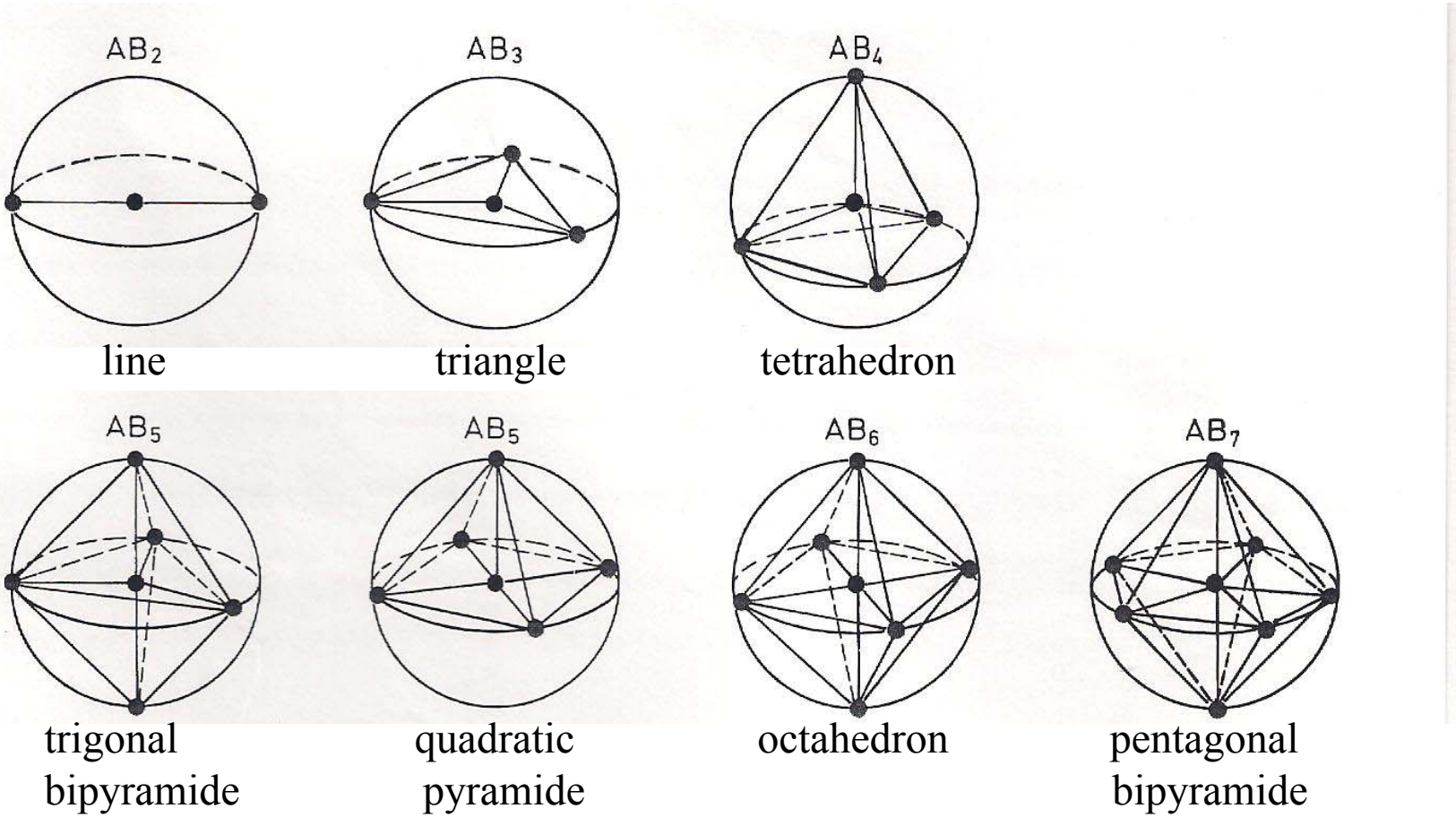
Point arrangements on a sphere with maximum distances



AB_n represent molecules AX_mE_n (A = central atom, X = ligand atom, E = free electron pair). The horizontal and axial positions of AB_5 are not equivalent.

How to use VSEPR

VSEPR = (V)alence (S)hell (E)lectron (P)air (R)epulsion
The VSEPR Theory was developed by Gillespie & Nyholm. With this theory it is possible to determine nearly every molecular structure. The general idea of this concept is to handle the free electron pairs of the central atom of a molecule as ligands. **The ligands and electron pairs are arranged with a maximal distance to each other.**

The following rules are important to determine the correct molecular structure on the basis of this concept:

1. Draw the complete Lewis structure of the molecule
2. Localize the central atom by using the Lewis concept
3. Count the number of ligands and add the number of free electron pairs of the central atom (Coordination number)
4. a) Determine the Ψ-polyhedra (maximal distance between all ligands and free electron pairs)
   b) A free electron pair needs more space than a ligand (the bond angles in a molecule with free electron pairs are different from those with only ligands but with the same coordination number)
   c) multiple bonds count as one ligand but they need more space than single bonds
   d) ligands with a higher electronegativity attract the binding electrons and decrease their required space
5. "Remove" the free electron pairs from the Ψ-polyhedra to determine the real structure of the molecule
6. For central atoms of 3. period or higher, the lone pair will occupy a nonbonding orbital and bnding will be through p orbitals with bond angles near 90 ^{o}.

Examples for the most important structures

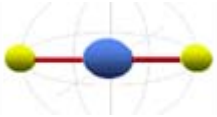
a) without free electron pairs

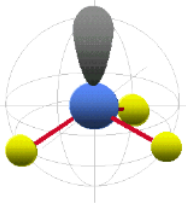
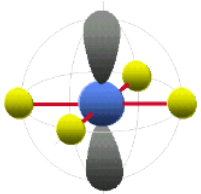
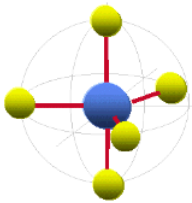
Coordination Number	Ψ-polyhedra	Number of free electron pairs	Real structure	examples
2	linear	0	linear	$BeCl_2$
3	trigonal planar	0	trigonal planar	SO_3^{2-}
4	tetrahedral	0	tetrahedral	CH_4
5	trigonal bipyramidal	0	trigonal bipyramidal	PCl_5
6	octahedral	0	octahedral	SF_6

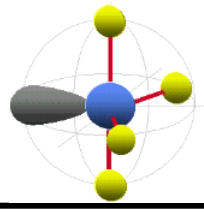
b) with free electron pairs:

4	tetrahedral	2	bent	H_2O
4	Tetrahedral	1	trigonal pyramidal	H_3O^+
5	trigonal bipyramidal	2	T-shaped	ClF_3
5	trigonal bipyramidal	1	seesaw	SF_4
6	octahedral	2	square planar	ICl_4^-
6	octahedral	1	square pyramidal	BrF_5

Some examples

Molecule	**Type**	**Ψ-Geometry**	**Geometry**
CO_2	AX_2	linear 	linear
NO_2^-	AX_2E	trig. pl. 	bent
NO_3^-	AX_3	trig. pl. 	trig. pl.

Molecule	Type	Ψ-Geometry	Geometry
SO_3^{2-}	AX_3E	tetr. 	trig. py.
XeF_4	AX_4E_2	oct. 	quad. pl.
PCl_5 (g)	AX_5	trig. bipy. 	trig. bipy

Molecule	Type	Ψ-Geometry	Geometry
SF_4	AX_4E	trig. bipy. 	disphenoidal

For further information see www.shef.ac.uk/chemistry/vsepr

Molecular geometries using the VSEPR model

Electron pairs	ψ-polyhedron	Type	Shape	Examples
2	ψ- linear	AB_2	linear	HgX_2, CdX_2, ZnX_2, $BeCl_2$
3	ψ- dreieckig	AB_3	dreieckig	BX_3, GaI_3
		AB_2E	V-förmig	$SnCl_2$
4	ψ- tetraedrisch	AB_4	tetraedrisch	BeX_4^{2-}, BX_4^-, CX_4, NX_4^+, SiX_4, GeX_4, AsX_4
		AB_3E	trigonal-pyramidal	NX_3, OH_3^+, PX_3, AsX_3, SbX_3, P_4O_6
		AB_2E_2	V-förmig	OX_2, SX_2, SeX_2, TeX_2

Electron pairs	ψ-polyhedron	Type	Shape	Examples
5	ψ- trigonal-bipyramidal	AB_5	trigonal-bipyramidal	PCl_5, PF_5, PCl_3F_2, $SbCl_5$
		AB_4E	tetraedrisch verzerrt	SF_4, SeF_4, SCl_4
		AB_3E_2	T-förmig	ClF_3, BrF_3
		AB_2E_3	linear	ICl_2^-, I_3^-, XeF_2
5	ψ- quadratisch-pyramidal	AB_5	quadratisch-pyramidal	SbF_5
6	ψ- oktaedrisch	AB_6	oktaedrisch	SF_6, SeF_6, TeF_6, PCl_6^-, PF_6^-, SiF_6^{2-}, $Te(OH)_6$
		AB_5E	quadratisch-pyramidal	ClF_5, BrF_5, IF_5
		AB_4E_2	quadratisch-planar	ICl_4^-, I_2Cl_6, BrF_4^-, XeF_4
7	ψ- pentagonal-bipyramidal	AB_7	pentagonal-bipyramidal	IF_7