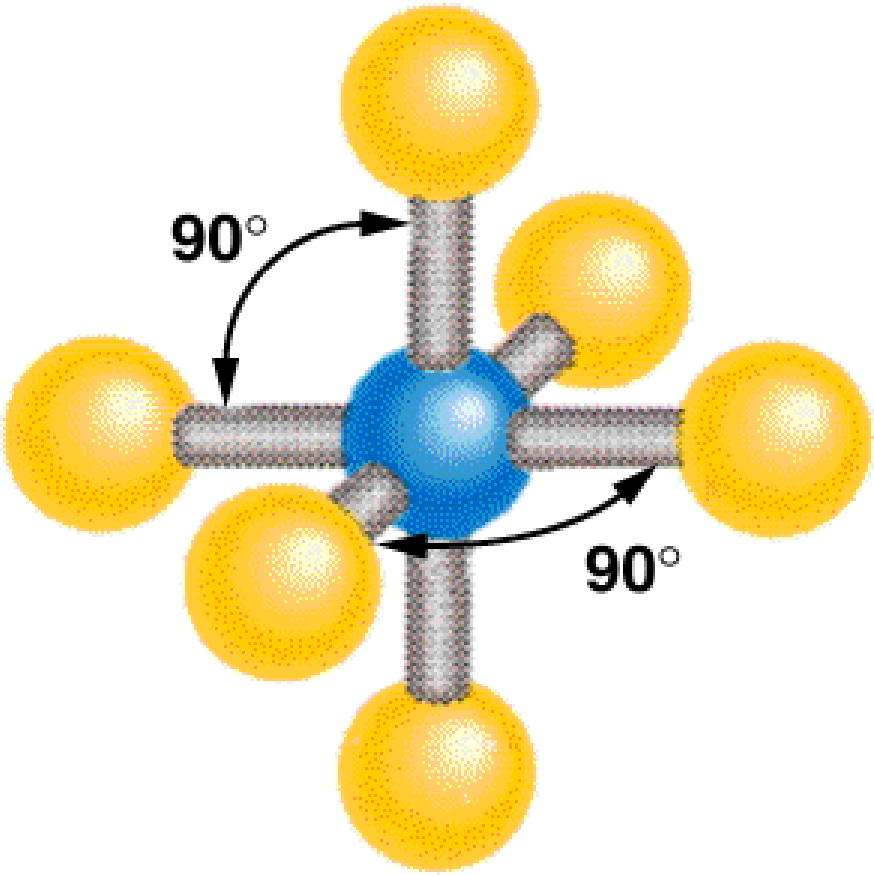




Sulfur Hexafluoride

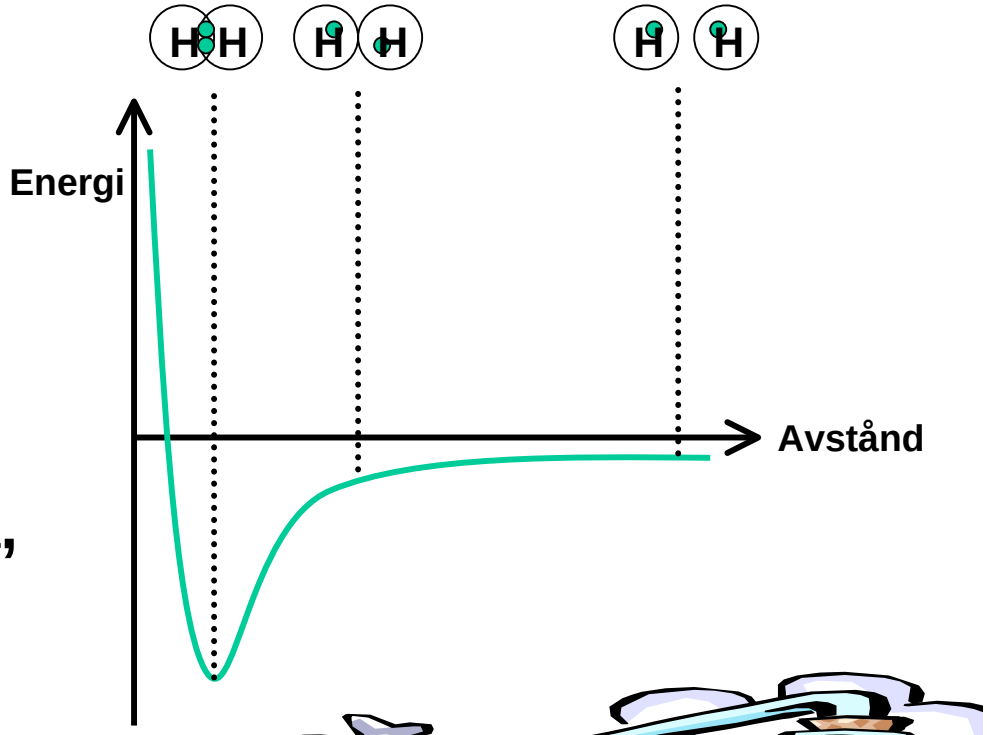


Octahedral



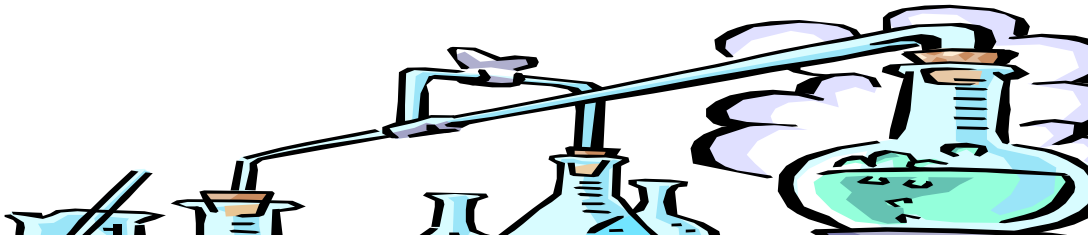
Kovalent bindning

- **Det är orbitalernas överlappning som utgör bindningen.**
  - **På långt avstånd ingen attraktion.**
  - **På lagom avstånd skapas bindning.**
  - **Om atomerna kommer för nära överlappar kärnorna, vilket är mycket ogynnsamt.**



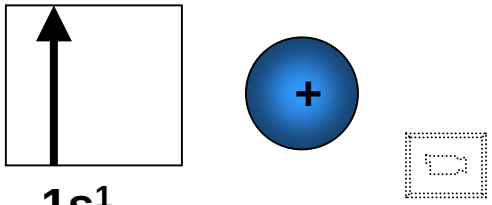
VB-teori - Valence bond theory

- **Valence bond theory**
  - **Elektronerna i en molekyl befinner sig i respektive atoms atomorbitaler.**
  - **Bindningar skapas genom att de olika atomorbitalerna överlappar varandra, det vill säga när två orbitaler delar ett gemensamt område i rymden.**
  - **Varje individuell atom är en del i molekylen och tillsammans skapar atomerna molekylens bindningar.**

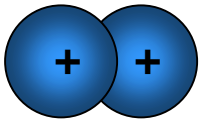


Kovalent bindning

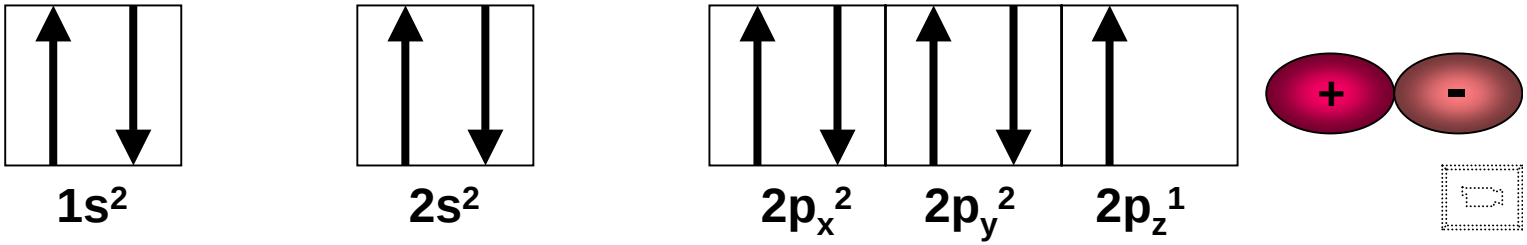
H



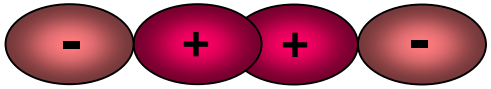
H_2



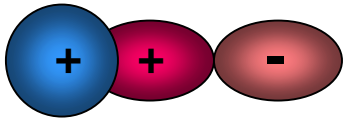
F

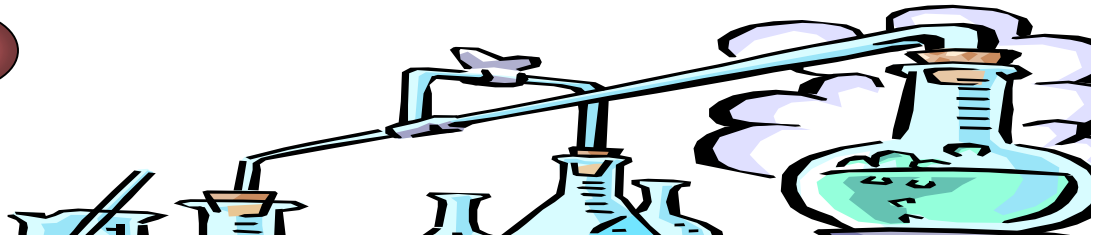


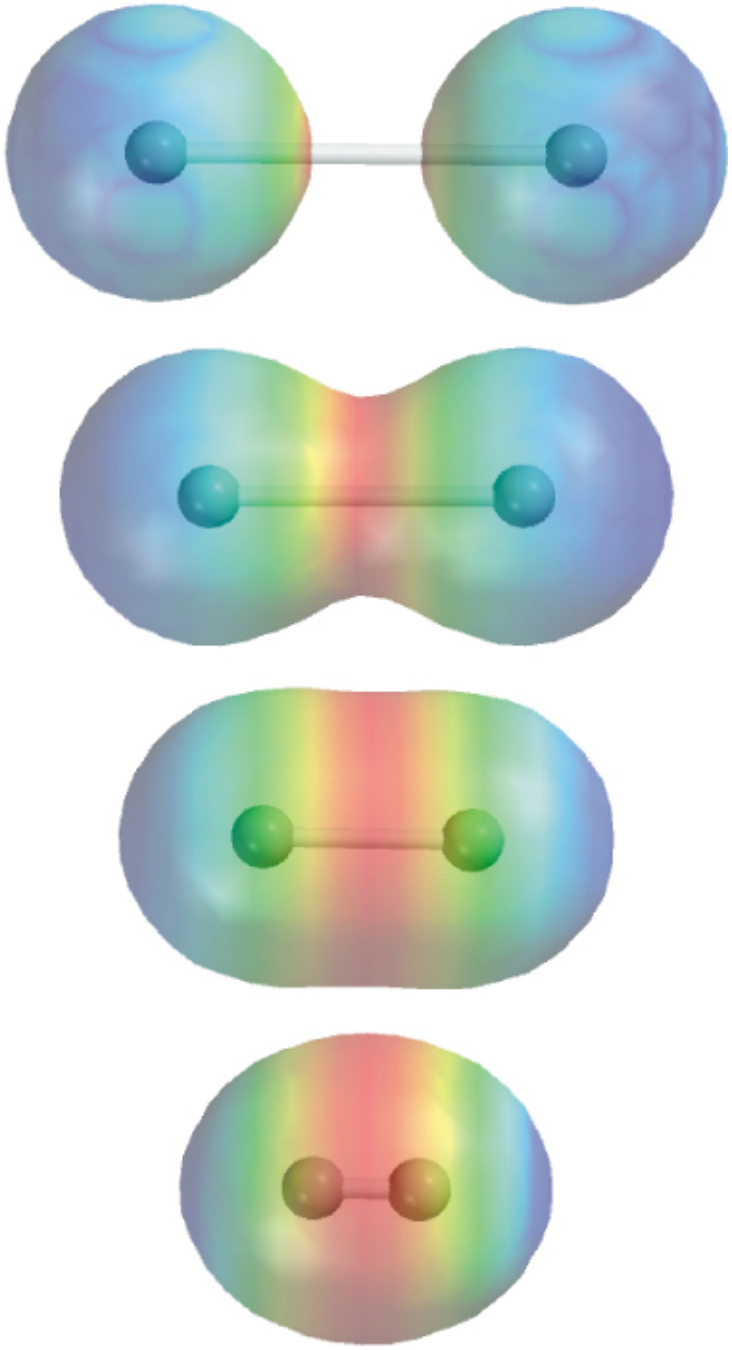
F_2



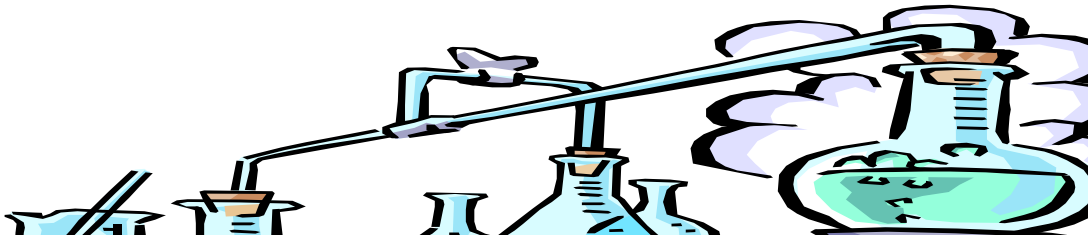
HF





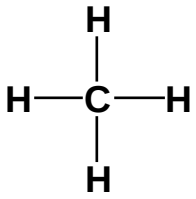


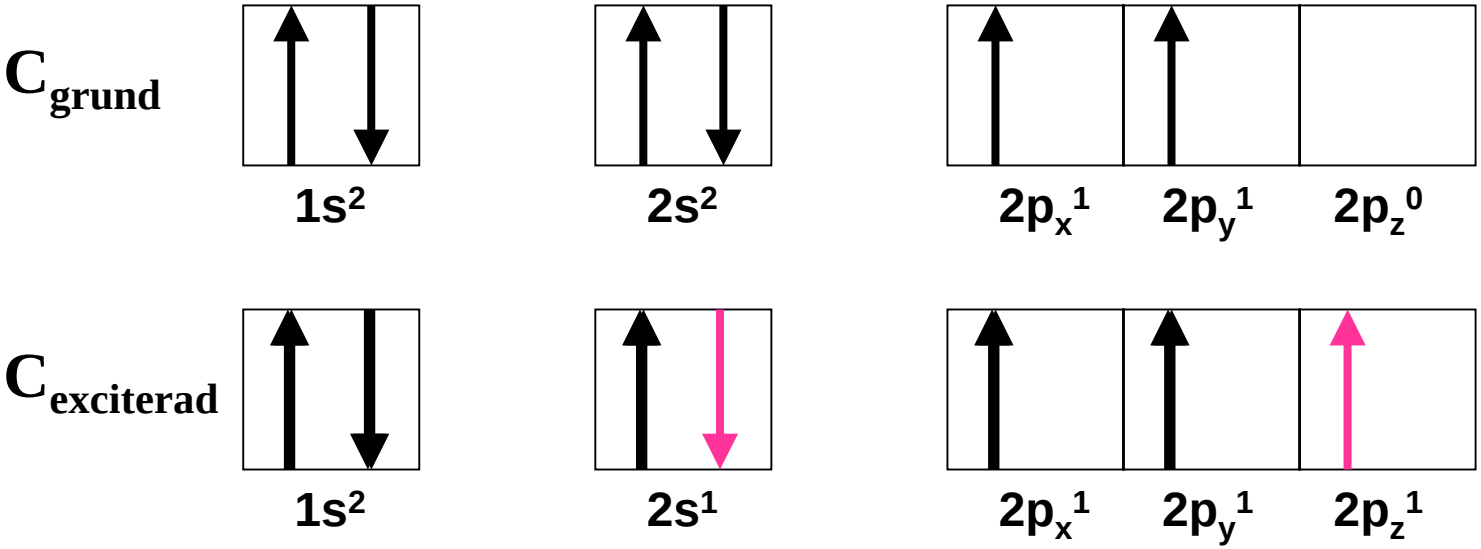
Förändring i elektron-densitet när två väte-atomer närmar sig varandra

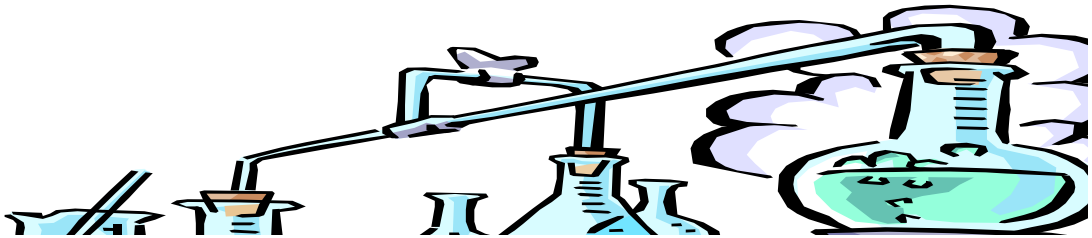


Hybridisering

- **Hur ser metan ut?**

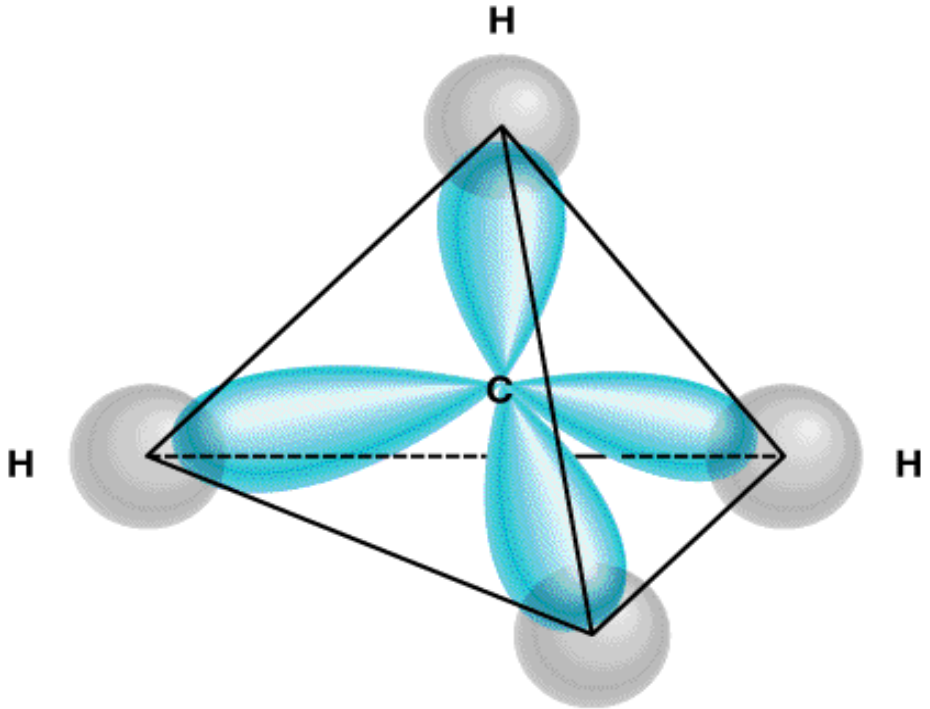




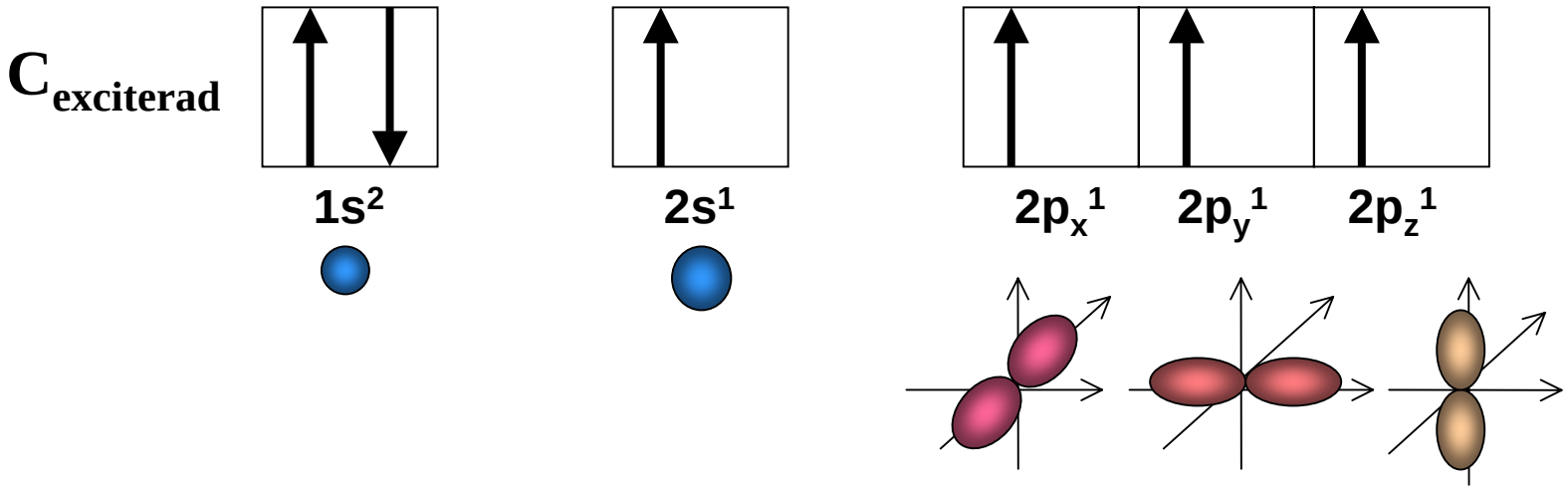


Hybridisering

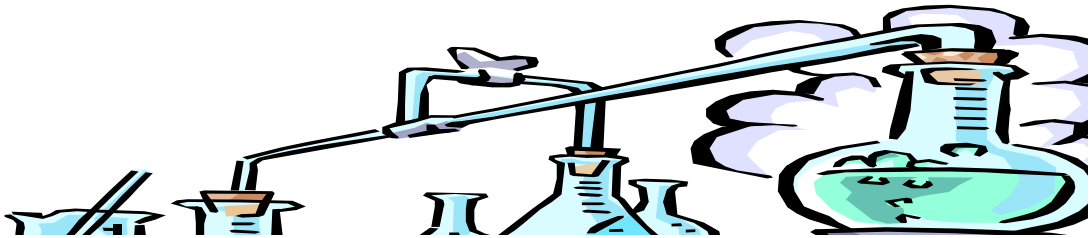
- **Kolatomen i CH_4 är sp^3-hybridiserad.**



Hybridisering

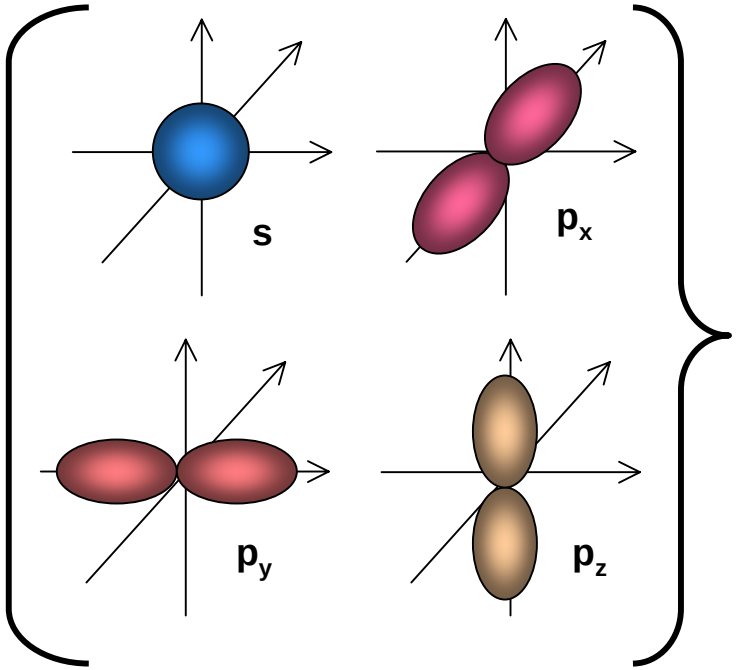


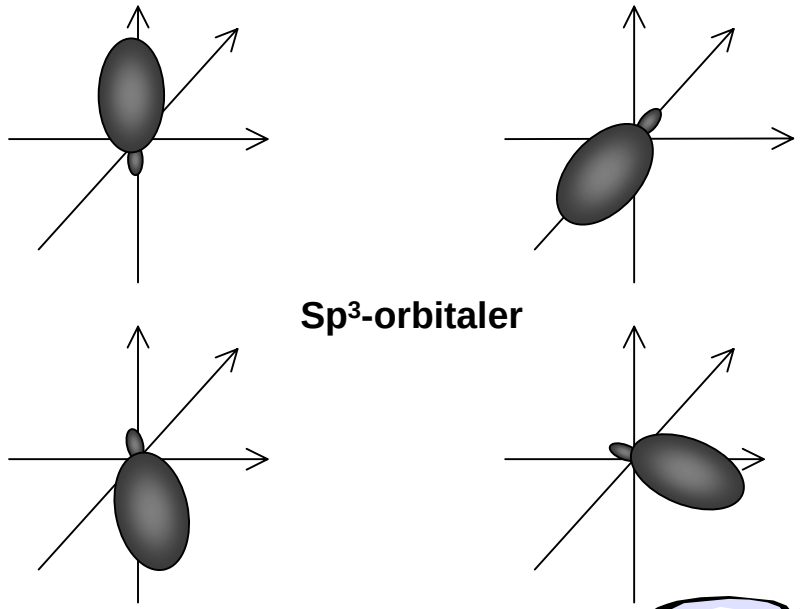
- **Fyra orbitaler kan nu vara med och skapa kovalenta bindningar till väte. Men alla bindningar i metan är ju lika?!**



Hybridisering

- **En s- och tre p-orbitaler omvandlas till fyra sp^3-orbitaler.**





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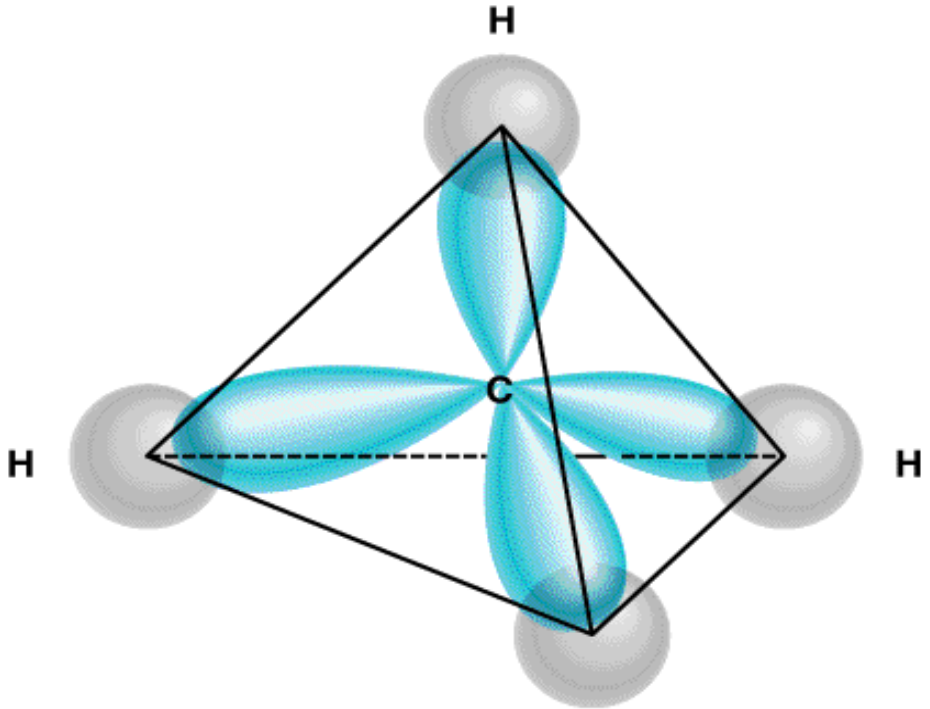
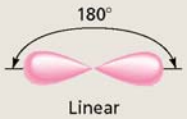
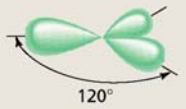
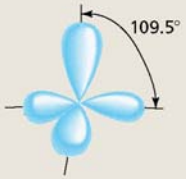
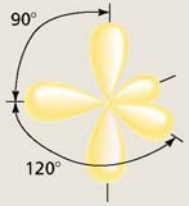
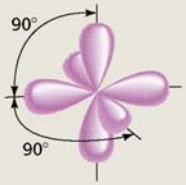
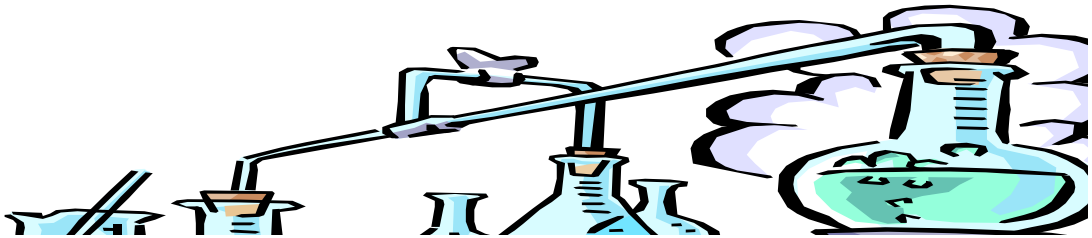


Hybridisering

Table 10.4 Important Hybrid Orbitals and Their Shapes

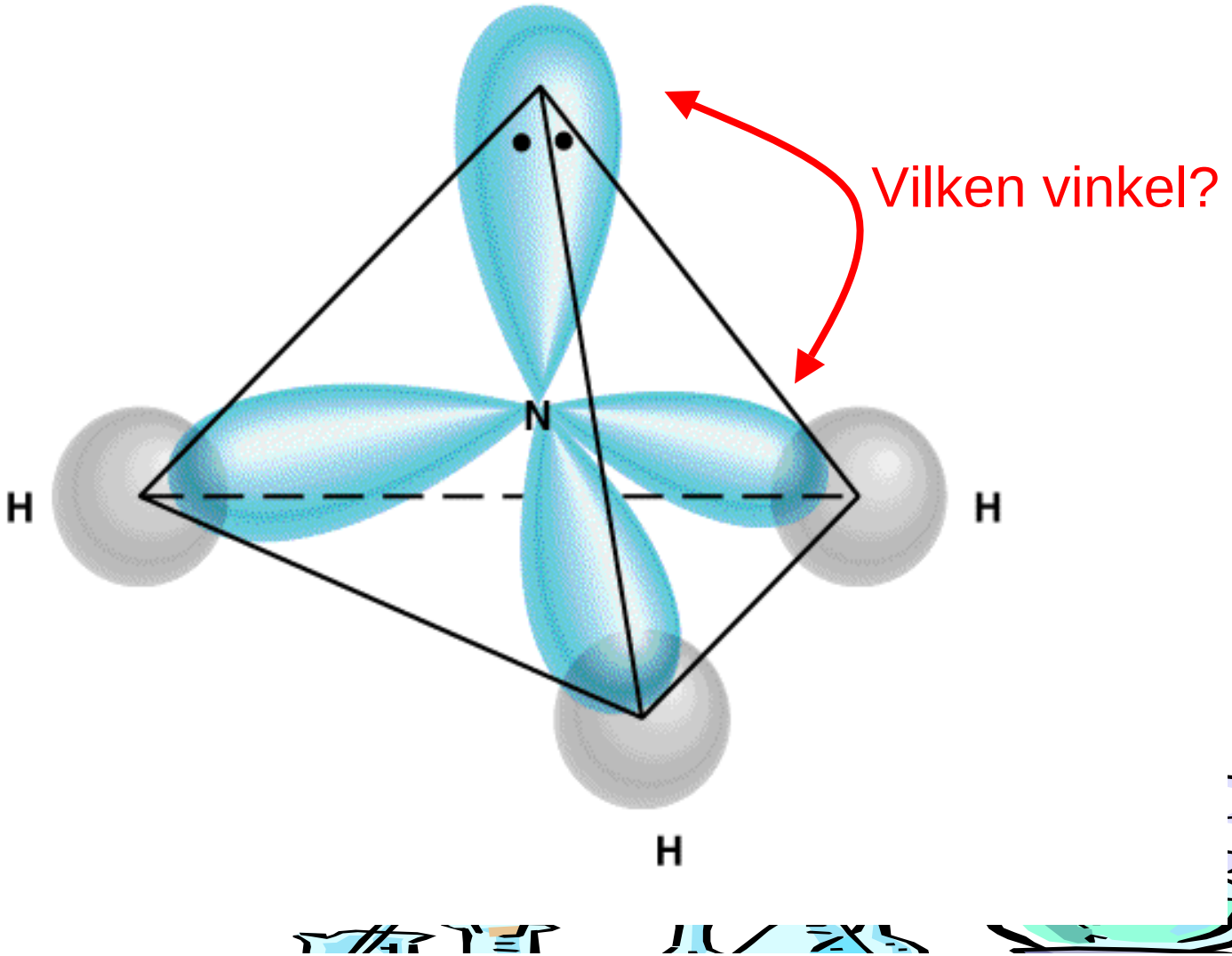
Pure Atomic Orbitals of the Central Atom	Hybridization of the Central Atom	Number of Hybrid Orbitals	Shape of Hybrid Orbitals	Examples
s, p	*sp*	2	 Linear	$BeCl_2$
s, p, p	sp^2	3	 Planar	BF_3
s, p, p, p	sp^3	4	 Tetrahedral	CH_4, NH_4^+
s, p, p, p, d	sp^3d	5	 Trigonal bipyramidal	PCl_5
s, p, p, p, d, d	sp^3d^2	6	 Octahedral	SF_6

- **Hybridorbitalerna strävar efter att vara så långt ifrån varandra som möjligt i rymden.**
  - **Jmf. VSPER-teorin**



Hybridisering

- NH_3



Det periodiska systemet

1 1A												13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 **H**	2 2A																2 **He**
3 **Li**	4 **Be**											5 **B**	6 **C**	7 **N**	8 **O**	9 **F**	10 **Ne**
11 **Na**	12 **Mg**	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**
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**	57 **La**	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**	89 **Ac**	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110	111	112	(113)	114	(115)	116	(117)	118

Representative elements

Noble gases

Transition metals

Zinc
Cadium
Mercury

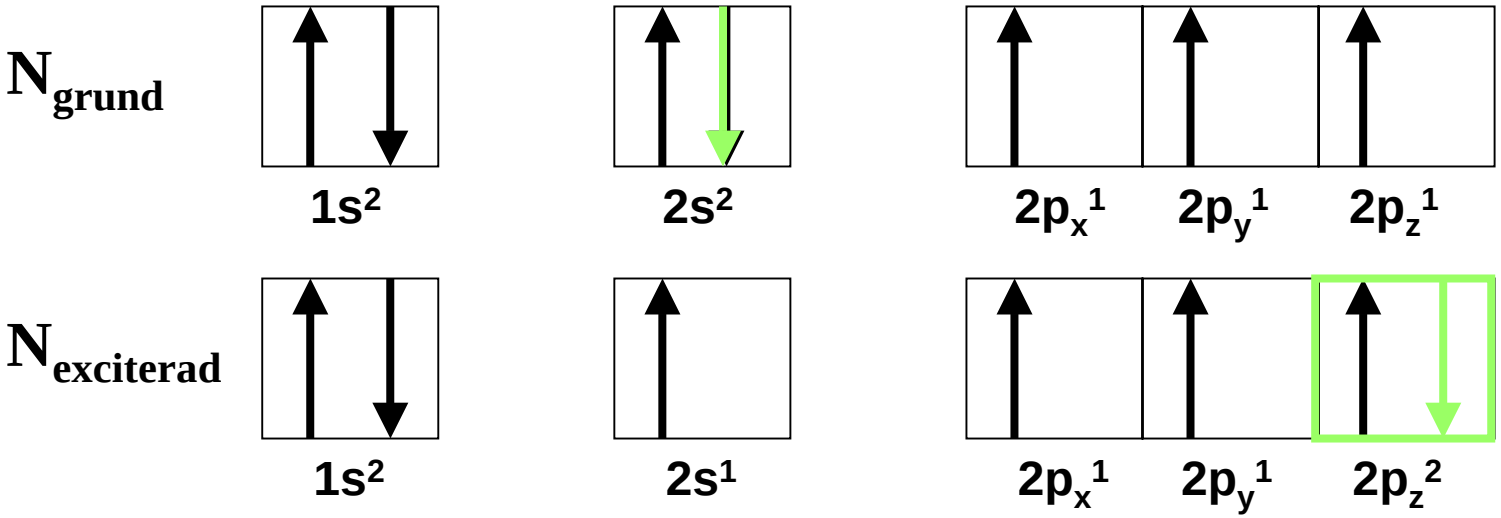
Lanthanides

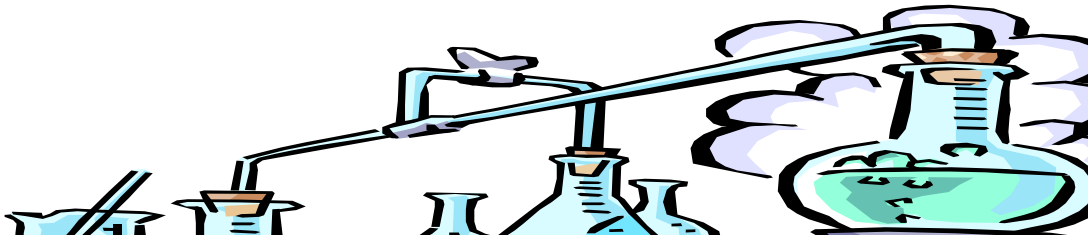
Actinides

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**	71 **Lu**
90 **Th**	91 **Pa**	92 **U**	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**	103 **Lr**

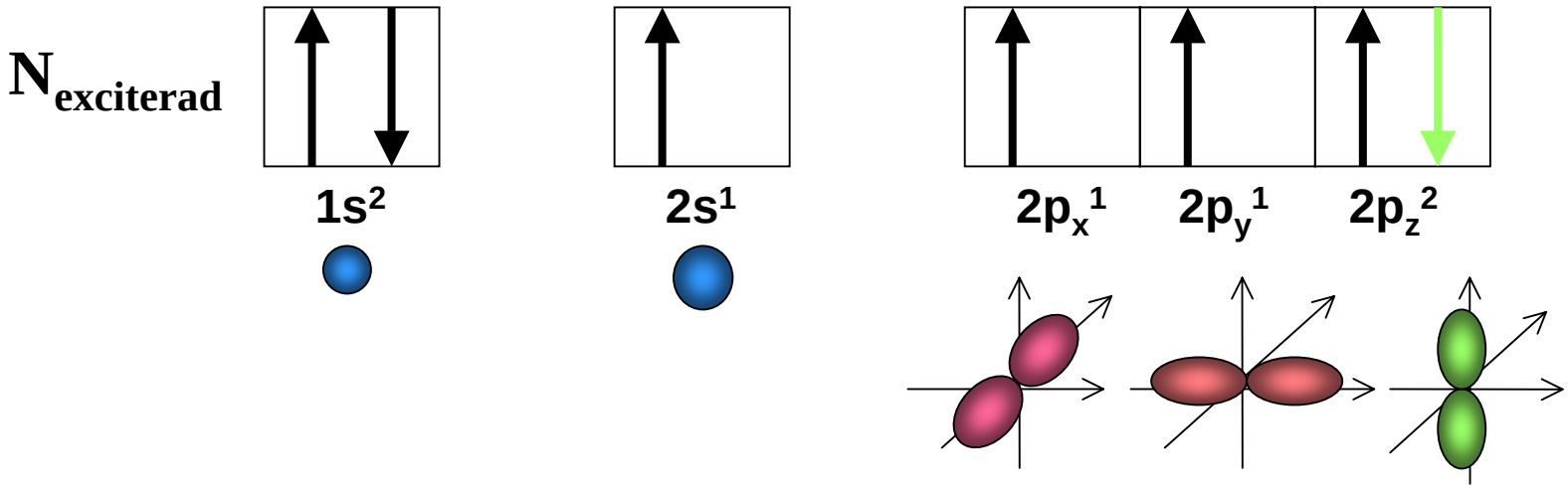
Hybridisering

- **Vilken hybridisering har NH_3?**
  - **Även NH_3 är tetrahedrisk till formen, därför kan vi anta att N är sp^3-hybridiserad.**

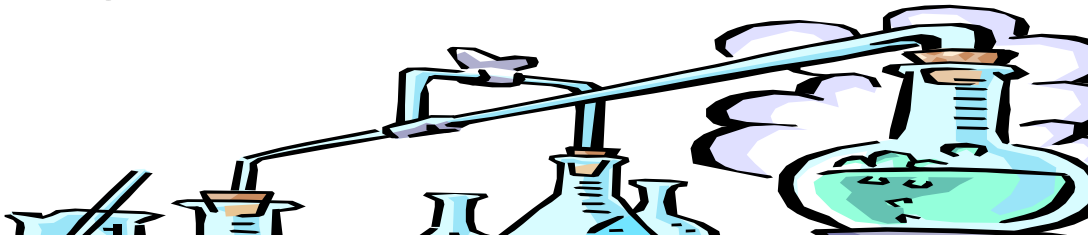




Hybridisering

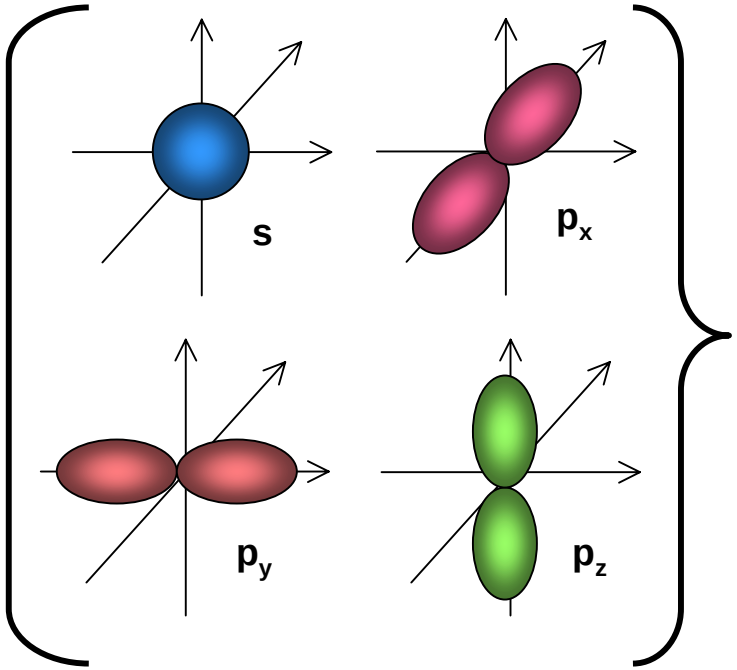


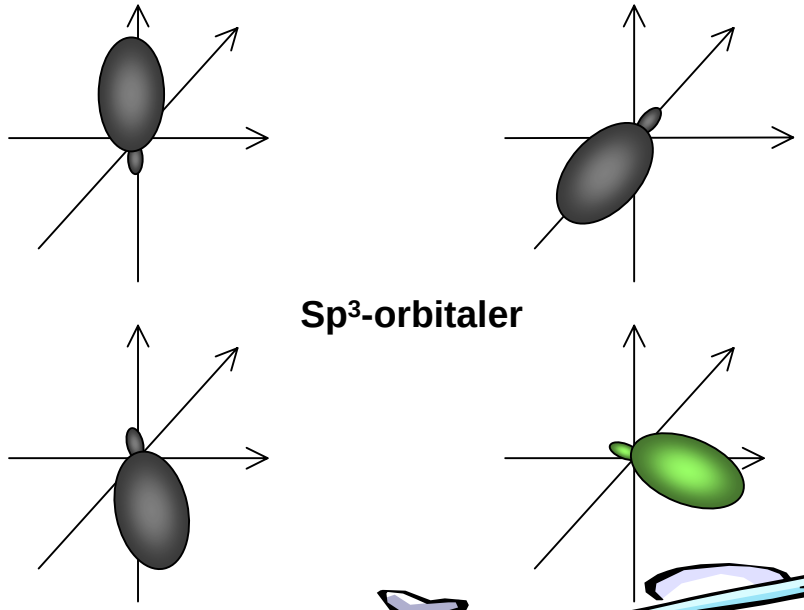
- **Fyra orbitaler kan nu vara med och skapa kovalenta bindningar till väte. Men NH_3 har ju bara tre bindningar och ett fritt elektronpar?!**



Hybridisering

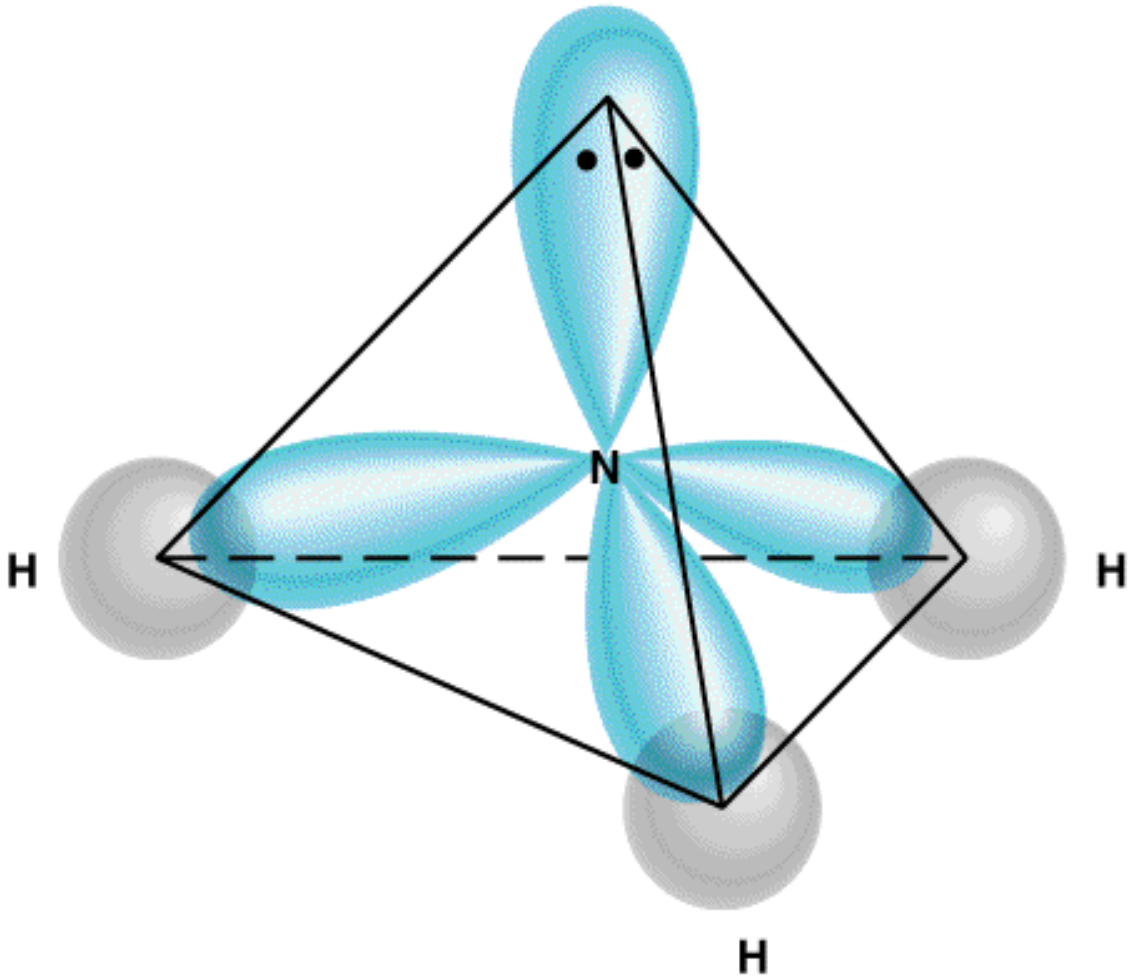
- **En s- och tre p-orbitaler omvandlas till fyra sp^3-orbitaler. I en av orbitalerna finns två elektroner, denna sp^3-orbital blir det fria elektronparet.**



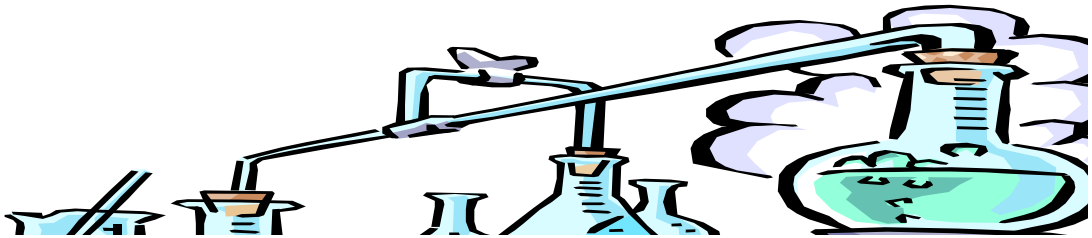


Hybridisering

- NH_3



Lite repetition



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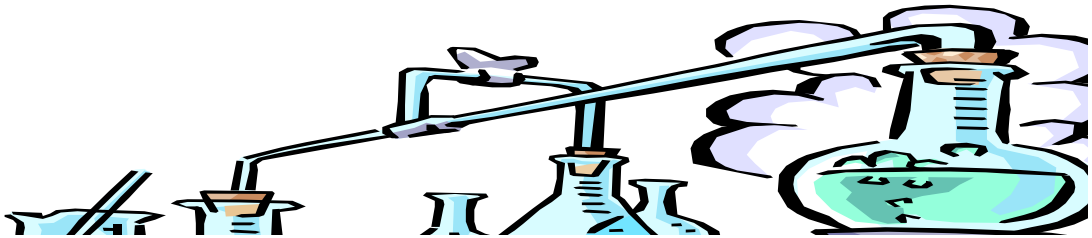
- **Valence bond theory**
  - **Elektronerna i en molekyl befinner sig i respektive atoms atomorbitaler.**
  - **Bindningar skapas genom att de olika atomorbitalerna överlappar varandra, det vill säga när två orbitaler delar ett gemensamt område i rymden.**
  - **Varje individuell atom är en del i molekylen och tillsammans skapar atomerna molekylens bindningar.**



Hybridisering

Table 10.4 Important Hybrid Orbitals and Their Shapes

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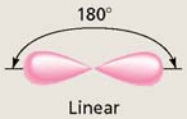
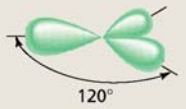
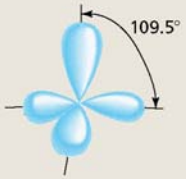
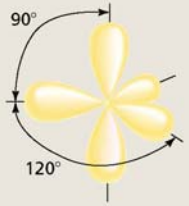
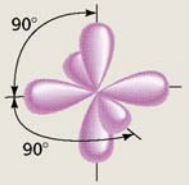
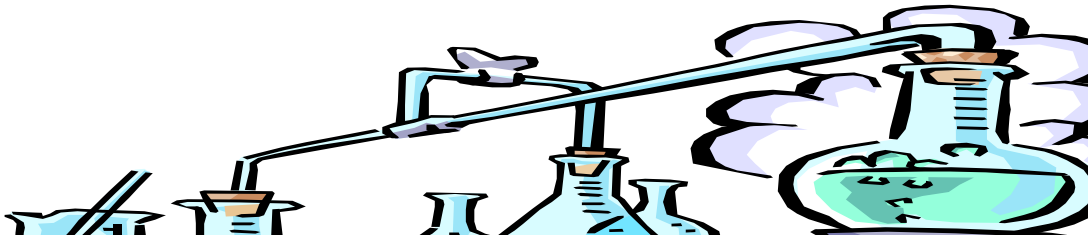
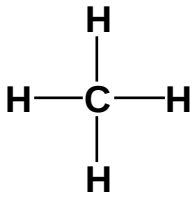
s, p	*sp*	2	 Linear	$BeCl_2$
s, p, p	sp^2	3	 Planar	BF_3
s, p, p, p	sp^3	4	 Tetrahedral	CH_4, NH_4^+
s, p, p, p, d	sp^3d	5	 Trigonal bipyramidal	PCl_5
s, p, p, p, d, d	sp^3d^2	6	 Octahedral	SF_6

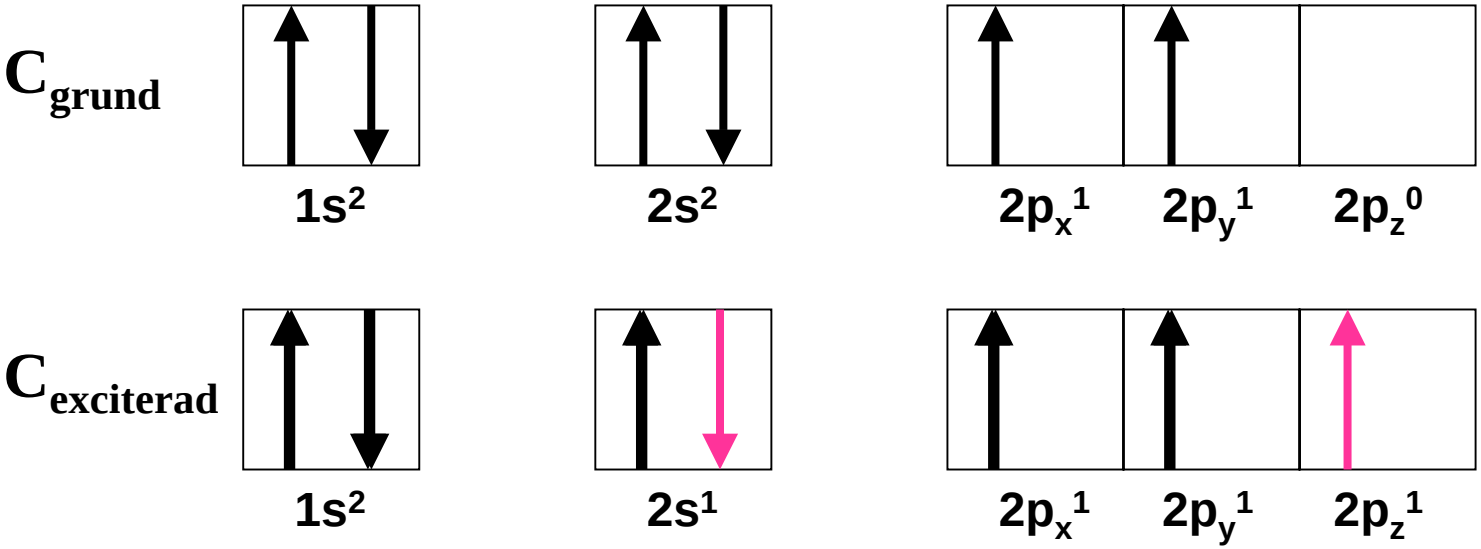
- **Hybridorbitalerna strävar efter att vara så långt ifrån varandra som möjligt i rymden.**
  - **Jmf. VSPER-teorin**

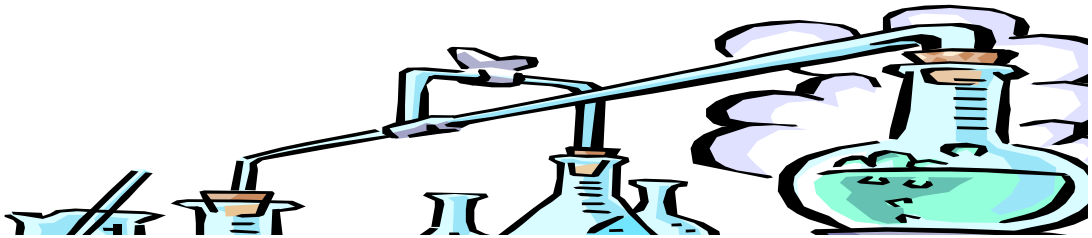


Hybridisering

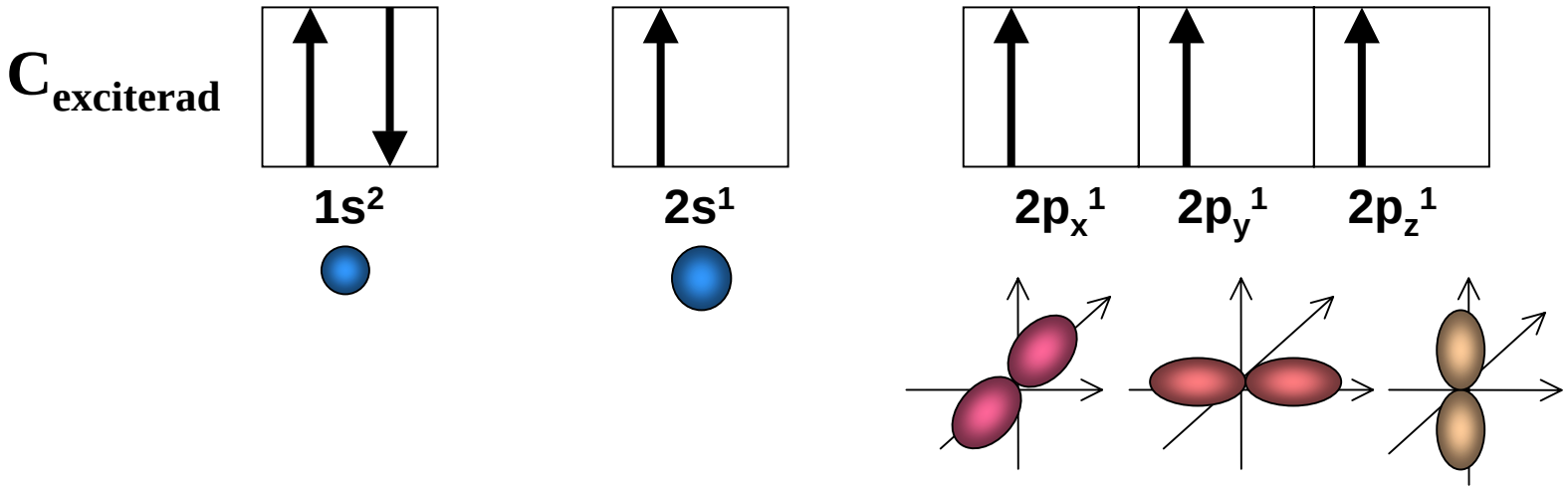
- **Hur ser metan ut?**



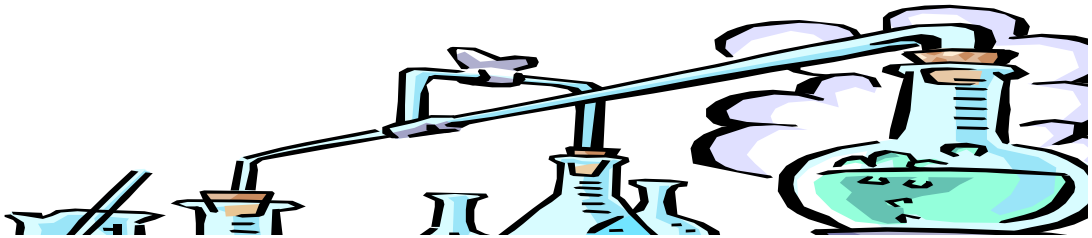




Hybridisering

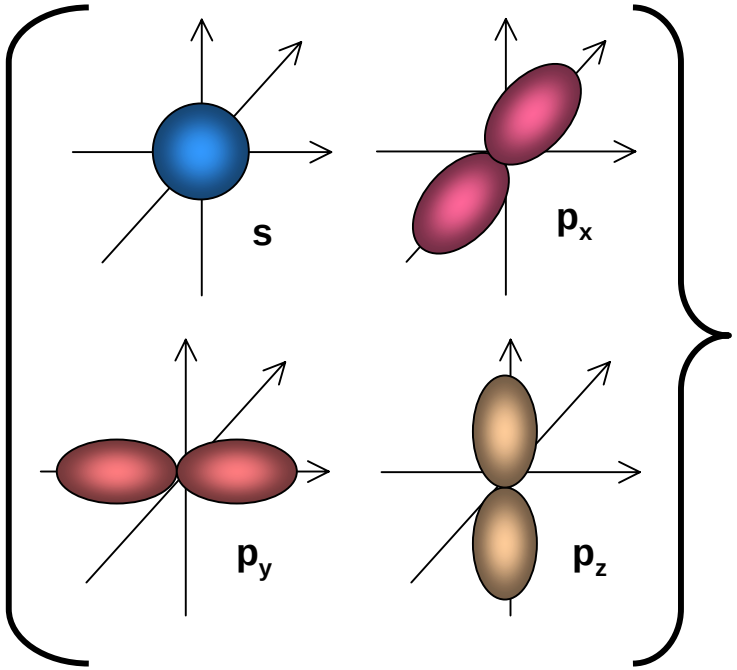


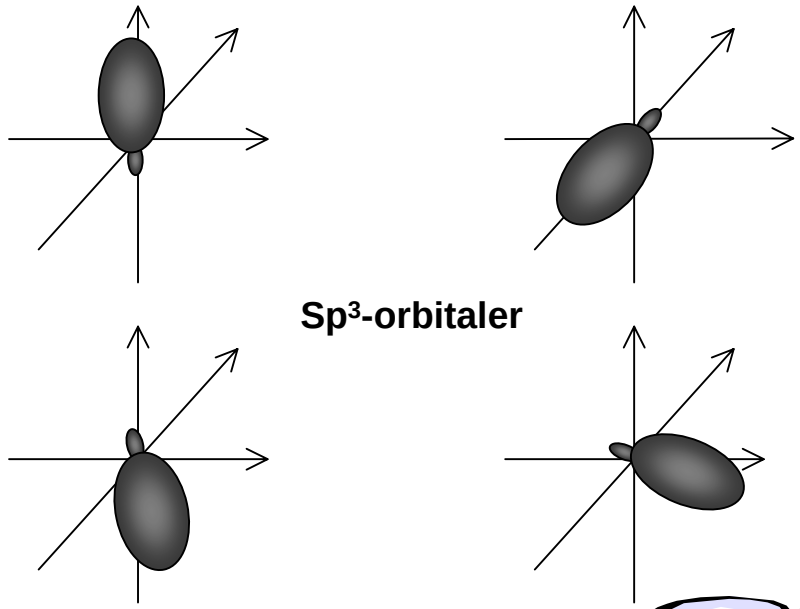
- **Fyra orbitaler kan nu vara med och skapa kovalenta bindningar till väte. Men alla bindningar i metan är ju lika?!**



Hybridisering

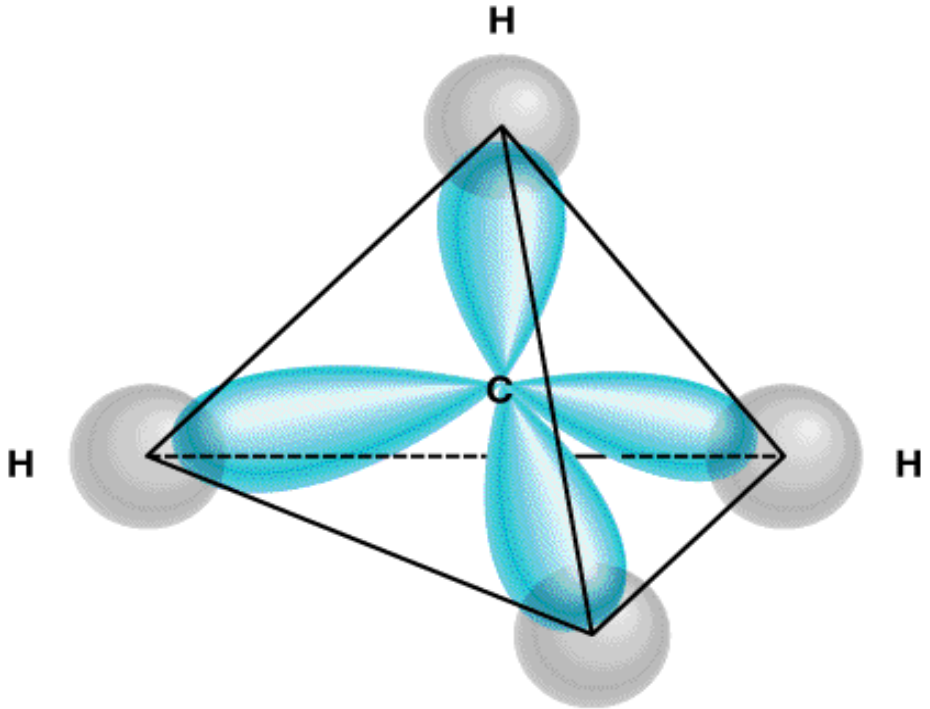
- **En s- och tre p-orbitaler omvandlas till fyra sp^3-orbitaler.**





Hybridisering

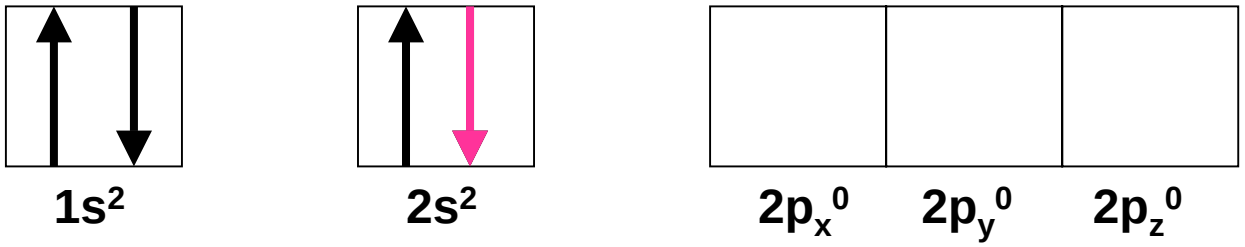
- **Kolatomen i CH_4 är sp^3-hybridiserad.**



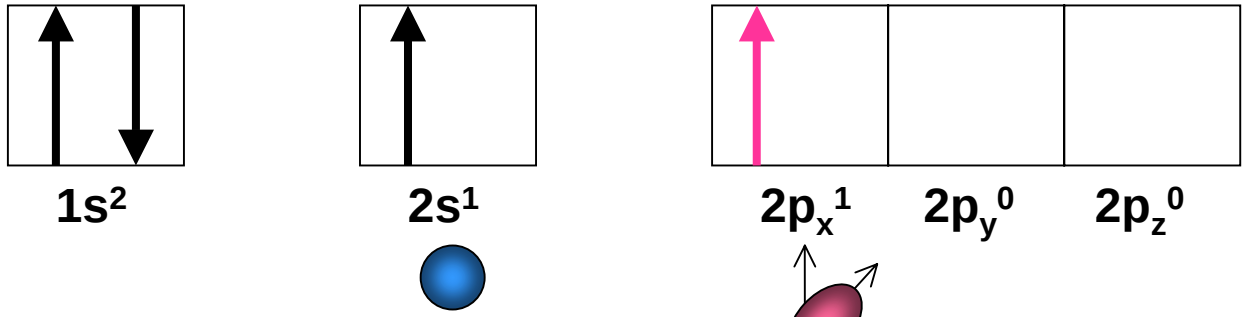
Hybridisering

- $BeCl_2$

Be_{grund}

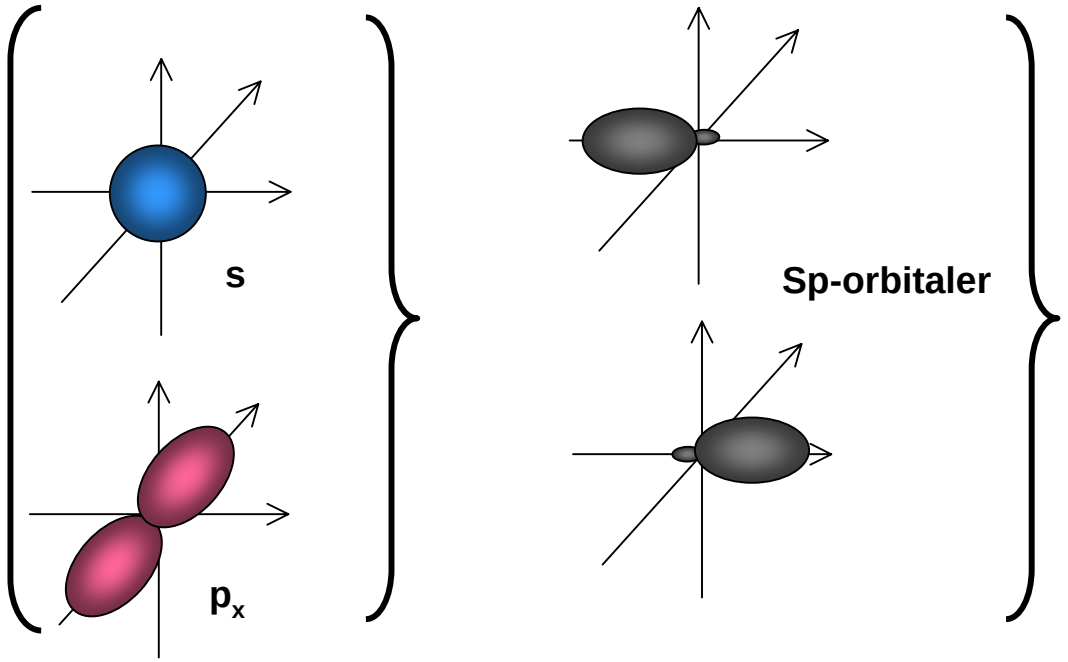


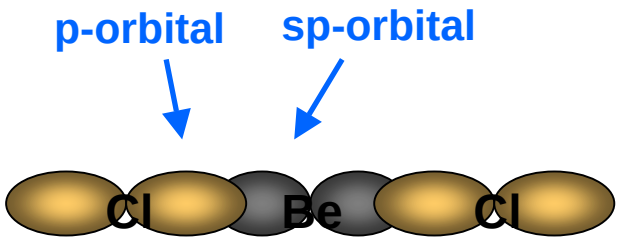
$Be_{exciterad}$



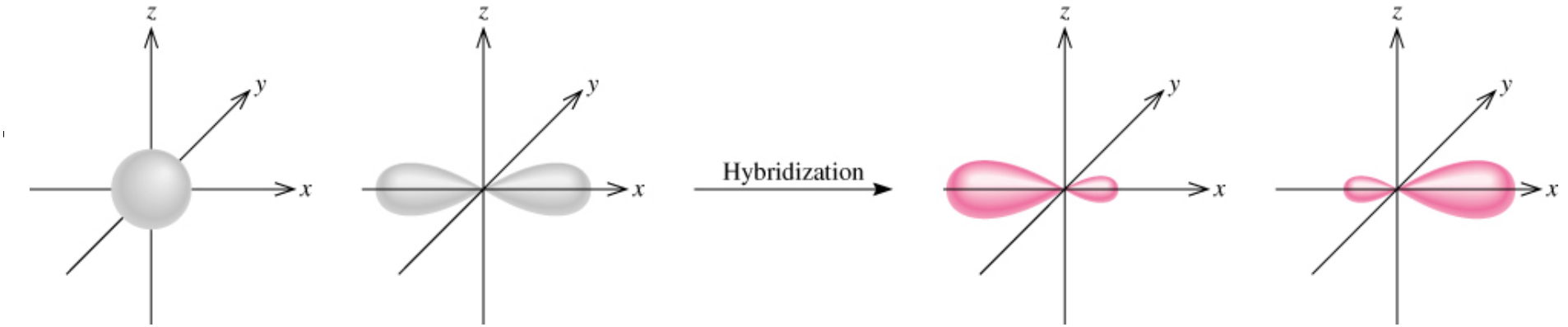
Hybridisering

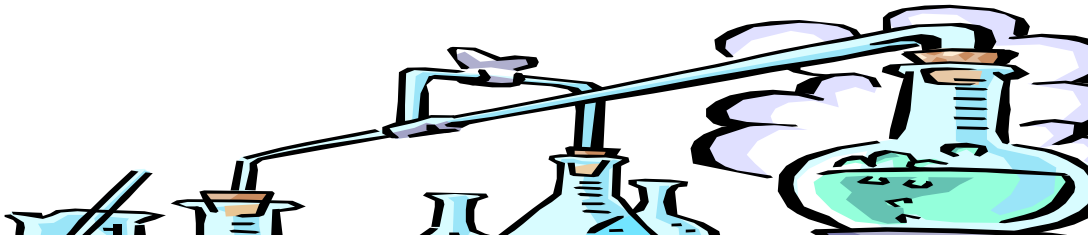
- **$BeCl_2$**
  - **En s- och en p-orbital kombineras till två sp-orbitaler. Be-atomen är sp-hybridiserad.**





Bildning av sp orbitaler

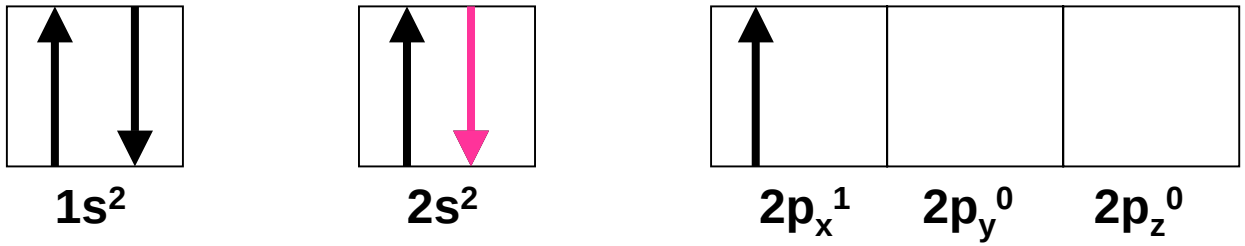




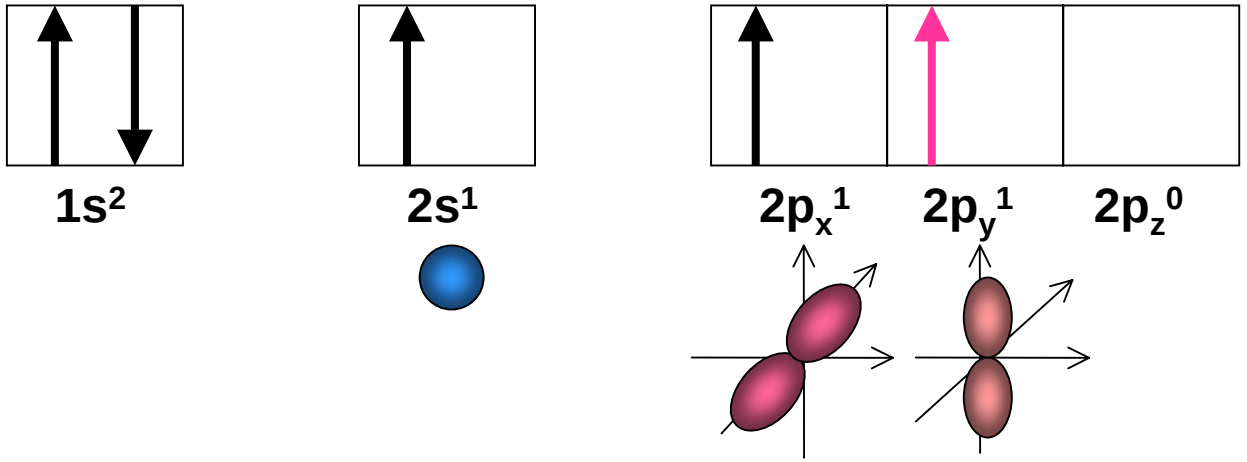
Hybridisering

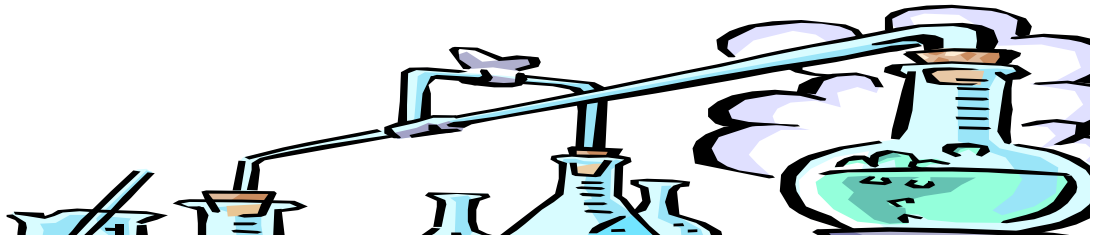
- BF_3

B_{grund}



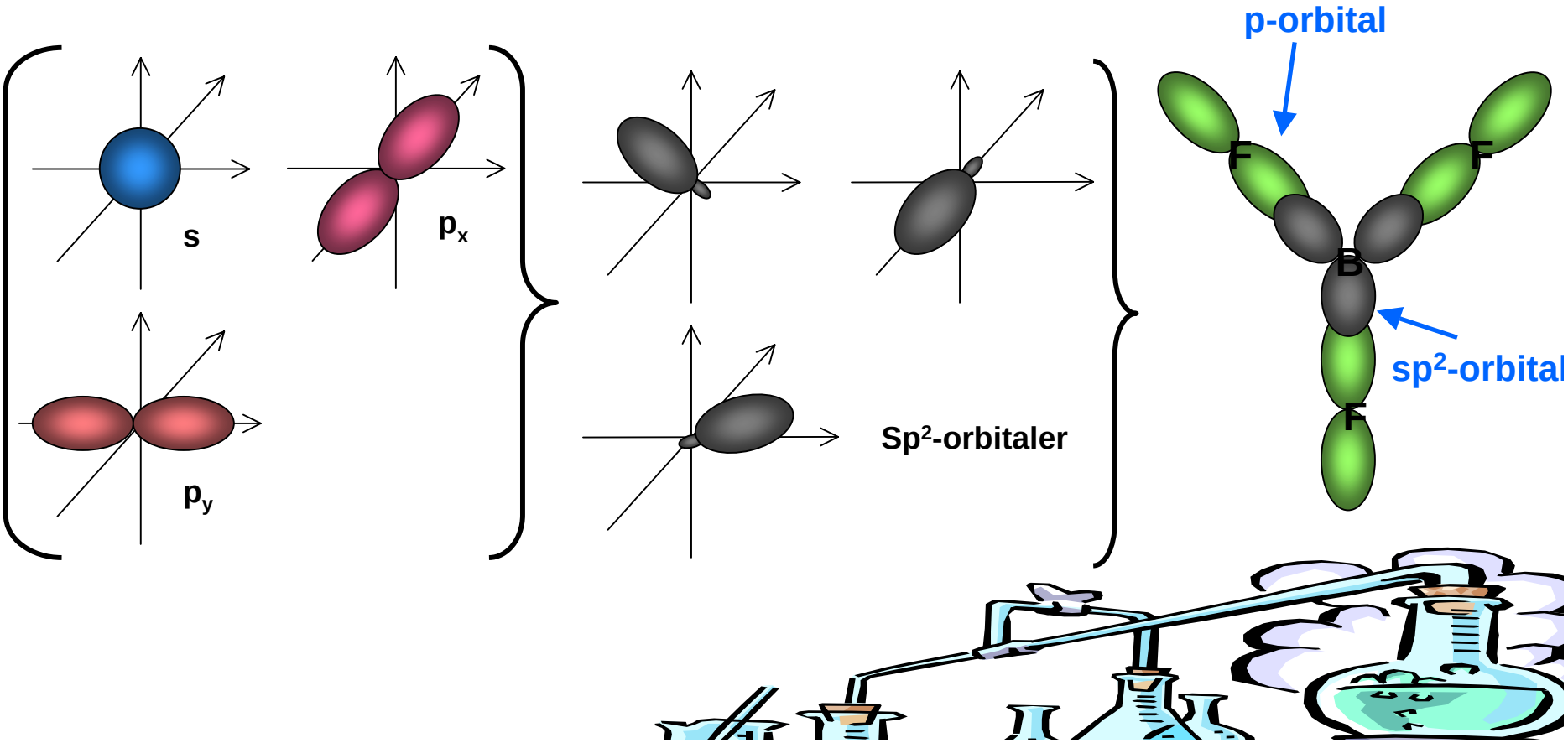
$B_{exciterad}$





Hybridisering

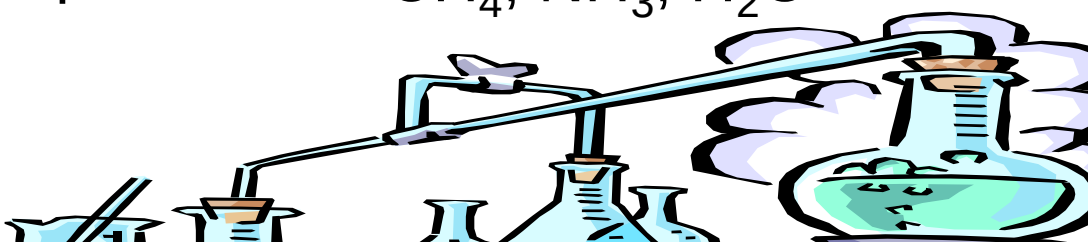
- BF_3
  - En s- och två p-orbitaler kombineras till tre sp^2-orbitaler. B-atomen är sp^2-hybridiserad.



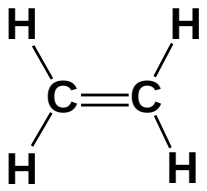
Hur vet man hybridiseringen?

- Räkna antalet fria elektronpar och antalet atomer bundna till centralatomen

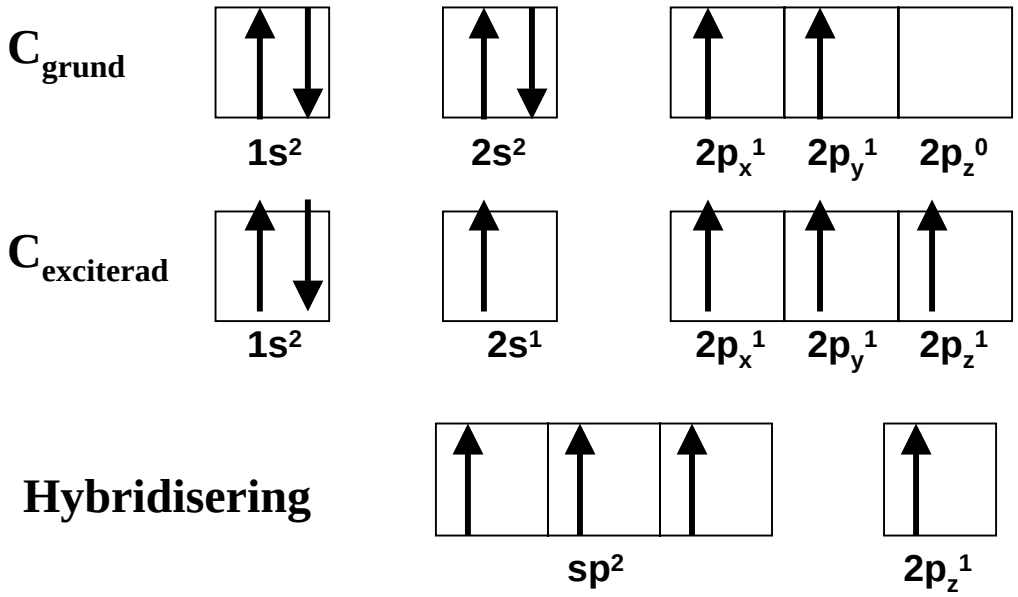
# fria e-par + # bundna atomer	hybridisering	exempel
2	sp	$BeCl_2$
3	sp^2	BF_3
4	sp^3	CH_4, NH_3, H_2O



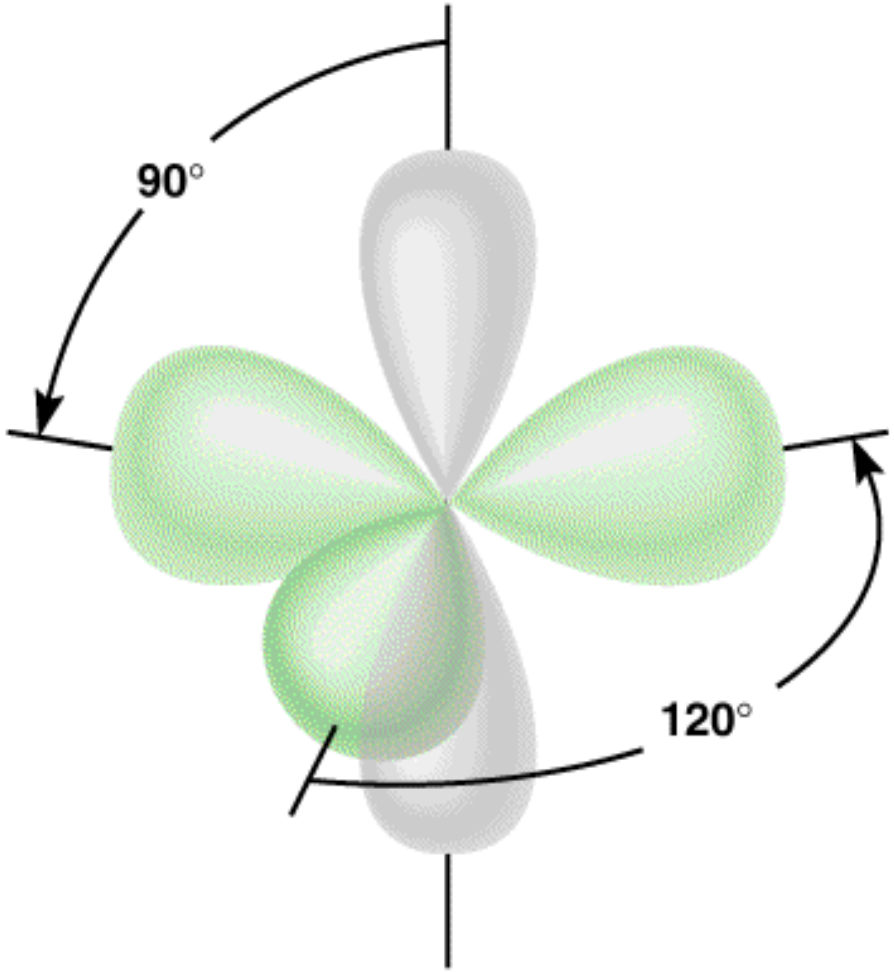
Dubbelbindning



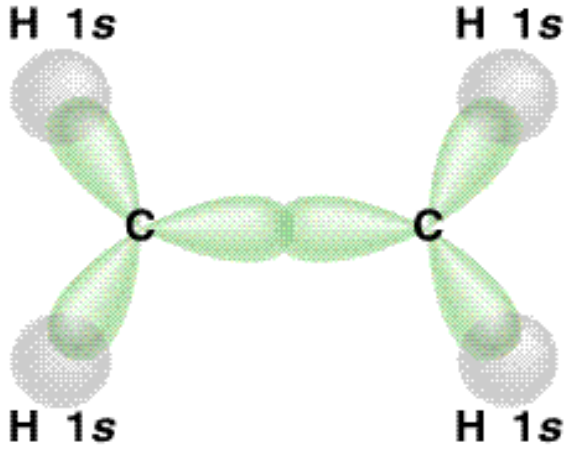
- **Eten**
  - **Liknar BF_3 utseendemässigt, plan molekyl, bindningsvinkel 120°. Sp^2-hybridiserade kol?**

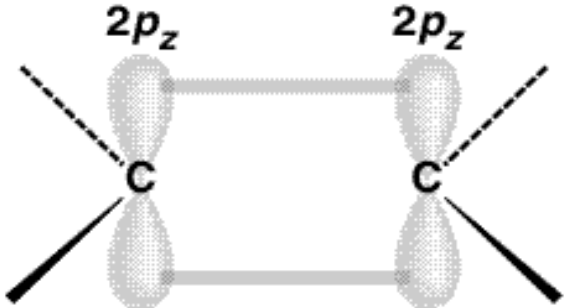


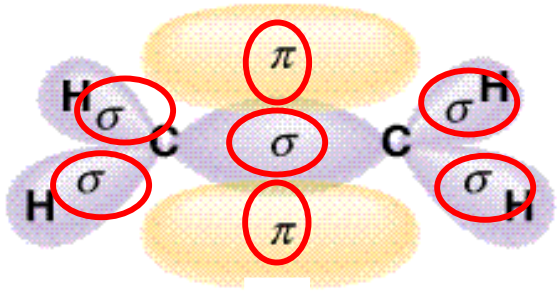
$2p_z$ orbitalen ligger vinkelrätt mot sp^2 planet



Etens dubbelbindning







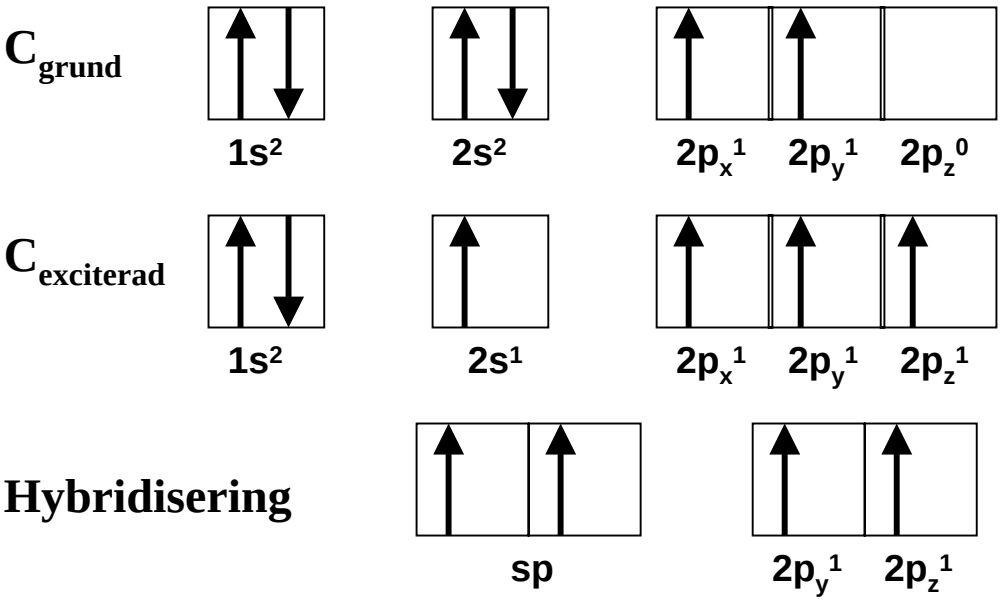
π-elektrondensitet ovanför och under kärnplanet

σ-elektrondensitet mellan atomkärnorna

Trippelbindning

H—C≡C—H

- **Etyn (Acetylen)**
  - **Liknar $BeCl_2$ utseendemässigt, linjär molekyl, bindningsvinkel 180º. Sp-hybridiserade kol?**



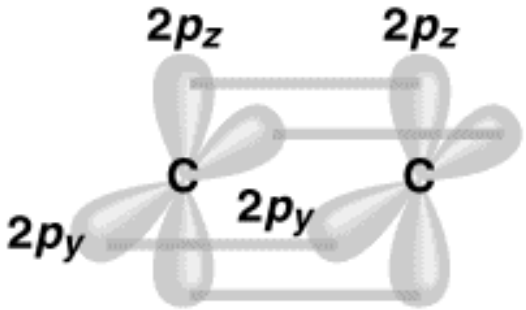
Sp + två p-orbitaler blir över!

Trippelbindning

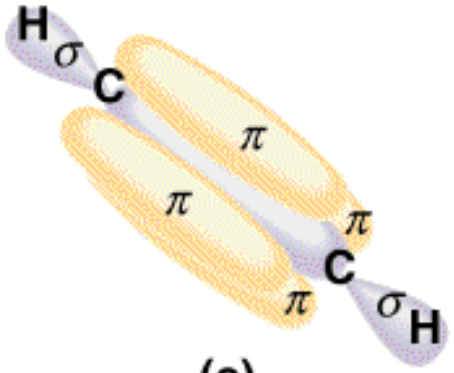
H—C≡C—H

- **Etyn**

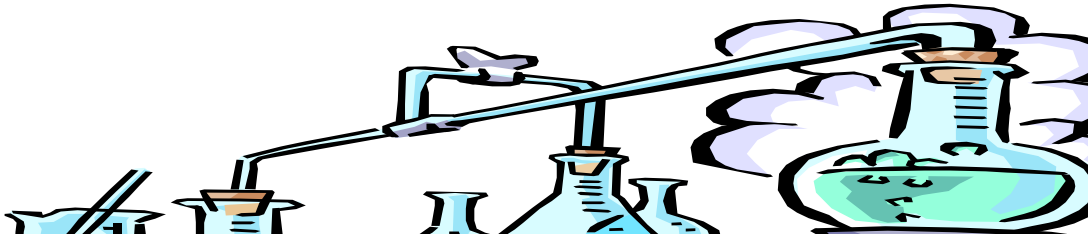
(a)



(b)

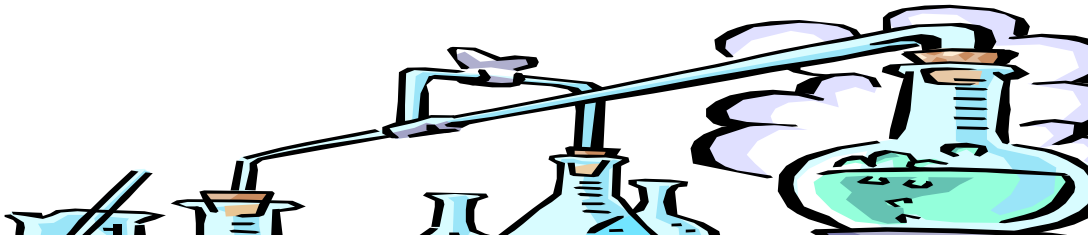


(c)



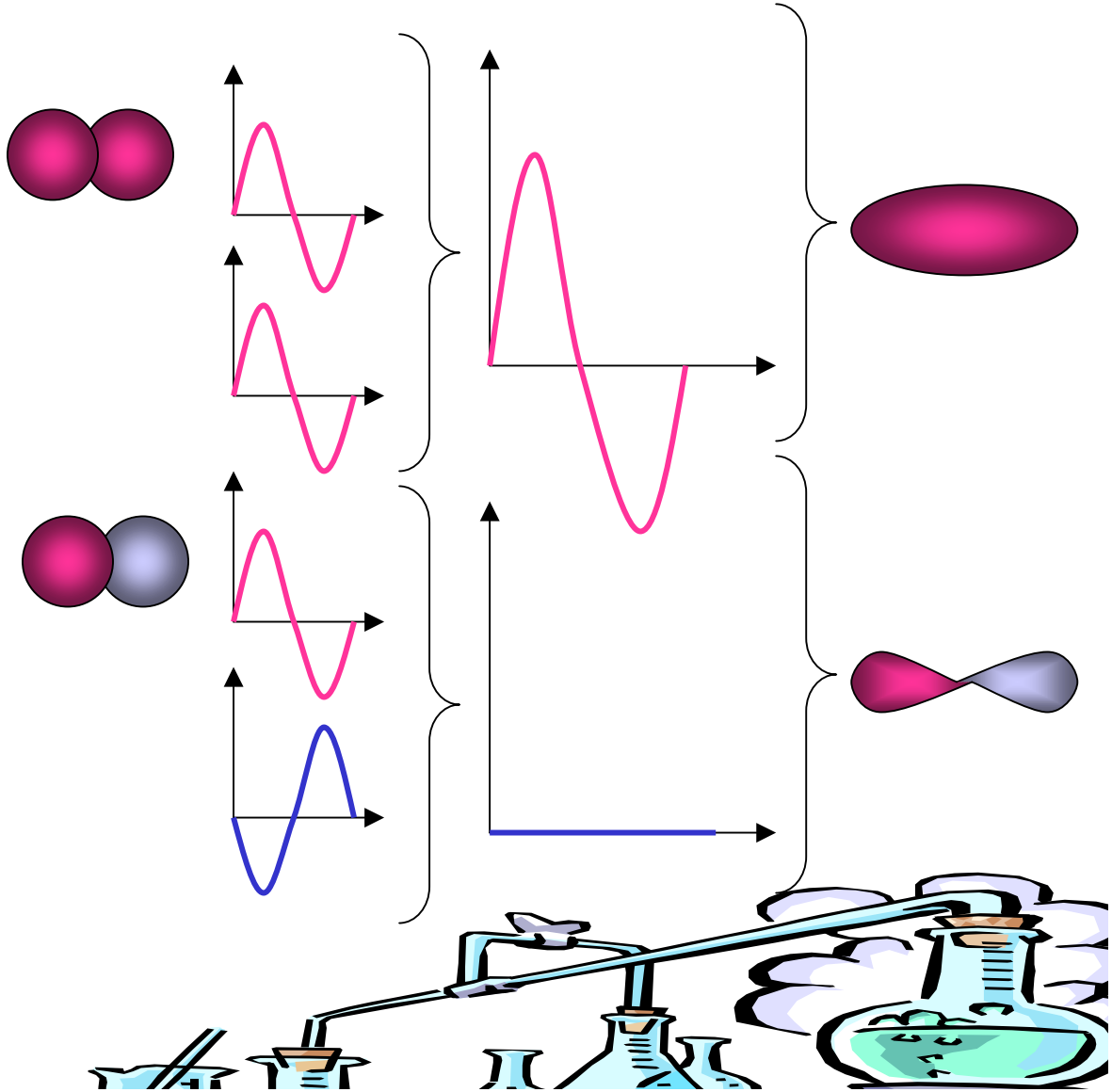
MO-teori

- **MO-teori (Molecular orbital)**
  - **Molekylorbitaler skapas av de i molekylen ingående atomernas atomorbitaler.**
  - **Varje elektron deltar i en orbital som är karakteristisk för molekylen som helhet.**
    - **Om orbitalerna som överlappar varandra är i samma fas skapas en bindning, de kallas bindande orbitaler. De bindande orbitalerna har låg energi.**
    - **Om orbitalerna som överlappar varandra är i motsatt fas skapas ingen bindning, de kallas antibindande orbitaler. De antibindande orbitalerna har hög energi och är ostabila.**



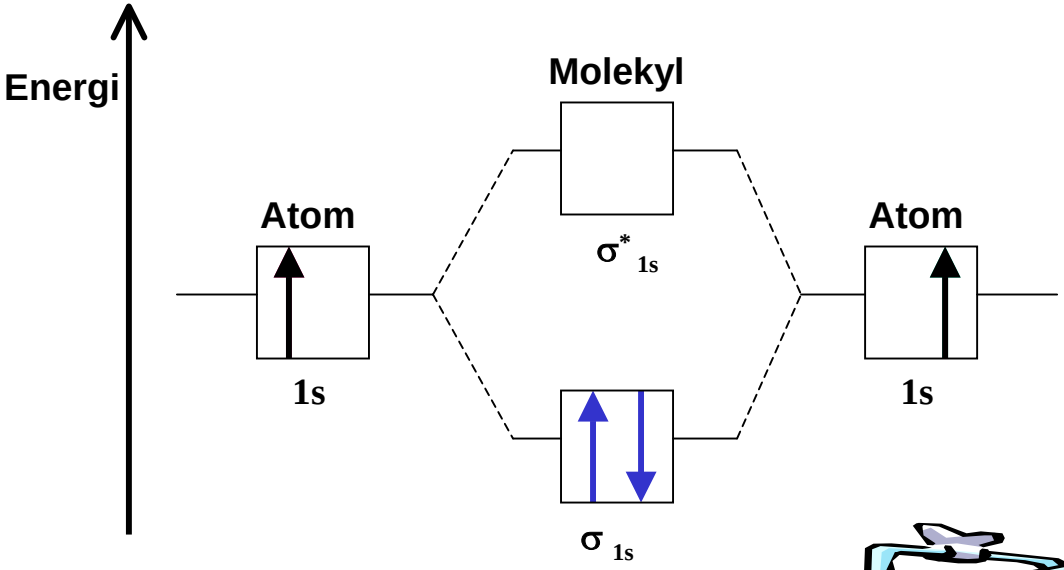
MO-teori

- **Bindande orbitaler (σ)**
- **Antibindande orbitaler (σ*)**



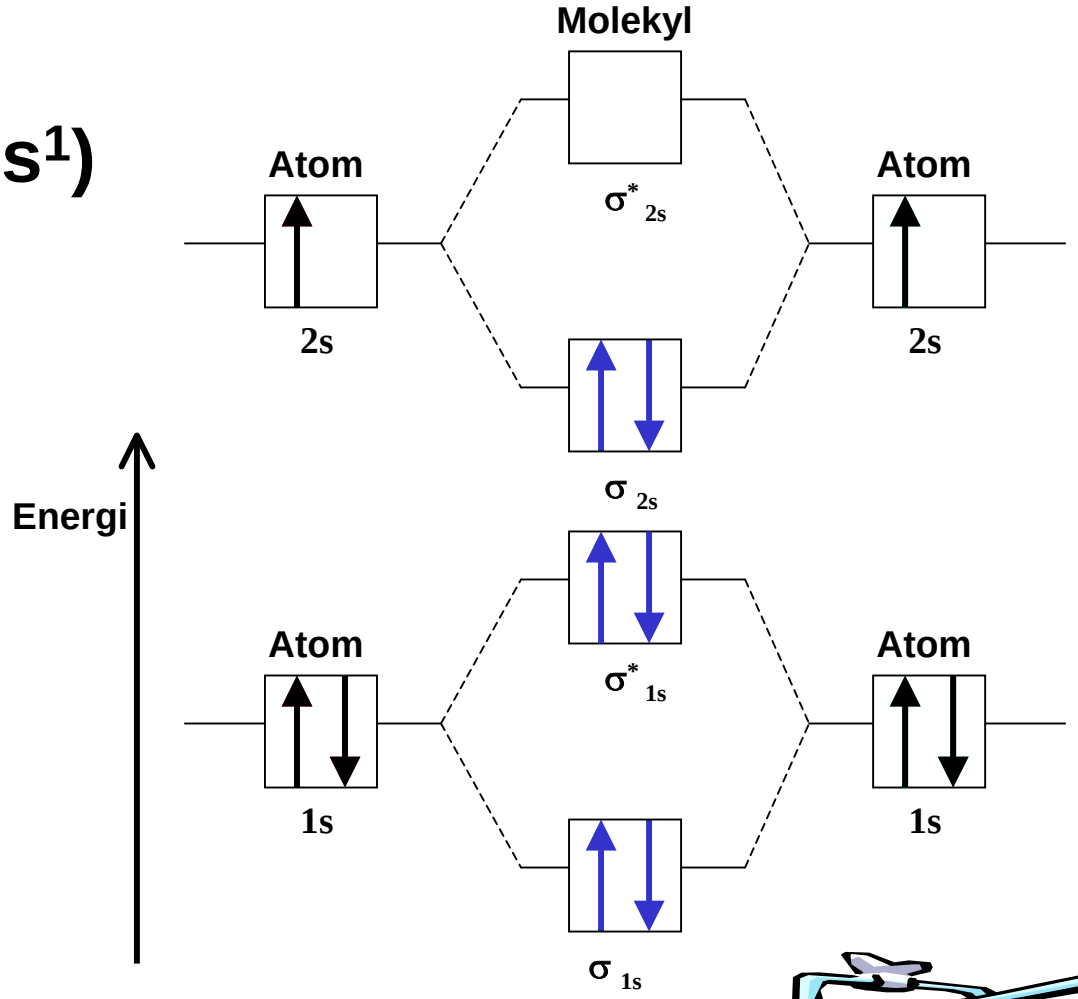
MO-teori

- H_2 ($1s^1$)
  - Energinivåerna för bindande respektive anti-bindande molekylorbitaler i en molekyl:



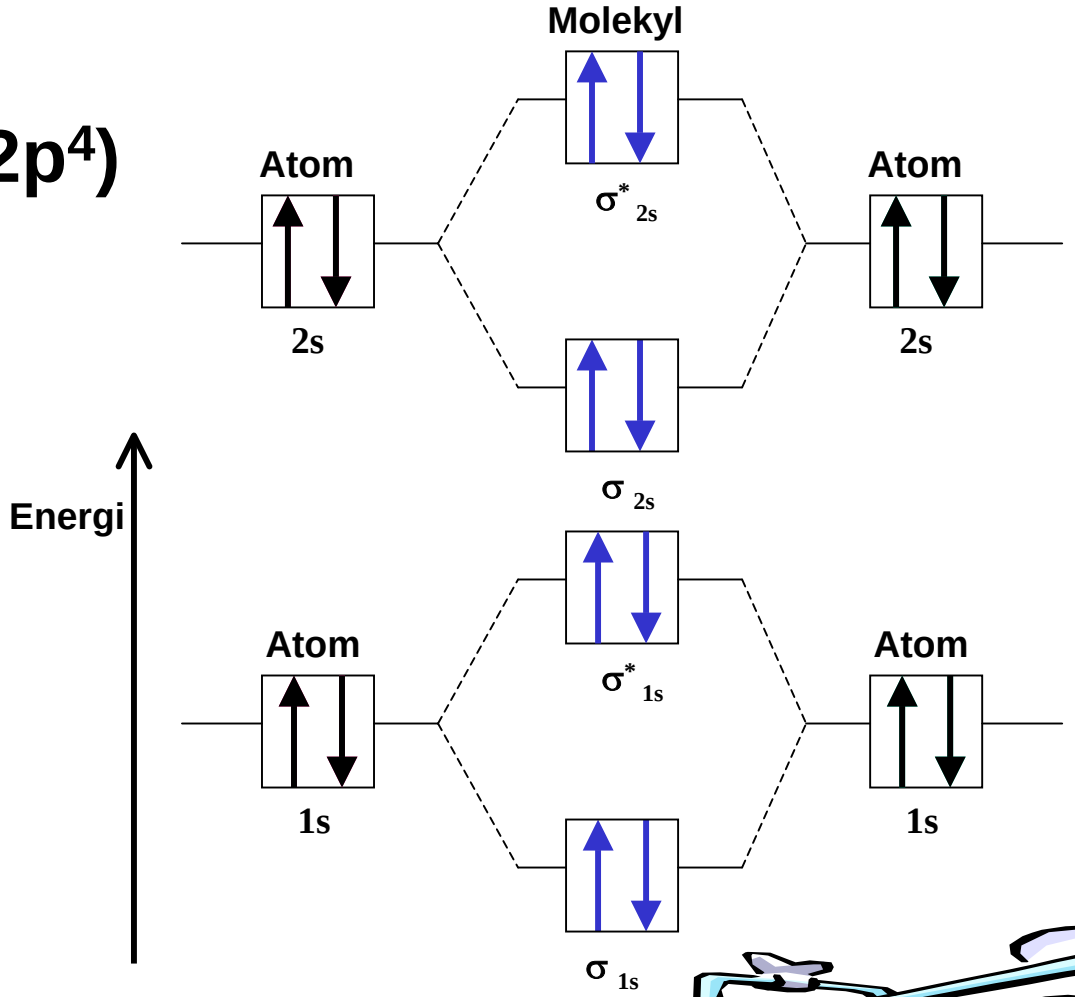
MO-teori

- Li_2 ($1s^2\ 2s^1$)

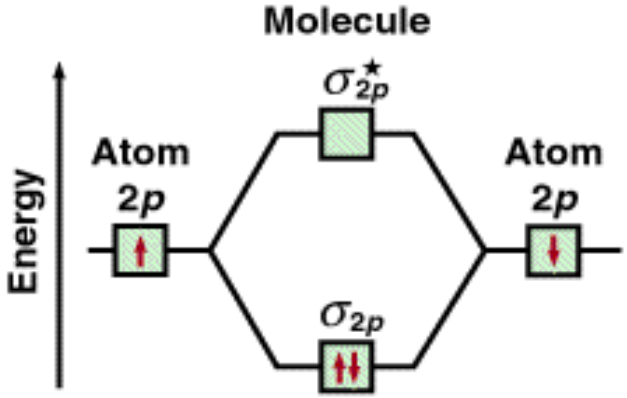


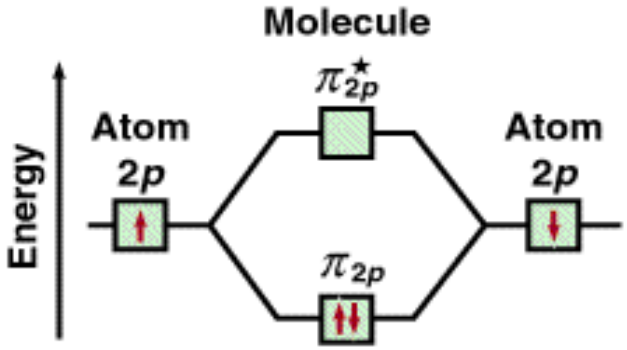
MO-teori

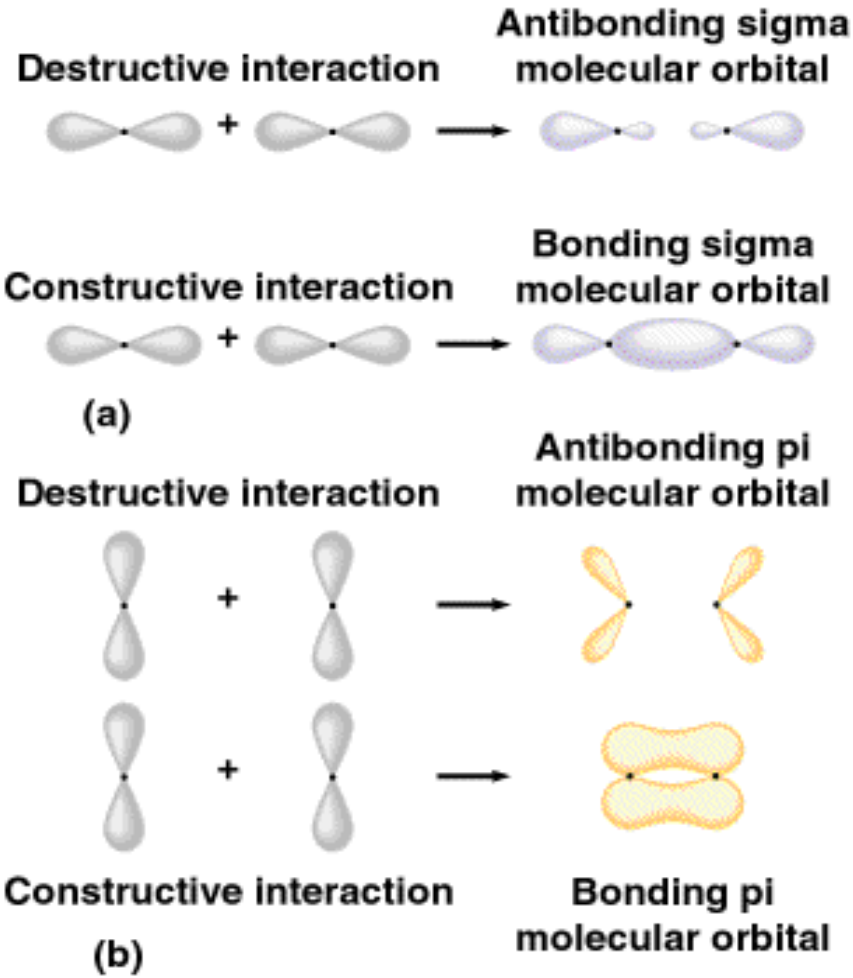
- O_2 ($1s^2\ 2s^2 2p^4$)



Bindande och icke bindande π orbitaler

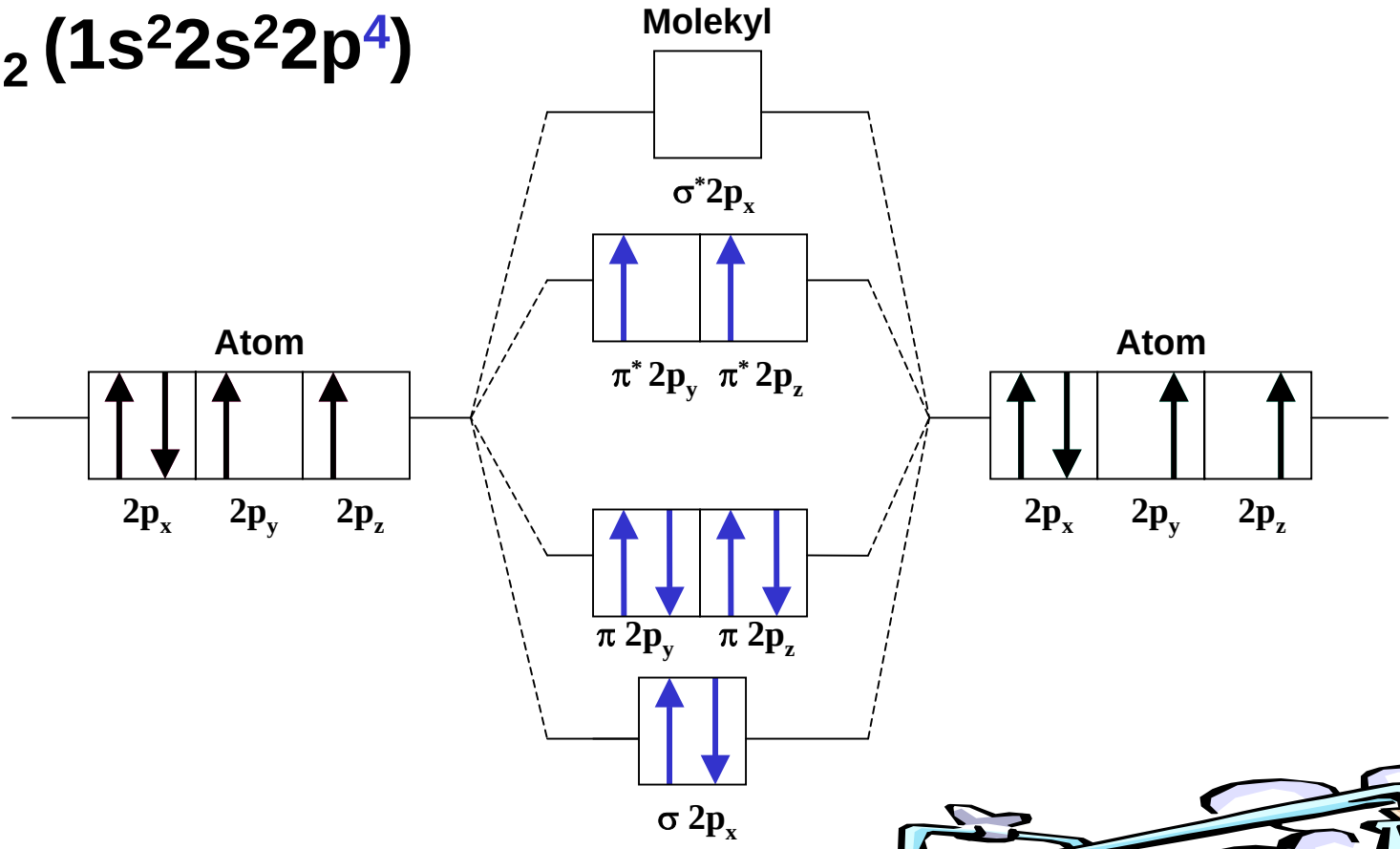






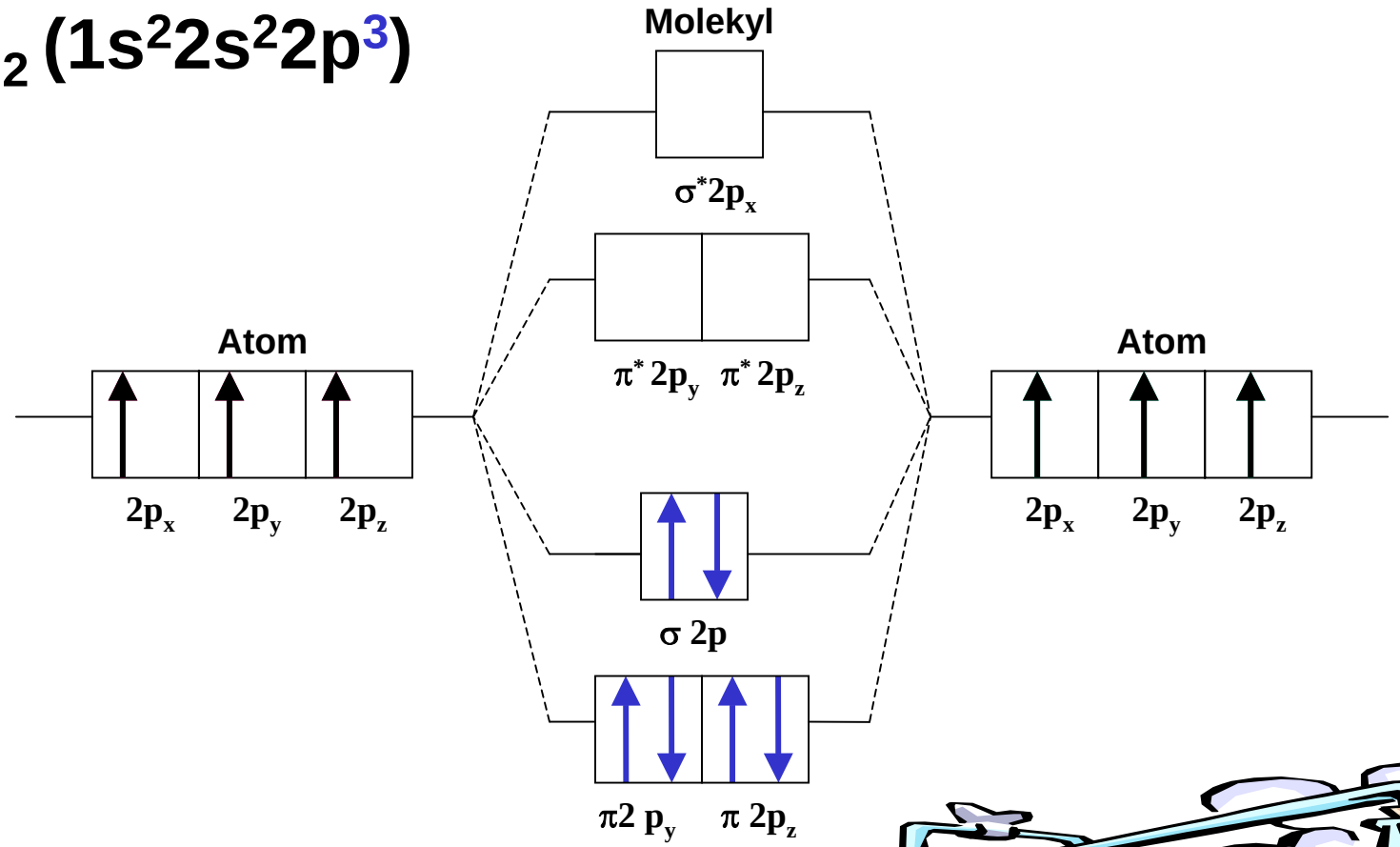
MO-teori

- O_2 ($1s^2 2s^2 2p^4$)



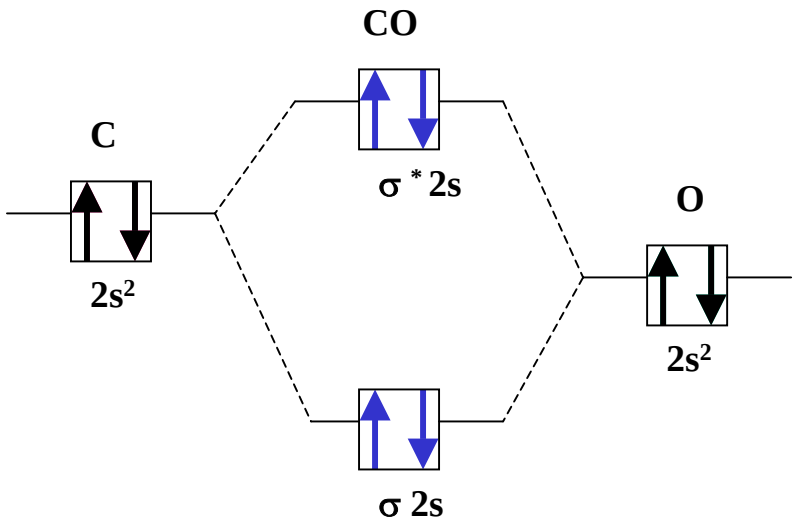
MO-teori

- N_2 ($1s^2 2s^2 2p^3$)



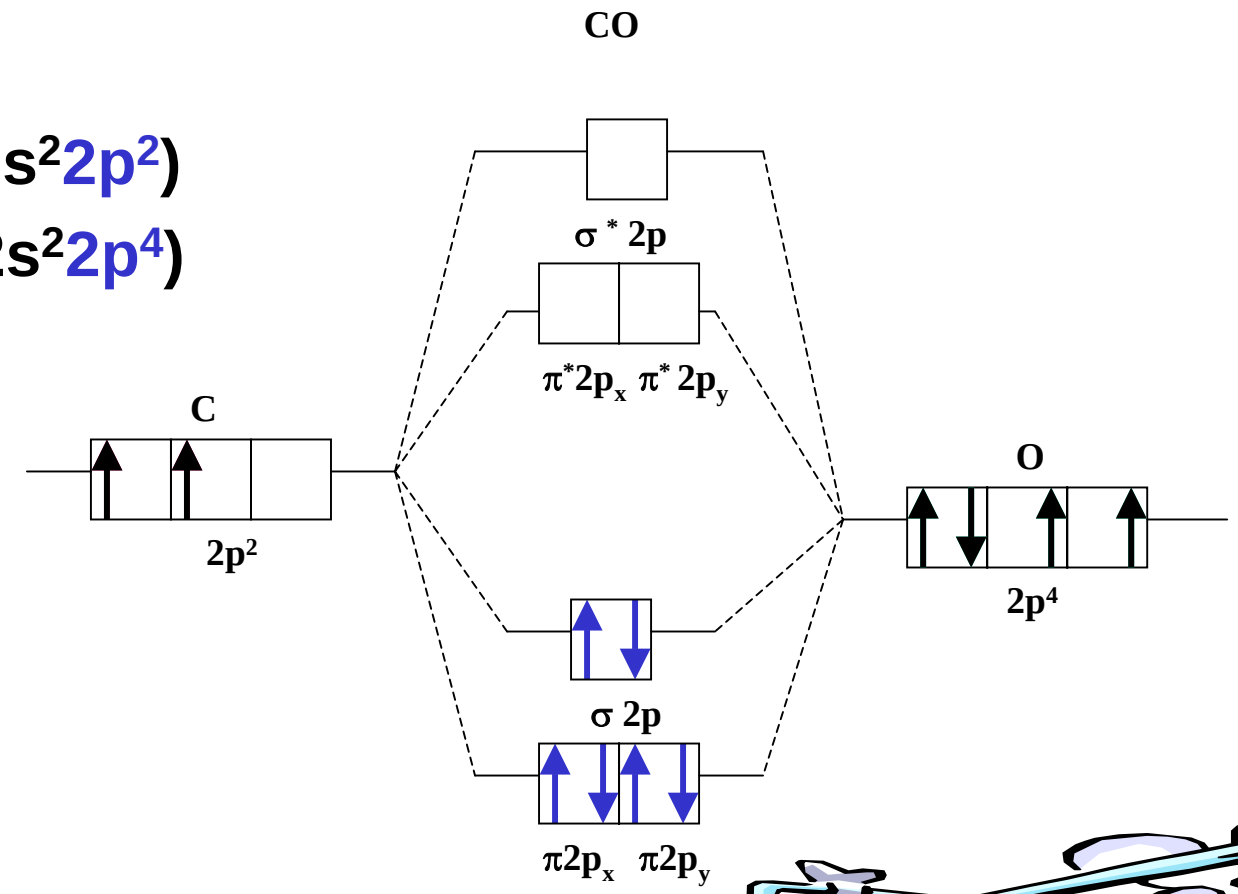
MO-teori

- **CO**
  - C ($1s^2 2s^2 2p^2$)
  - O ($1s^2 2s^2 2p^4$)

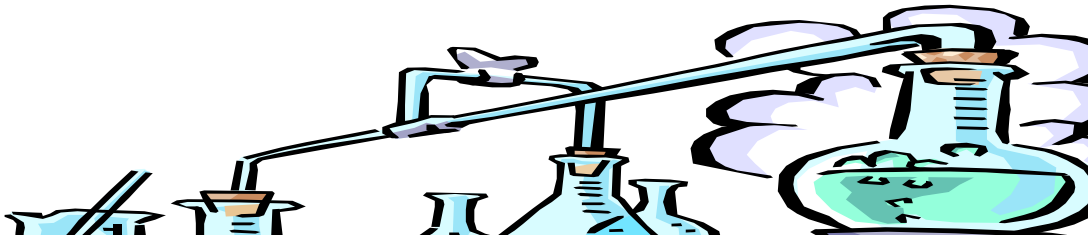


MO-teori

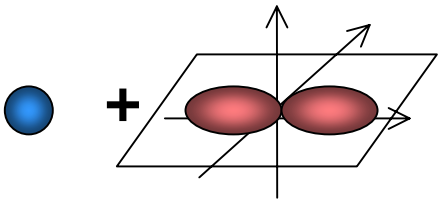
- **CO**
  - **C ($1s^2 2s^2 2p^2$)**
  - **O ($1s^2 2s^2 2p^4$)**

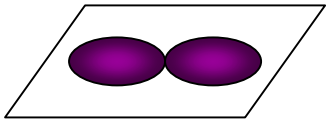


Lite repetition



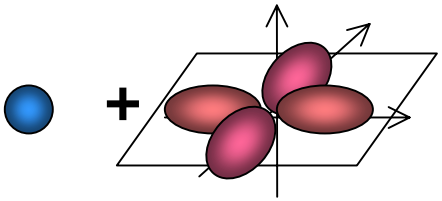
Hybridisering

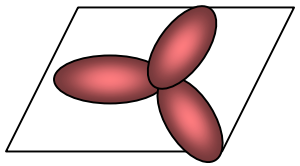




2 st sp-orbitaler

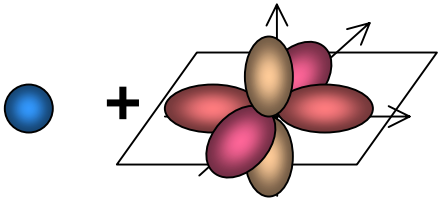
180°, linjär

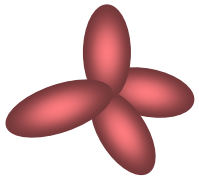




3 st sp^2-orbitaler

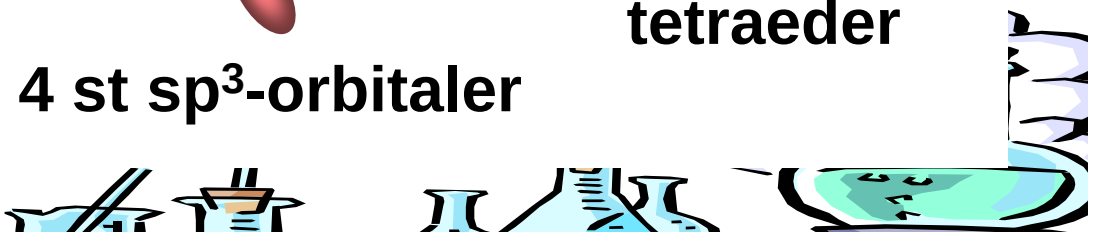
120°, plan triangulär





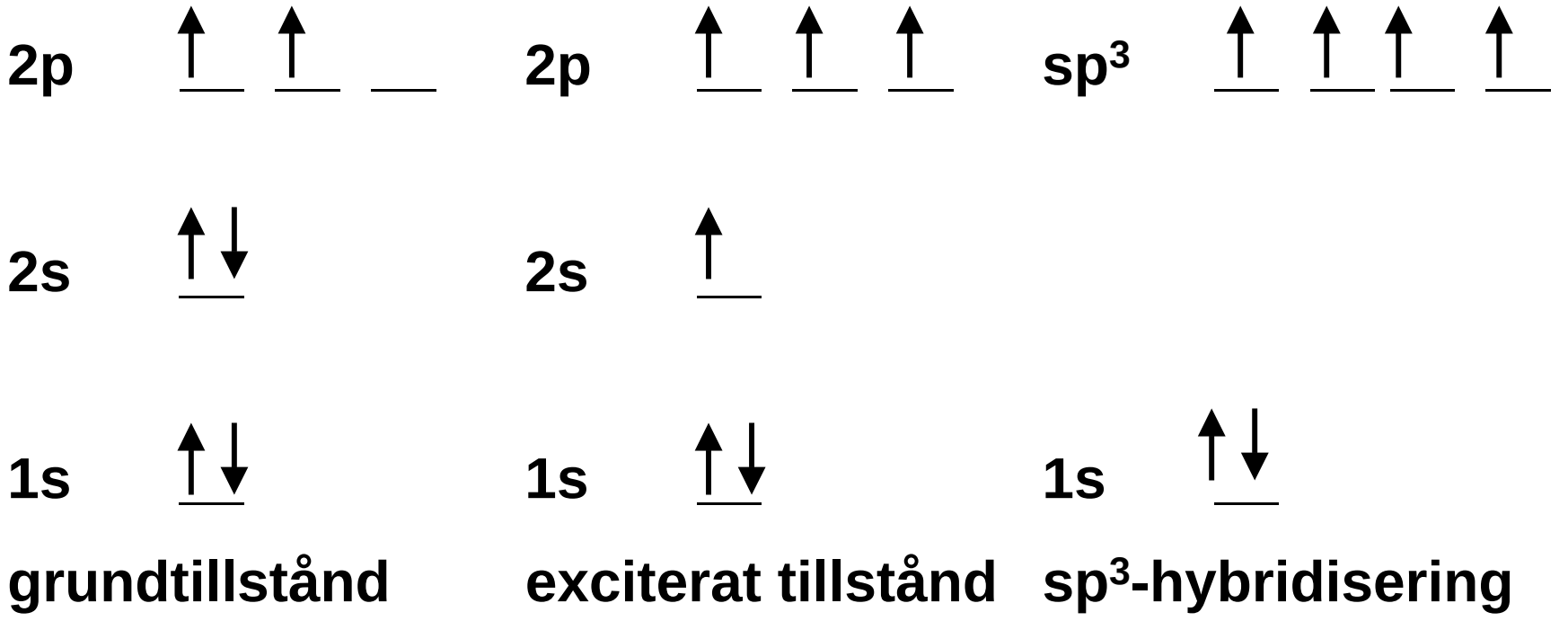
4 st sp^3-orbitaler

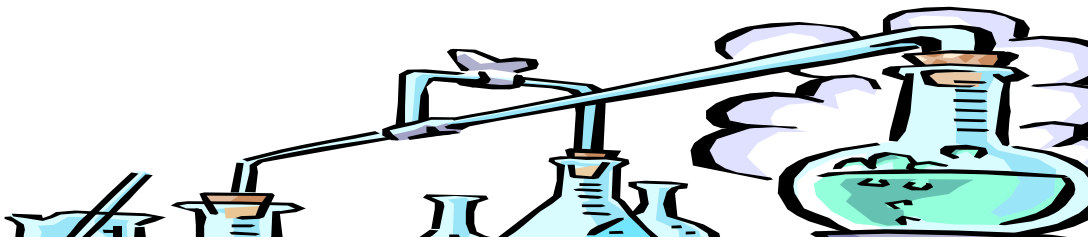
109.5° tetraeder



Hybridisering - kolatomen

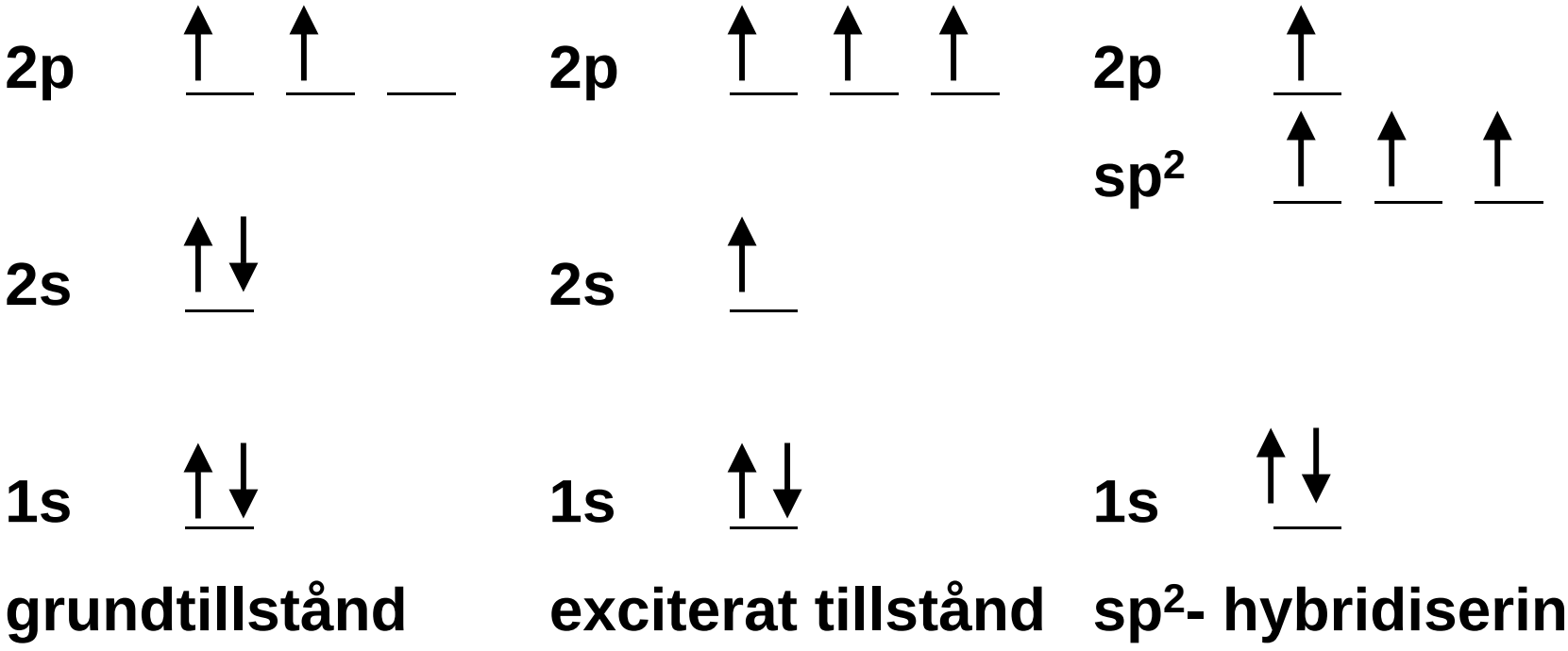
- **sp^3-hybridisering:**

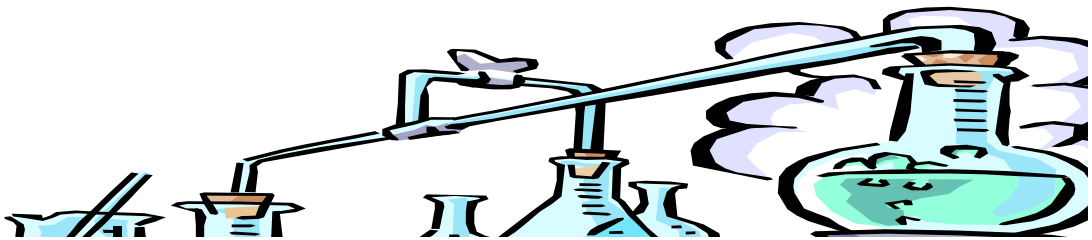




Hybridisering - kolatomen

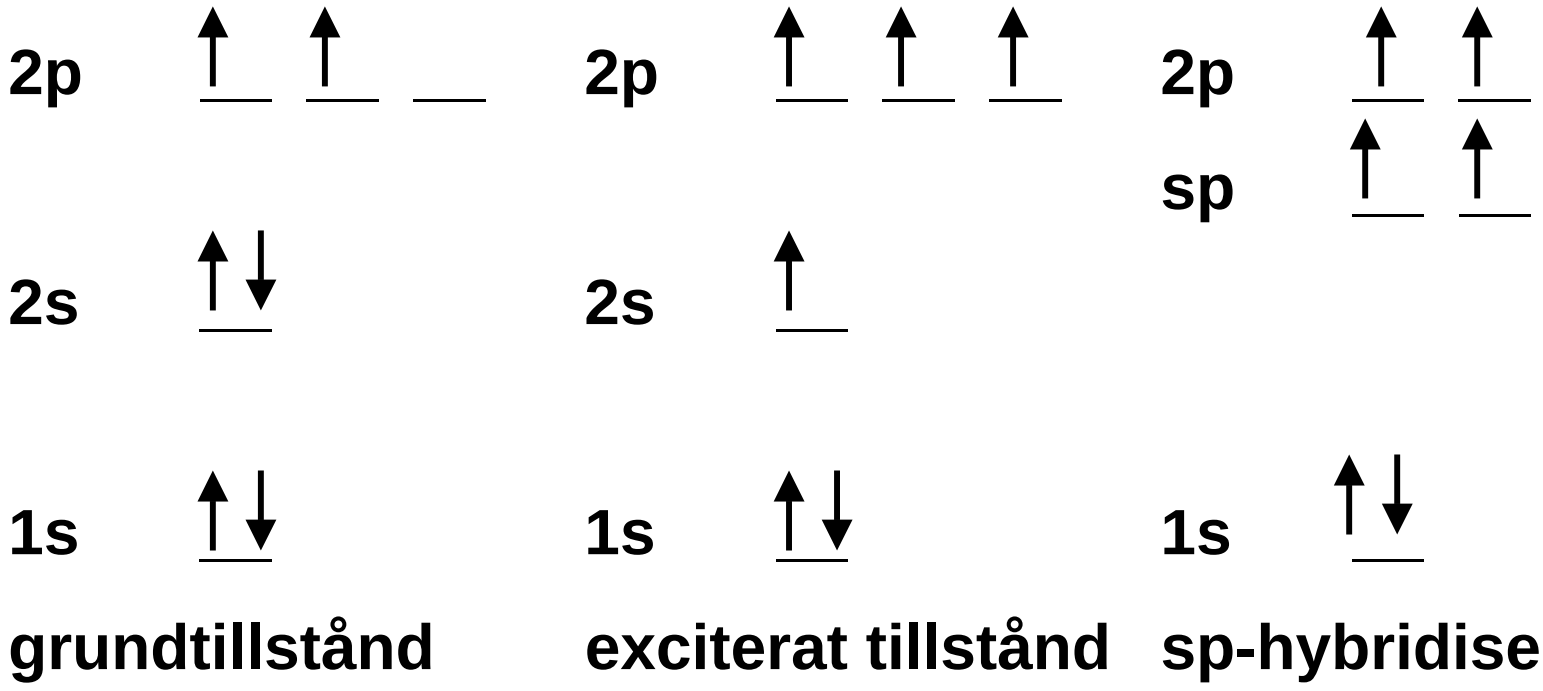
- **sp^2-hybridisering:**

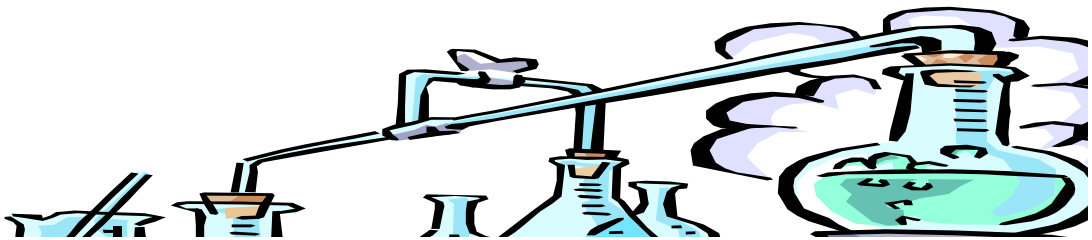




Hybridisering - kolatomen

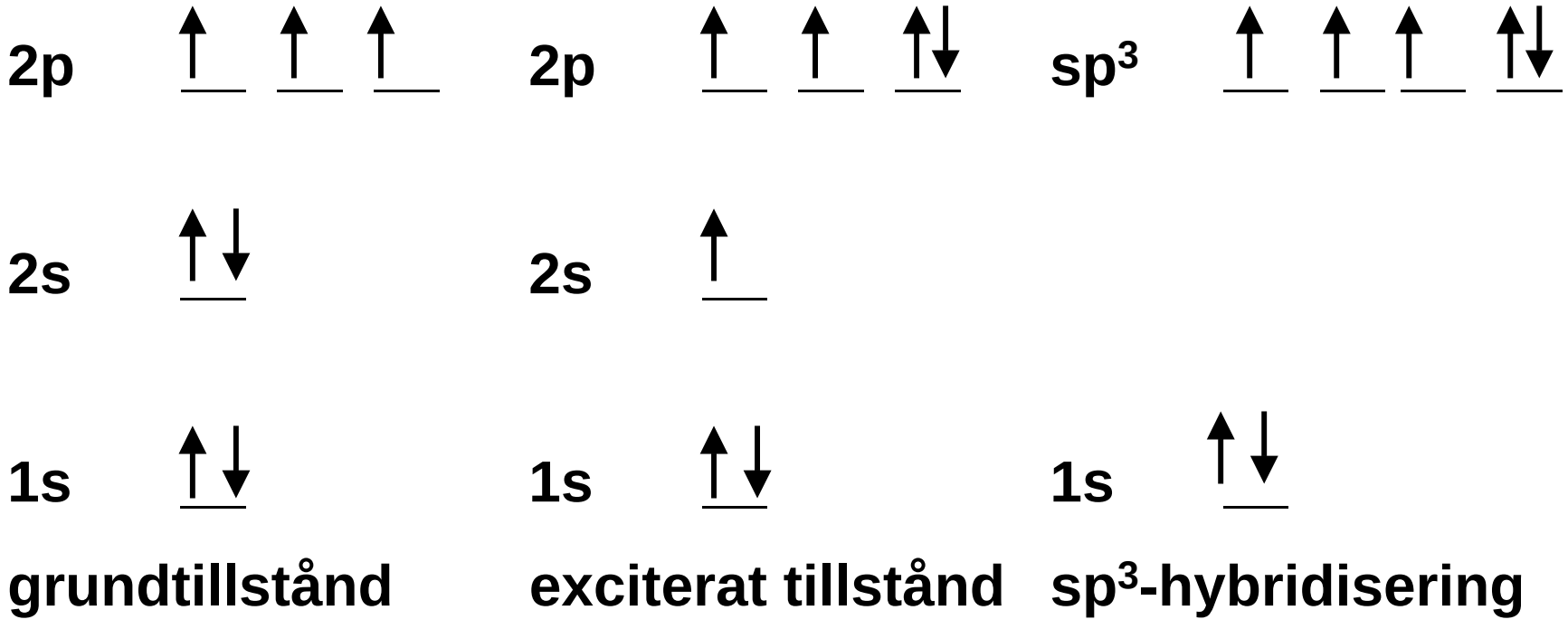
- **sp-hybridisering:**

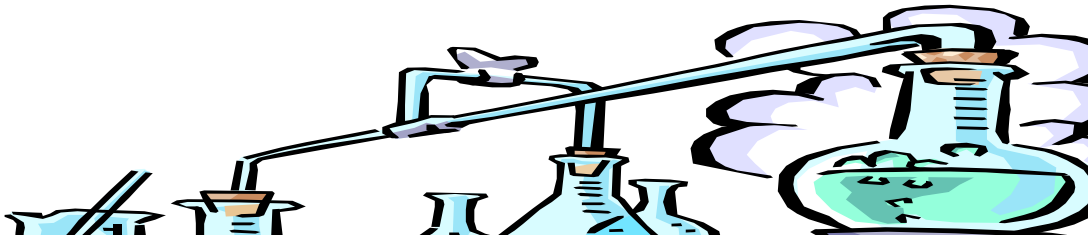




Hybridisering - kväveatomen

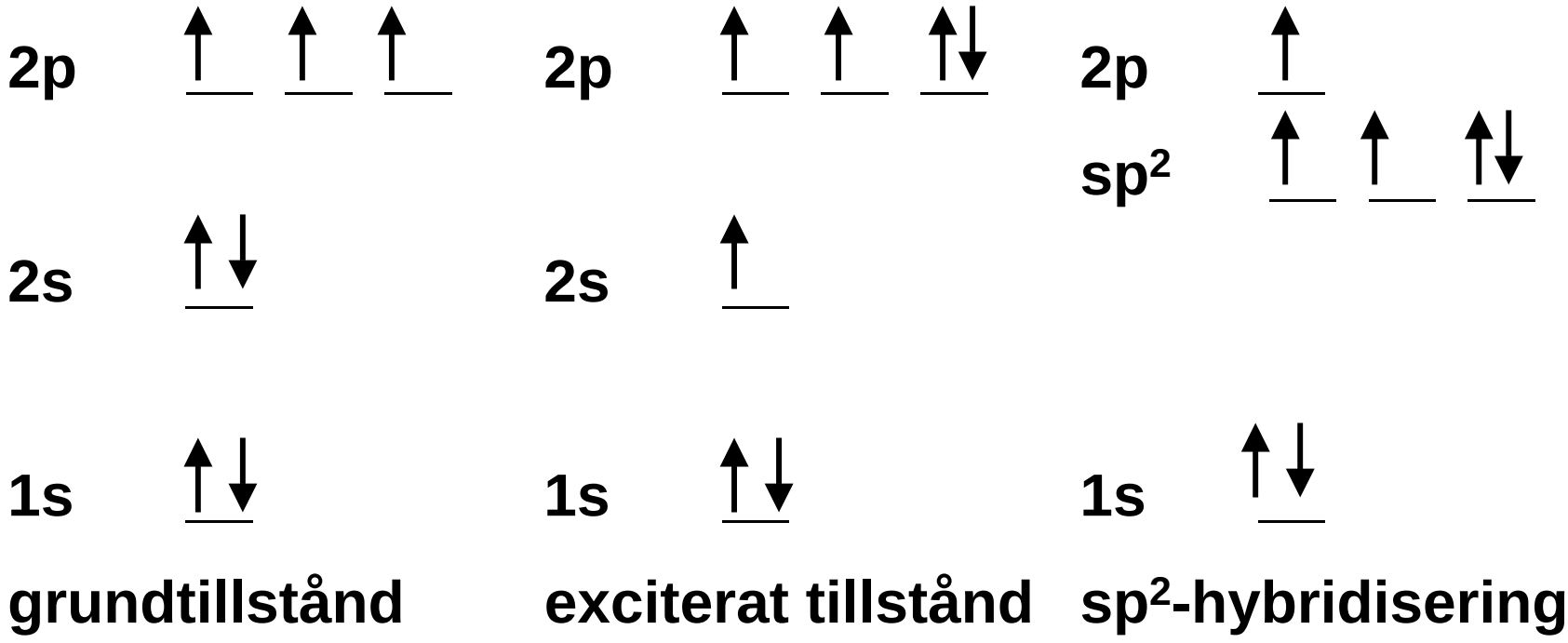
- **sp^3-hybridisering:**

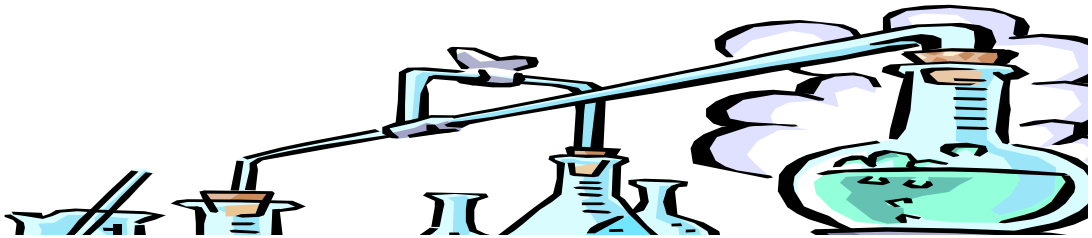




Hybridisering - kväveatomen

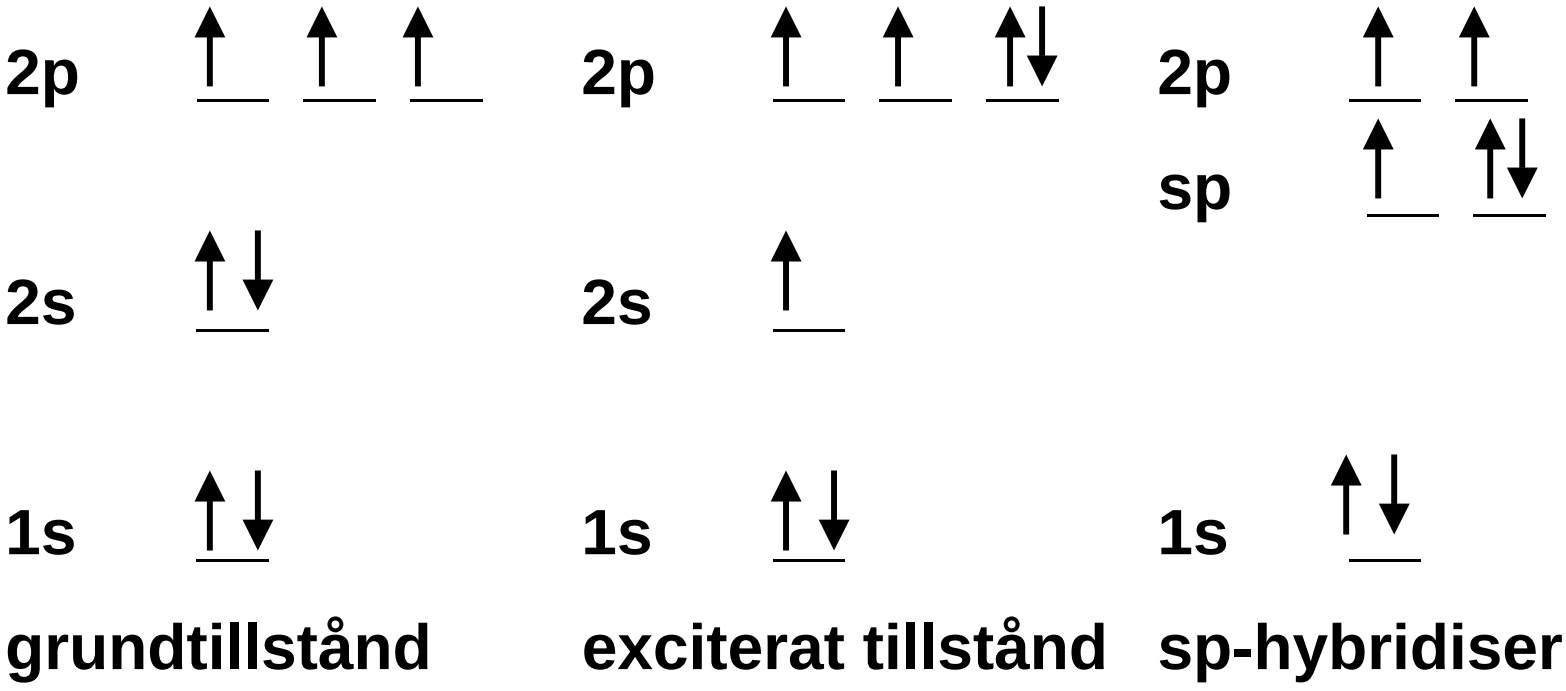
- **sp^2-hybridisering:**

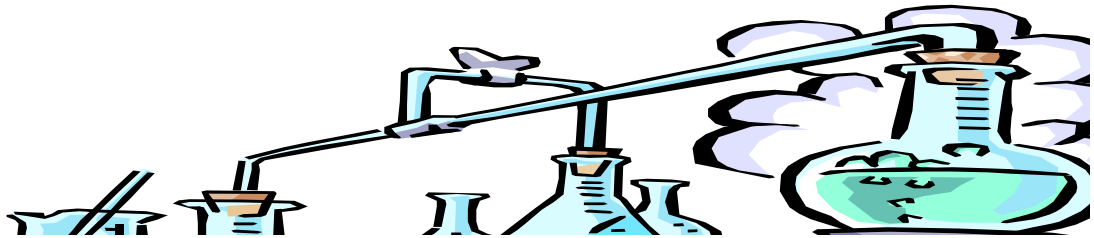




Hybridisering - kväveatomen

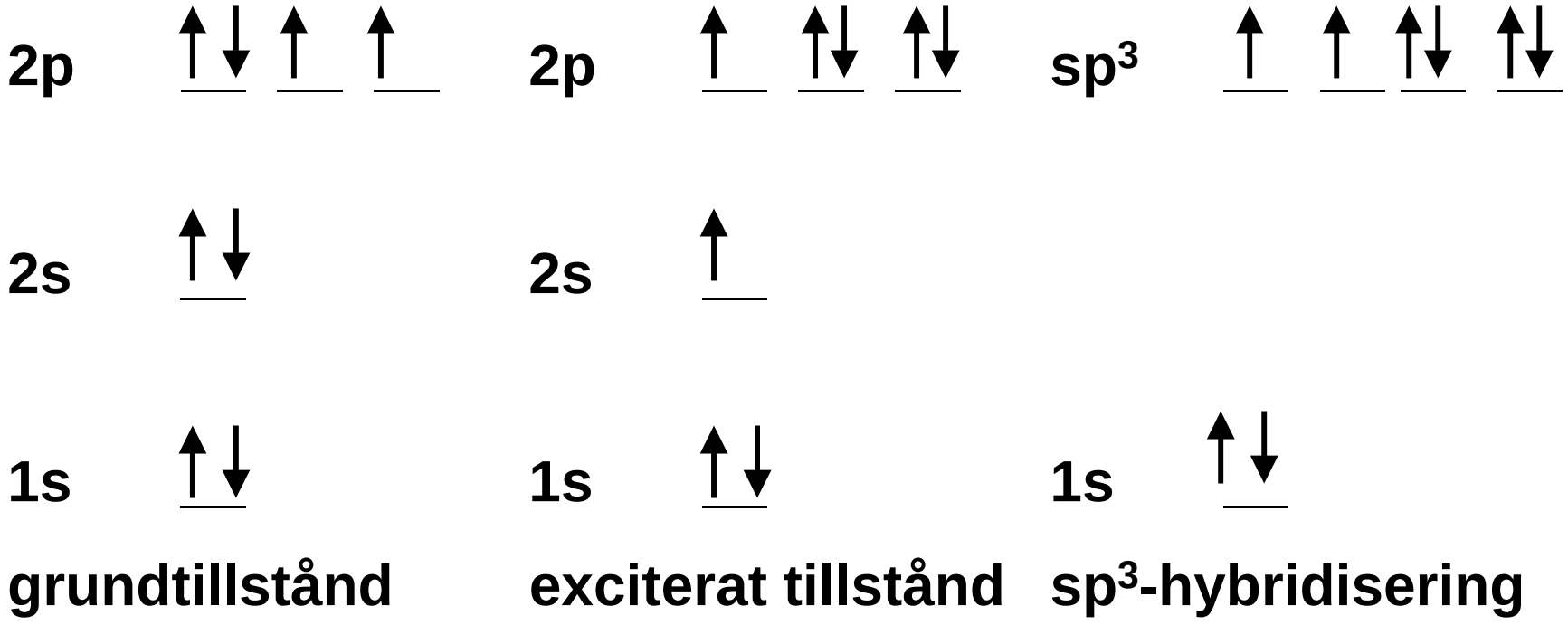
- **sp-hybridisering:**

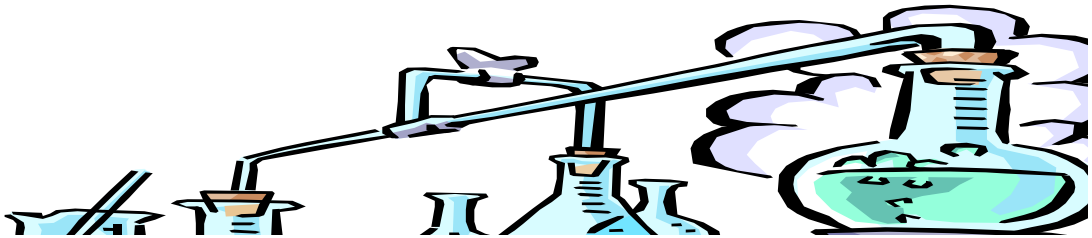




Hybridisering - syreatomen

- **sp^3-hybridisering:**





Hybridisering - syreatomen

- **sp^2-hybridisering:**