World chemicals turnover **in 2010** was valued at **2353 billion Euros** with China being the major producer of most of the bulk chemicals.

Among industrially important inorganic chemicals and chemical compositions, those based on the p block elements constitute a major component if one keeps the organic carbon based compounds aside.

Among the top fifteen bulk inorganic chemicals/elements produced by chemical industries across the world, ten belong to the p block.

materials for infrastructure **clay bricks (200 billion bricks per year), cement (3600 mmt) glass (56 mmt) Natural zeolites (3 mmt).**

Three major organic chemicals produced in the word in 2013

ethylene (156 mmt)
propylene (80 mmt)
methanol (65 mmt)

1million metric ton (mmt) =1 000 000 000 kilograms (10 crore kg!)

S. No	Bulk Inorganic Chemical/Element/ Composition	Year of reference	Quantity (world production in million metric tons)	Major uses and applications
1	Cement	2013	3600	Construction
2	Iron (steel)	2013	958(1528)	Construction, ships, containers etc
3	Calcium carbonate/ Lime stone	2008	285	Metallurgy, building products, pulp and paper
4	Phosphate Rock	2016	261	Production of phosphate fertilizers
5	Sulfuric acid	2010	198	Production of phosphate fertilizers
6	Ammonia	2013	140	Fertilizers (80%), nitric acid synthesis
7	Sulfur	2010	77	Sulfuric acid manufacture
8	Sodium carbonate	2012	62	Glass, detergents and cleaners, as source of sodium ion
9	Nitric acid	2013	60	Ammonium nitrate for use in fertilizers and explosives
10	Sodium hydroxide	2004	60	Paper, detergents, Bayer process for aluminum
11	Glass	2010	56	Construction, buildings, automobile
12	Chlorine	2010	56	Ethylene dichloride, propylene oxide, isocyanates
13	Hydrogen	2013	50	Ammonia and methanol synthesis, petroleum refinery
14	Phosphoric acid	2009	46	Phosphate fertilizers
15	Aluminum	2012	45	Construction, airplanes etc

1million metric ton (mmt) =1 000 000 000 kilograms (10 crore kg!)

Common inorganic fertilizers

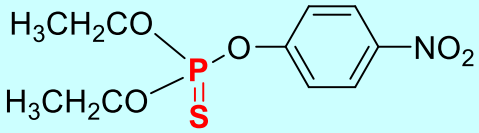
The multibillion dollar chemical equation!

$Ca_5(PO_4)_3X + 5\ H_2SO_4 + 10\ H_2O \rightarrow 3\ H_3PO_4 + 5\ CaSO_4 \cdot 2\ H_2O + HX$

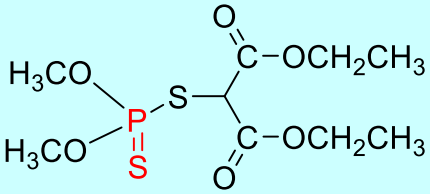
X=F (fluorapatite) OH hydroxyapatite)

Chemical name of fertilizer	Industrial Name	Formula	NPK value
Ammonia	Ammonia	NH_3	82-00-00
Urea	Urea	$(H_2N)_2CO$	46-00-00
Ammonium Sulfate	Ammonium sulfate	$(NH_4)_2SO_4$	21-00-00
Calcium nitrate	Norvegian Saltpeter	$Ca(NO_3)_2$	15-00-00
Ammonium nitrate	Ammonium nitrate	NH_4NO_3	33-00-00
Mono ammonium phosphate	Mono ammonium phosphate	$(NH_4)H_2PO_4$	11-48-00
Diammonium phosphate	Diammonium phosphate	$(NH_4)_2HPO_4$	18-46-00
Mono calcium phosphate	Triple superphosphate	$Ca(H_2PO_4)_2$	00-44-00
Mono calcium phosphate + gypsum	Single superphosphate	$Ca(H_2PO_4)_2 + 2\ CaSO_4$	00-17-00

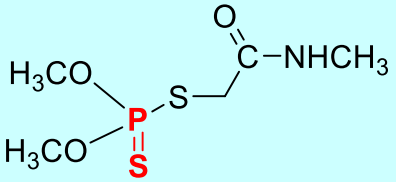
Examples of pesticides/nerve gases based on phosphorus and chlorine



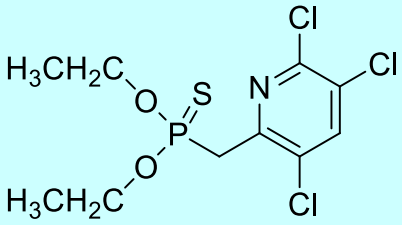
Parathion



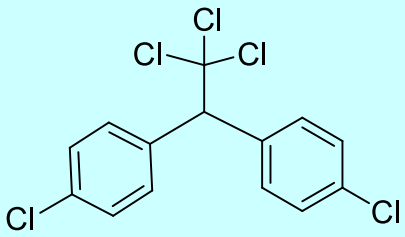
Malathion



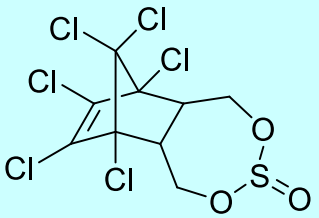
Roger
(Dimethoate)



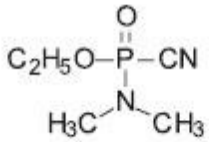
Chlorpyriphos



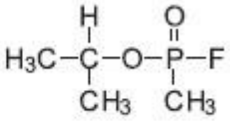
DDT



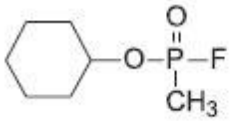
Endosulfan



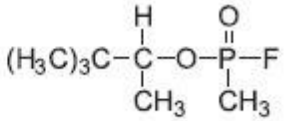
Tabun



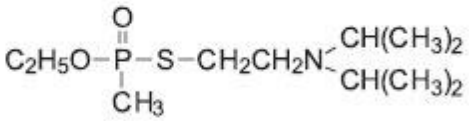
Sarin



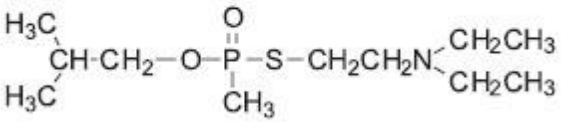
Cyclosarin



Soman



VX



VR

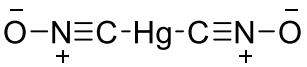
Figure 8. Structures of the main neurotoxic chemical warfare agents.

Solar energy materials

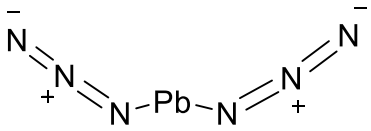
Name Material	Bandgap (300K) eV	Conv. efficiency (%)	Type	Advantages	Disadvantages
c-Si **Monocrystalline silicon**	1.1	19-22.5	Wafers (cut from cylindrical ingots)	High conversion efficiency, long life. Performs in low light	Very expensive, loss of material during cutting of ingots
p-Si **Polycrystalline silicon**	1.1	13.0-16.0	casting molten silicon	Process simple and less costly than c-Si. Lower heat tolerance than c-Si.	Less efficient due to lower purity , lower space efficiency
a-Si **Amorphous silicon**	1.7-1.8	11.1	Thin films	Mass production easy, flexible, cheap	Mostly small scale applications (e.g. calculators)
CdTe **Cadmium telluride**	1.4	16.5-17.0	Thin films	Cost efficient . large scale installation possible	Cadmium is highly toxic, degrades
GaAs **Gallium Arsenide**	1.424	28.8	Thin films	world record for the highest-efficiency single-junction solar cell	High cost
CIGS **Copper indium gallium selenide**	1. to 1.7	19.5-20.8	Thin films	Flexible substrate, more efficient than CdTe	Less toxic than CdTe, Degrades
Multi Junction (MJ) **Indium gallium phosphide;** **Indium gallium arsenide;** **Germanium**	1.9 1.4 0.7	40.7	Thin films	Highest conversion efficiency. Application preferred in space	Most expensive. Degrades fast

The complete spectrum of sunlight, from infrared to ultraviolet, covers a bandgap range from approximately 0.5 eV to about 2.9 eV (red light 1.7 eV and blue light 2.7 eV).

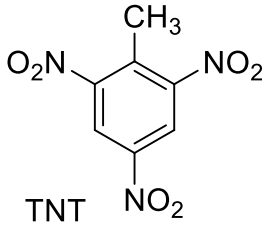
Common explosives and their velocities of detonation



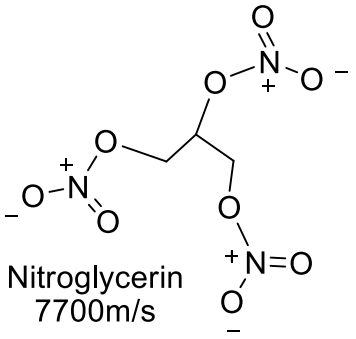
Mercury fulminate
4250 m/s



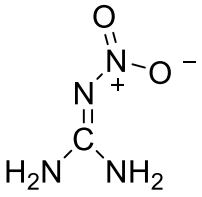
Lead Azide
4630 m/s



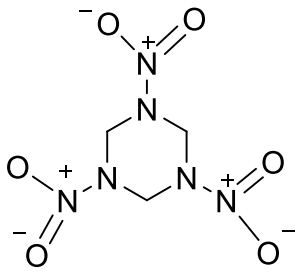
TNT
6900 m/s



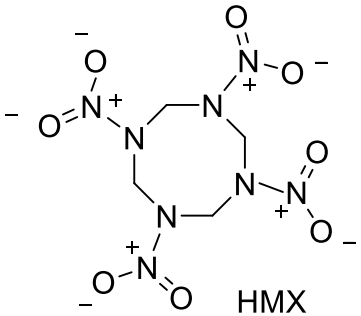
Nitroglycerin
7700m/s



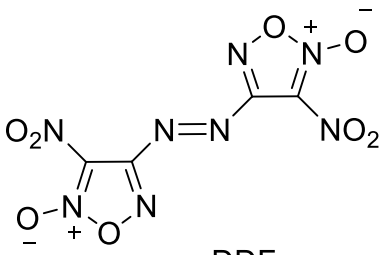
NItroguanadine
8200 m/s



RDX
8750 m/s



HMX
9400 m/s



DDF
10,000m/s

Higher velocity of detonation (VoD)
Higher density
Zero oxygen balance (OB%) indicating a good fuel to oxidizer ratio. This indicates the degree to which an explosive can be oxidized.
Higher value of heat of explosion Q_v.
Higher volume of gases generated.

Nuclear materials based on the p block

Lead can effectively attenuate certain kinds of radiation because of its relatively **high density (11.3)** and high atomic number. It is quite **effective at stopping gamma rays, and X-rays.** Lead's high density is caused by the combination of its high atomic mass and the relatively small size of its bond lengths and atomic radius.

isotope	Cross section for thermal neutron capture (barn)	Half life	Natural abundance
Indium -115	100	4.41×10^{14} years	95.71%
Boron-10	200	Non radioactive	19.9%
Cadmium- 113	30,000	7.7×10^{15} years	12.22%
Xenon- 135	2,600,000	9.14 hours	0 (Xe-135 is a decay product

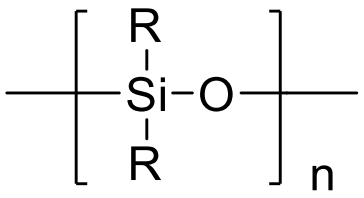
"**Half-thickness**" - the thickness of a material that will reduce its gamma ray exposure by half emitted by U-235

Lead	0.06 cm	Tungsten	0.04 cm
Concrete	4.24 cm	Lead Glass	0.08 cm
Water	12.44 cm	Aluminum	2.10 cm
Iron	0.80 cm	depleted uranium	0.04 cm

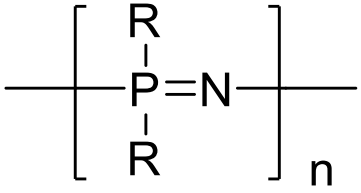
Transparent conducting oxides (TCOs)

Transparent conducting oxides (TCOs) are electrical conductive materials with comparably low absorption of electromagnetic radiation within the visible region of the spectrum. **Indium tin oxide** is one of the most widely used transparent conducting oxide because of its unique properties such as **good electrical conductivity (~10^4 S/cm)**, **very high optical transparency (75-90%),** as well as the ease with which it can be deposited as a thin film. Indium tin oxide is a mixture of In_2O_3 (90%) and SnO_2 (10%). The conductive and highly transparent surface created by ITO when applied as a coating to glass or other transparent surfaces, **reflect infrared rays while allowing visible and UV light to pass.** ITO which has a **stability upto 150 °C** is omnipresent in modern touch screen technology starting from automatic teller machines, touch screen mobile phones and tablet PCs. It is also used in flat panel LCD, OLED plasma and electro-chromatic displays, solar panels and even on the energy efficient windows of modern aircrafts for easy deicing.

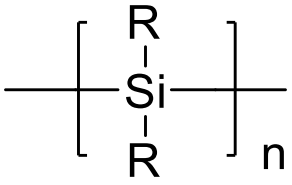
Inorganic polymers



Silicones



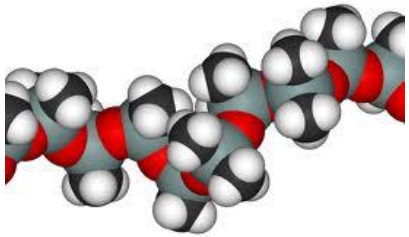
Polyphosphazenes



Polysilanes

Among the three, the one which has the highest market in terms of quantity are the silicones. The global market for silicones in terms of revenues was estimated to be worth $13,000 million in 2011 and is expected to reach $19,000 million by 2017. The silicone market is dominated by elastomers and fluids, together accounting for over 80% of the overall market. Silicones possess superior properties and characteristics which are extremely useful in the automotive, construction, medical and personal care and, electrical and electronics end-user industries

Industrial success of Silicones : PDMS



Hydrophobicity

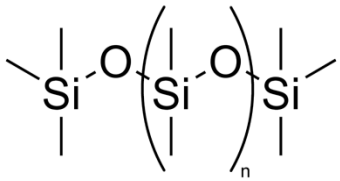
Oxygen permeability

Wide temp range

Low glass transition temp

Antifrothing

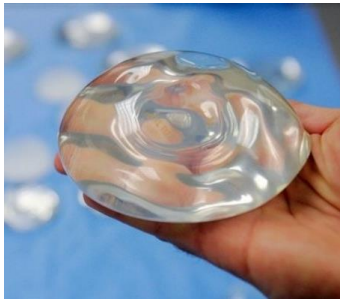
Non toxicity



First human foot print on moon

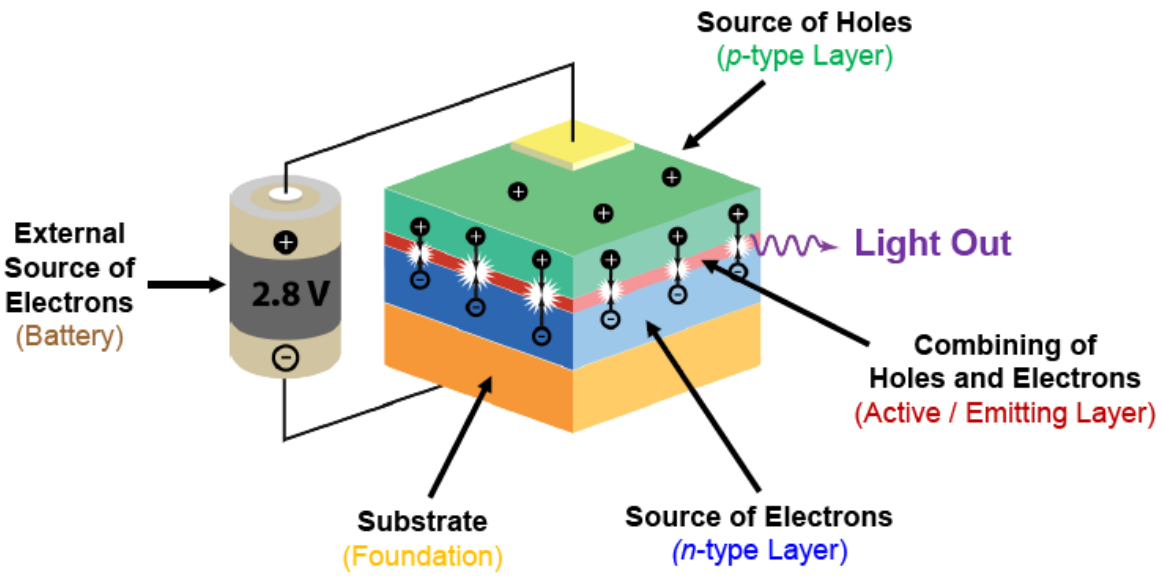
Moon temperature

(-153 to +107 °C)



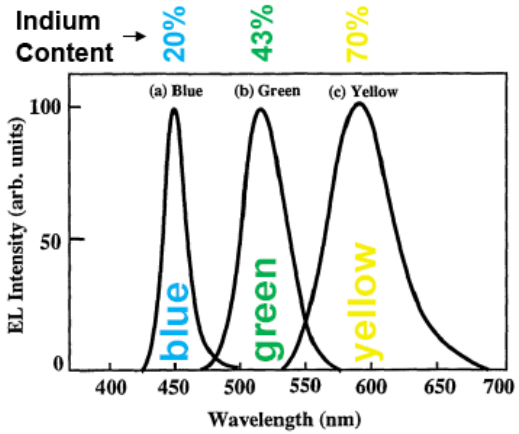
Light Emitting Diodes

A Light Emitting Diode (LED) **produces light of a single color** by combining holes and electrons in a semiconductor.

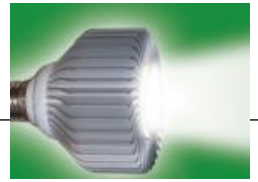
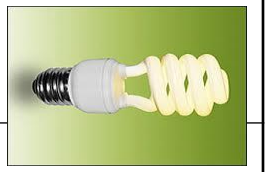


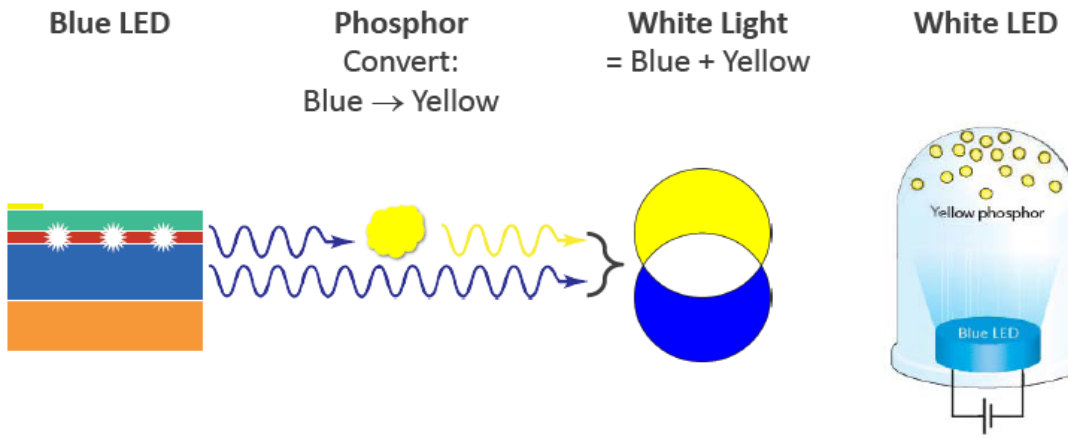
Semiconductor	Wavelength	Colour	V_F @ 20mA
GaAs	850-940nm	**Infra-Red**	1.2v
GaAsP	630-660nm	Red	1.8v
GaAsP	605-620nm	Amber	2.0v
GaAsP:N	585-595nm	Yellow	2.2v
AlGaP	550-570nm	Green	3.5v
SiC	430-505nm	Blue	3.6v
GaInN	450nm	White	4.0v

Electroluminescence



The main P-type dopant used in the manufacture of **Light Emitting Diodes** is Gallium and that the main N-type dopant used is As giving the resulting compound of Gallium Arsenide (GaAs) . Gallium Arsenide on its own as the semiconductor compound radiates large amounts of infra-red radiation from its junction when a forward current is flowing through it. But by adding Phosphorus, as a third dopant the wavelength of the emitted radiation is reduced to below 680nm giving visible red light to the human eye. Similarly GaN radiates blue / UV light. By introducing indium as a dopant one can get blue, green, yellow etc – by varying the band gap.

Energy Efficiency & Energy Costs	Light Emitting Diodes (LEDs)	Incandescent Light Bulbs	Compact Fluorescents
Life Span (average)	**50,000 hours**	**1,200 hours**	**8,000 hours**
Watts of electricity used (equivalent to 60 watt bulb).	**6 - 8 watts**	**60 watts**	**13-15 watts**
Kilo-watts of Electricity used (30 Incandescent Bulbs per year equivalent)	**329 KWh/yr.**	**3285 KWh/yr.**	**767 KWh/yr.**
Annual Operating Cost (30 Incandescent Bulbs per year equivalent)	**$32.85/year**	**$328.59/year**	**$76.65/year**
Environmental Impact			
Contains the TOXIC Mercury			
Carbon Dioxide Emissions (30 bulbs per year)	**451 pounds/year**	**4500 pounds/year**	**1051 pounds/year**

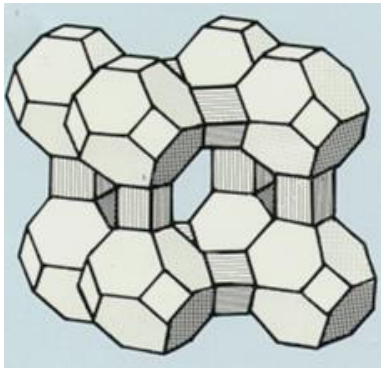


As reagents and catalysts

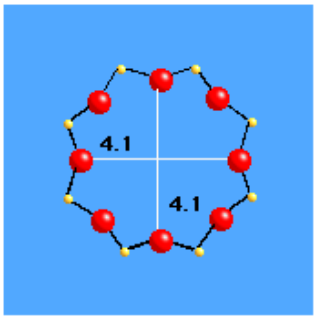
Lewis acid catalysts based on main group metals such as aluminum, boron, silicon, tin and antimony (BF_3, $SnCl_4$, SiF_4, SbF_5 and $AlCl_3$) are used extensively in reactions such as Friedel-Crafts and the aldol reaction, and various pericyclic processes that proceed slowly at room temperature, such as the Diels-Alder reaction, Claisen rearrangement and acetal formation.

The unusual catalytic activity shown by aluminosilicates such as zeolites and clays (e.g. montmorillonite) are unique to the p block elements. The open framework stable structures such as zeolites and ALPO can acts as **dehydration and shape selective catalysts.** Also of importance are methylating agents such as $AlMe_3$ and its partially hydrolyzed product methyl alumoxane (MAO) which find application as cocatalysts in olefin polymerization reactions

Linde A

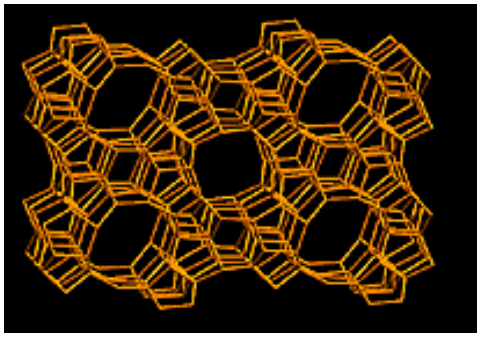


Si 50% - Al 50%
Cations Na, Ca
Polar
3-D straight channels

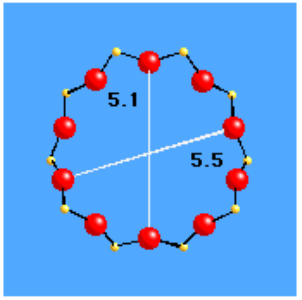


Ring 8

ZSM 5

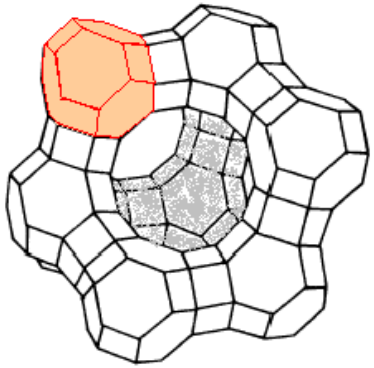


Si 93 %
non-polar
Hydrophobic
1-D channels

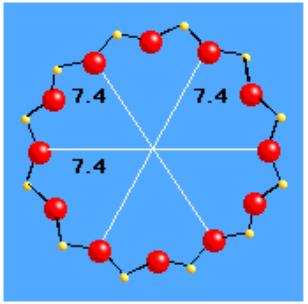


Ring 10

Faujasite

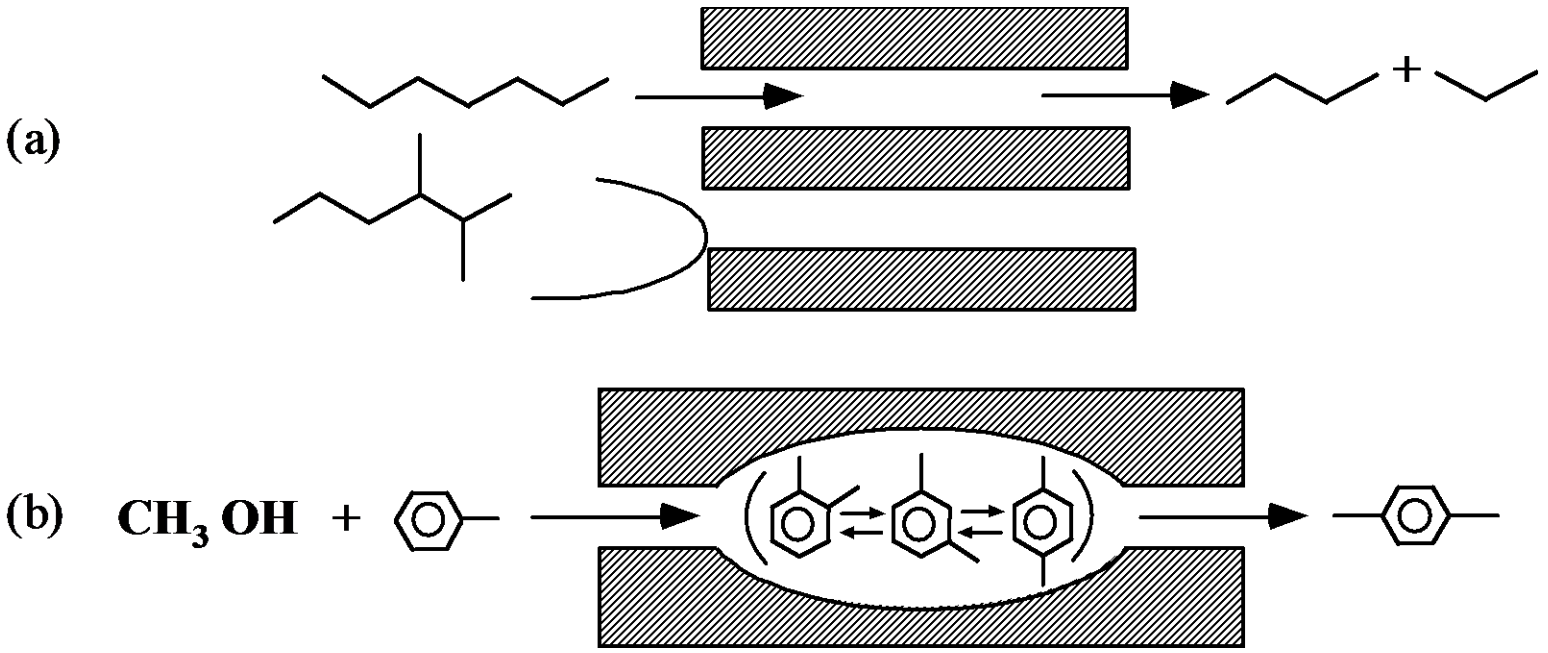


Si x% - Al y%
Cations Na, Ca
Polar
3-D entangled
channels



Ring 12

ZSM-5: Shape Selectivity in Catalysis



(a) reactant selectivity for cracking of a straight-chain versus branched C_7.

(b) product selectivity for p-xylene over o- and m- forms

Ammonium phosphates as Forest Fire retardants

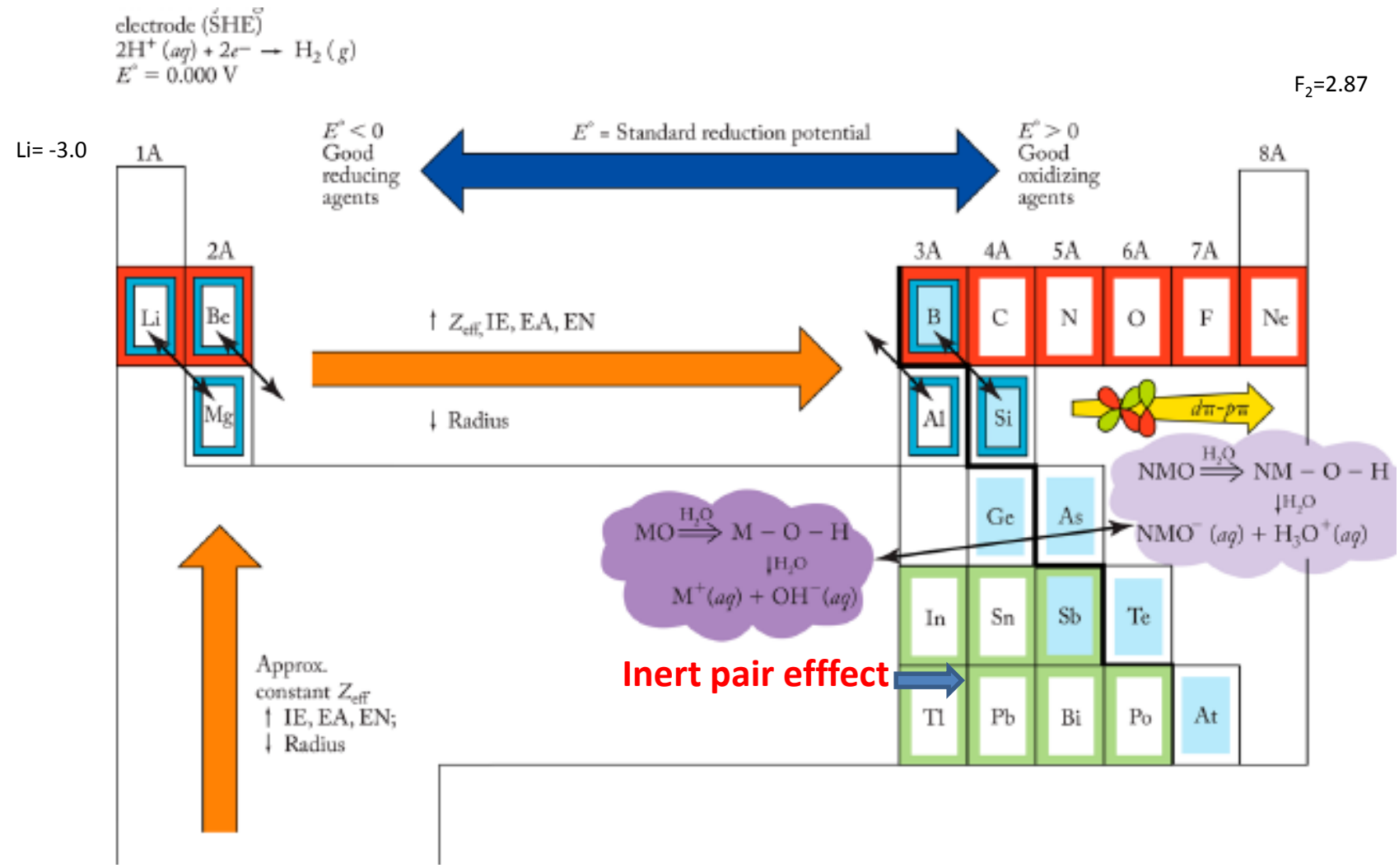
Patent

Diammonium phosphate 45%
Ammonium sulfate 45%
Sodium calcium borate
Sodium carbonate
Rhodamine B- 0.05%

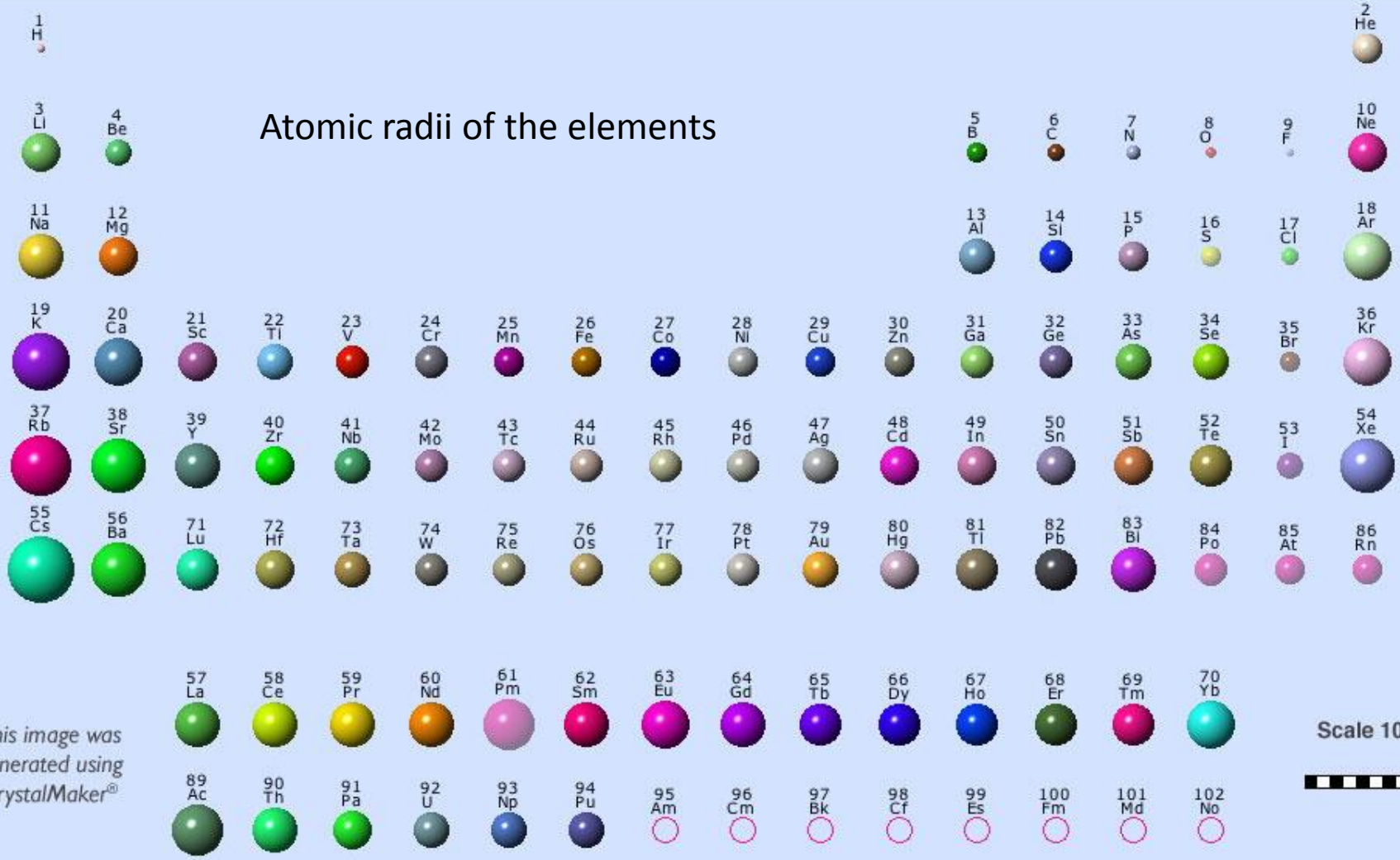
Phos check

Ammonium polyphosphate
Diammonium phosphate,
Diammonium sulfate,
Monoammonium phosphate,
Attapulgus clay,
Guar gum,
Red dye

Periodicity of properties of p block elements



Atomic radii of the elements



This image was generated using CrystalMaker®

Scale 10 Å

CrystalMaker®
Crystal Structures Software for Mac & Windows

These data are based on interatomic distances in the structures of the elements. (Radii for metals correspond to coordination numbers of 12.) Where no radius value can be found for a particular element, its radius has been set to a default value of 1 Å and a circle is plotted instead of a rendered sphere. Data from Vainshtein et al., 1995; values for O, F, S, Cl, Br, I, At, Po, Pm, Rn have been taken from Clementi et al.1963.

References: Vainshtein BK, Fridkin VM, Indenbom VL (1995) Structure of Crystals, 3rd Edition. Springer Verlag, Berlin.

Clementi E, Raimondi DL, Reinhardt WP (1963) Journal of Chemical Physics 38:2686-

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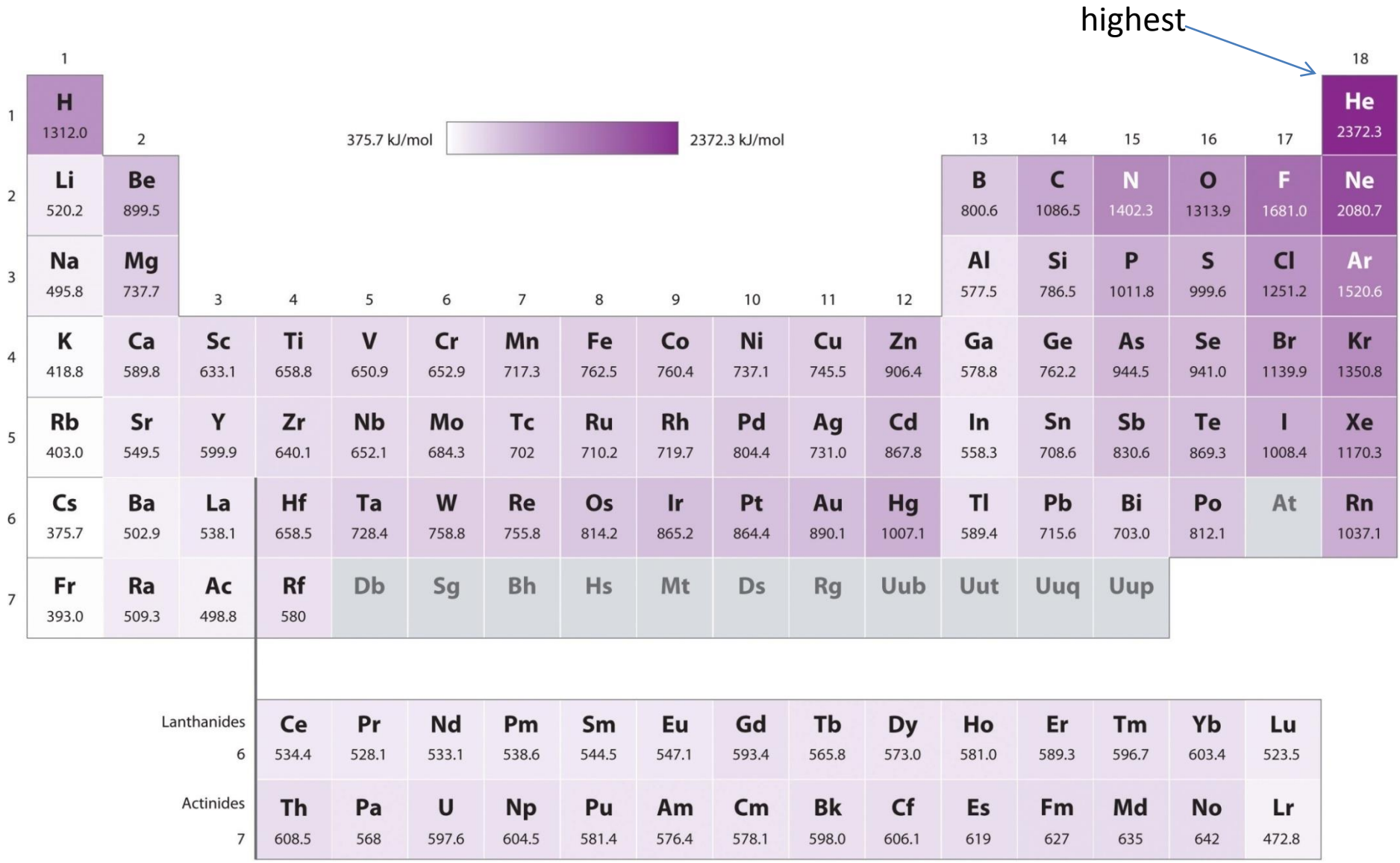
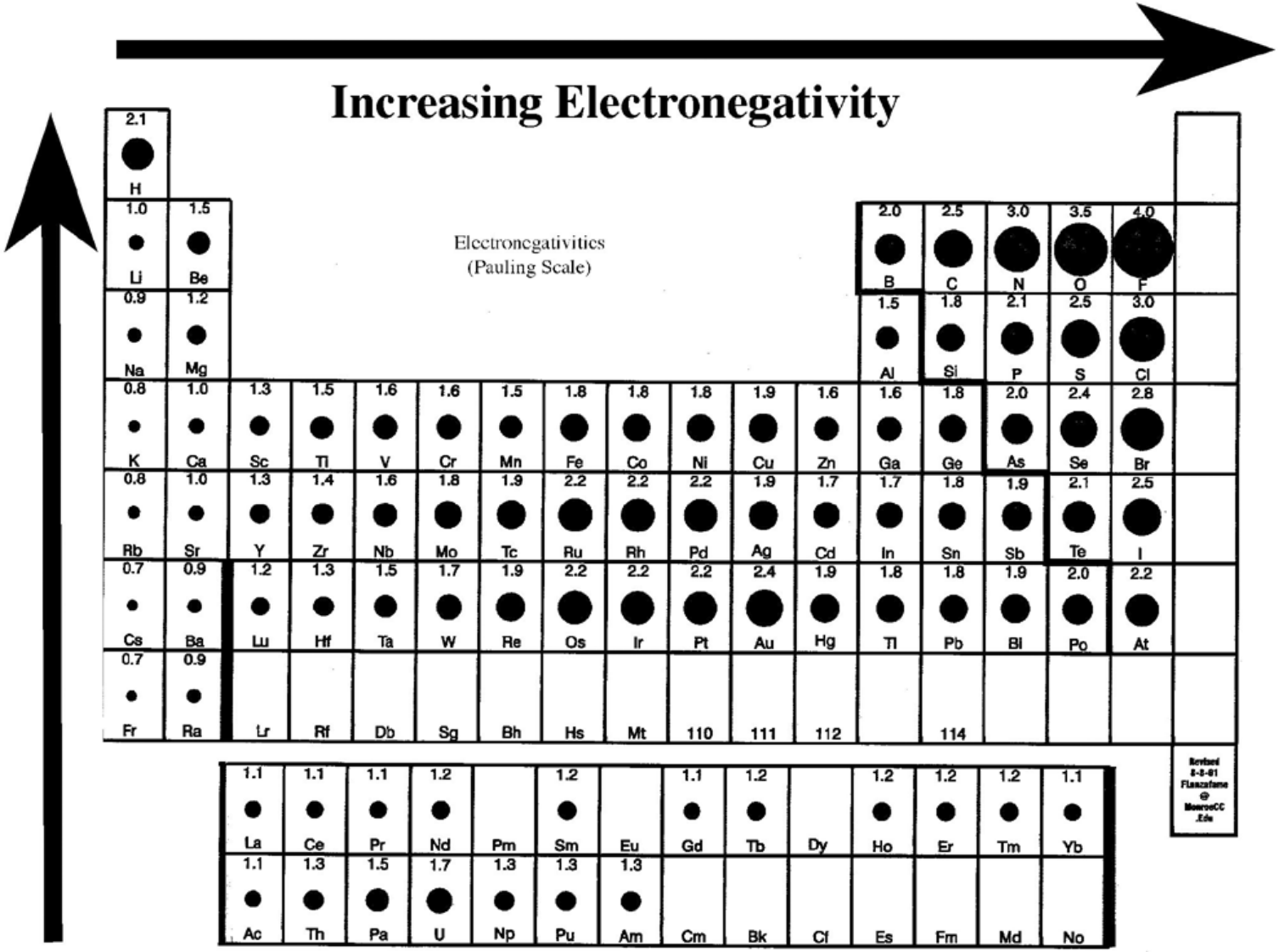
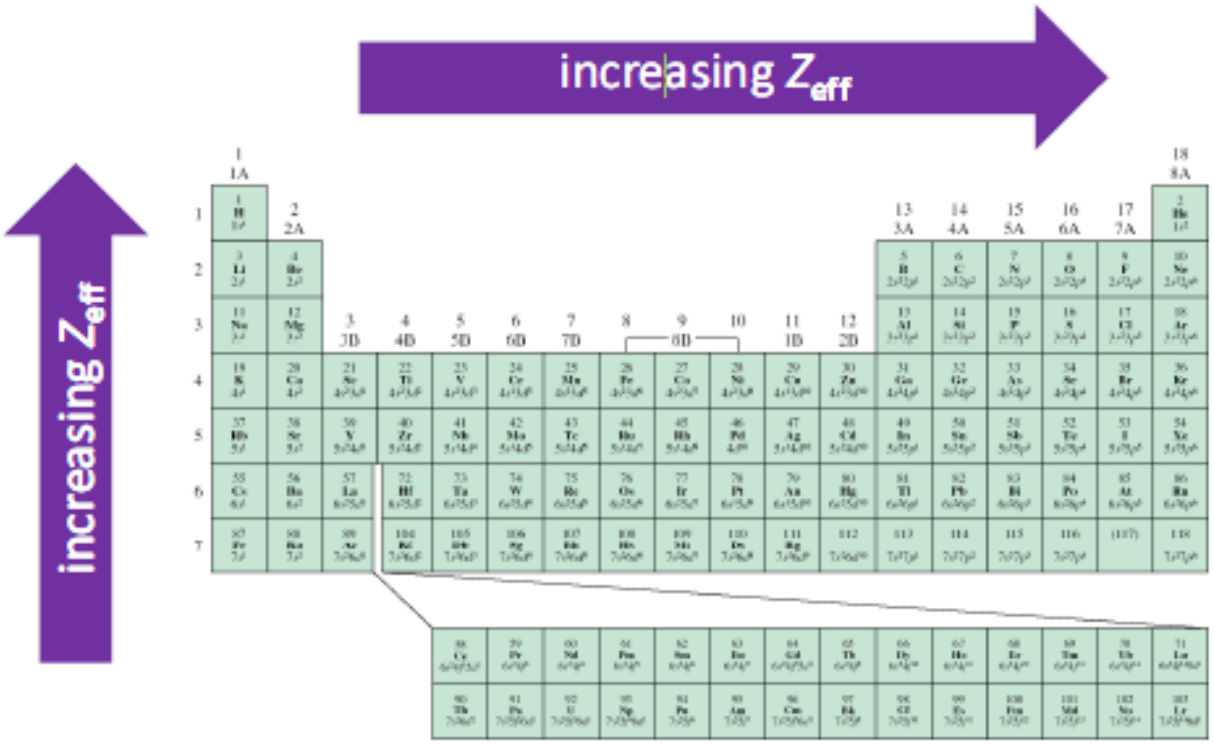
First Ionization energies



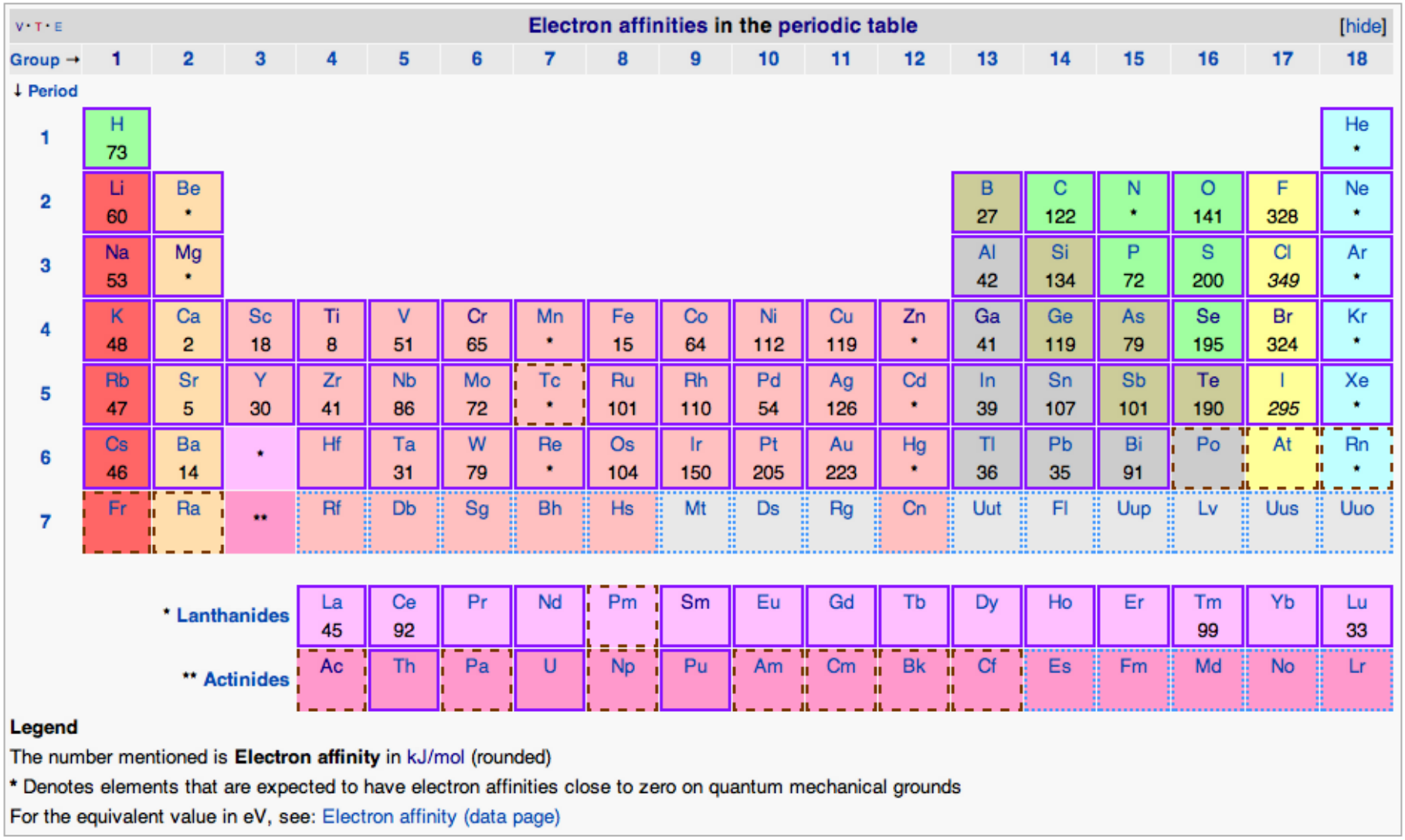

Increasing Electronegativity
Electronegativities
(Pauling Scale)
2.1 H
1.0 Li
1.5 Be
0.9 Na
1.2 Mg
0.8 K
1.0 Ca
1.3 Sc
1.5 Ti
1.6 V
1.6 Cr
1.5 Mn
1.8 Fe
1.8 Co
1.8 Ni
1.9 Cu
1.6 Zn
1.6 Ga
1.8 Ge
2.0 As
2.4 Se
2.8 Br
0.8 Rb
1.0 Sr
1.3 Y
1.4 Zr
1.6 Nb
1.8 Mo
1.9 Tc
2.2 Ru
2.2 Rh
2.2 Pd
1.9 Ag
1.7 Cd
1.7 In
1.8 Sn
1.9 Sb
2.1 Te
2.5 I
0.7 Cs
0.9 Ba
1.2 Lu
1.3 Hf
1.5 Ta
1.7 W
1.9 Re
2.2 Os
2.2 Ir
2.2 Pt
2.4 Au
1.9 Hg
1.8 Tl
1.8 Pb
1.9 Bi
2.0 Po
2.2 At
0.7 Fr
0.9 Ra
Lr
Rf
Db
Sg
Bh
Hs
Mt
110
111
112
114
2.0 B
2.5 C
3.0 N
3.5 O
4.0 F
1.5 Al
1.8 Si
2.1 P
2.5 S
3.0 Cl
1.1 La
1.1 Ce
1.1 Pr
1.2 Nd
Pm
1.2 Sm
Eu
1.1 Gd
1.2 Tb
Dy
1.2 Ho
1.2 Er
1.2 Tm
1.1 Yb
1.1 Ac
1.3 Th
1.5 Pa
1.7 U
1.3 Np
1.3 Pu
1.3 Am
Cm
Bk
Cf
Es
Fm
Md
No

net positive charge experienced by an electron in a multi-electron atom

Effective Nuclear Charge (Z_{eff})



	Na	<	Mg	<	Al	<	Si
Atomic Radii	186 pm		160		143		132



Electron affinities in the periodic table [hide]

Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
↓ Period																		
1	H 73																	He *
2	Li 60	Be *											B 27	C 122	N *	O 141	F 328	Ne *
3	Na 53	Mg *											Al 42	Si 134	P 72	S 200	Cl *349*	Ar *
4	K 48	Ca 2	Sc 18	Ti 8	V 51	Cr 65	Mn *	Fe 15	Co 64	Ni 112	Cu 119	Zn *	Ga 41	Ge 119	As 79	Se 195	Br 324	Kr *
5	Rb 47	Sr 5	Y 30	Zr 41	Nb 86	Mo 72	Tc *	Ru 101	Rh 110	Pd 54	Ag 126	Cd *	In 39	Sn 107	Sb 101	Te 190	I *295*	Xe *
6	Cs 46	Ba 14	*	Hf	Ta 31	W 79	Re *	Os 104	Ir 150	Pt 205	Au 223	Hg *	Tl 36	Pb 35	Bi 91	Po	At	Rn *
7	Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

* Lanthanides	La 45	Ce 92	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm 99	Yb	Lu 33
** Actinides	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Legend

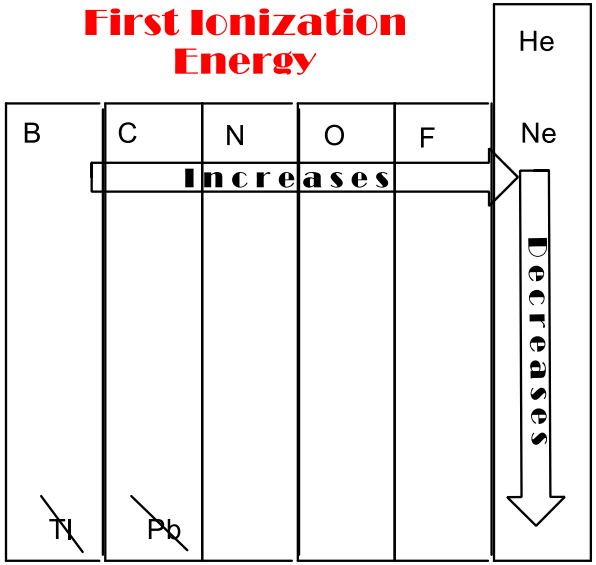
The number mentioned is **Electron affinity** in kJ/mol (rounded)

* Denotes elements that are expected to have electron affinities close to zero on quantum mechanical grounds

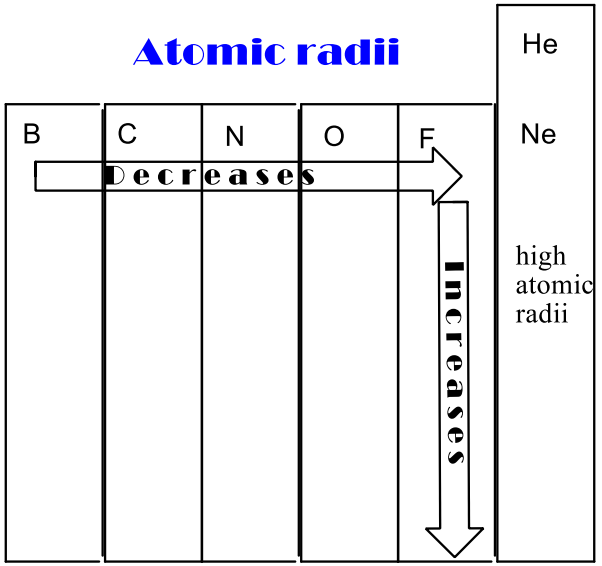
For the equivalent value in eV, see: Electron affinity (data page)

amount of energy released when an **electron** is added to a neutral atom

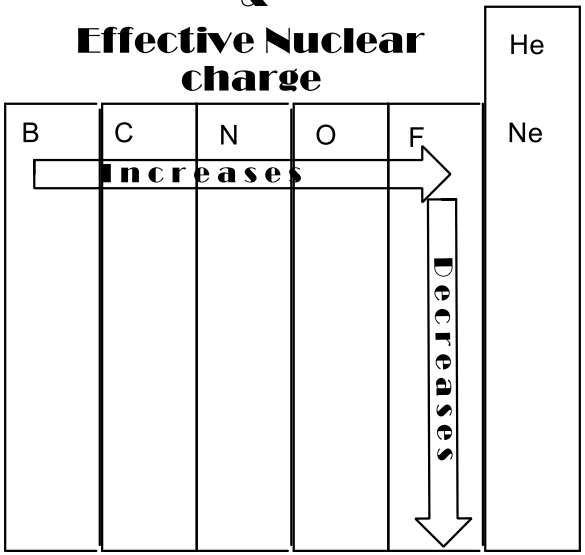
First Ionization Energy



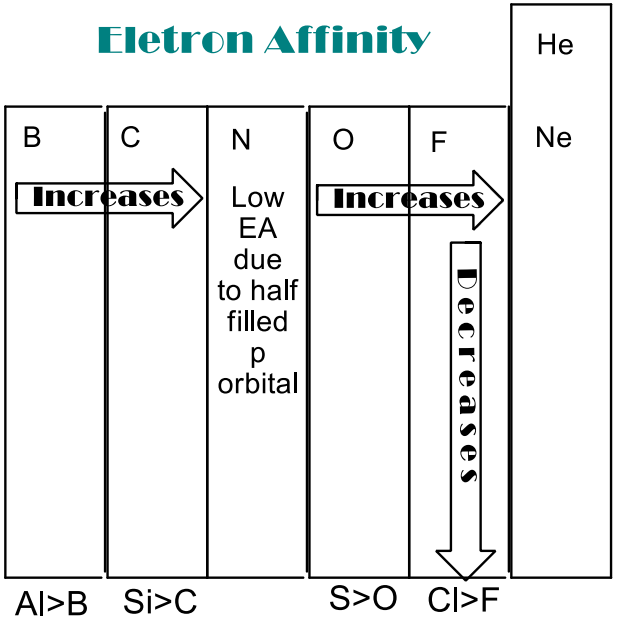
Atomic radii



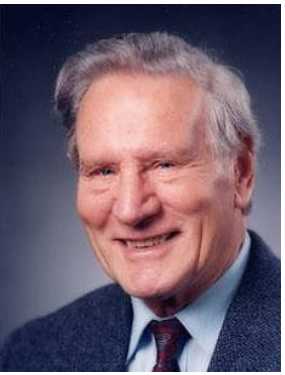
Electronegativity & Effective Nuclear charge



Eletron Affinity



smaller size of first row p block elements results in higher electron-electron repulsion when e's added



Ronald Gillespie
Mc Master Univ., Canada

Valence shell electron pair repulsion theory (VSEPR)

The rules are based on the ***Points on a sphere model*** as it envisages the arrangement of electron pairs as points on a spherical core. The rules have been quite successful in predicting the shape of compounds whose central atom is a p block element and not very useful in the case of compounds of transition metals .

The "**AXE** method" of electron counting
A represents the central atom and always has an implied subscript one.
X represents the number of ligands (atoms bonded to A).
E represents the number of lone *pairs* surrounding the central atom.

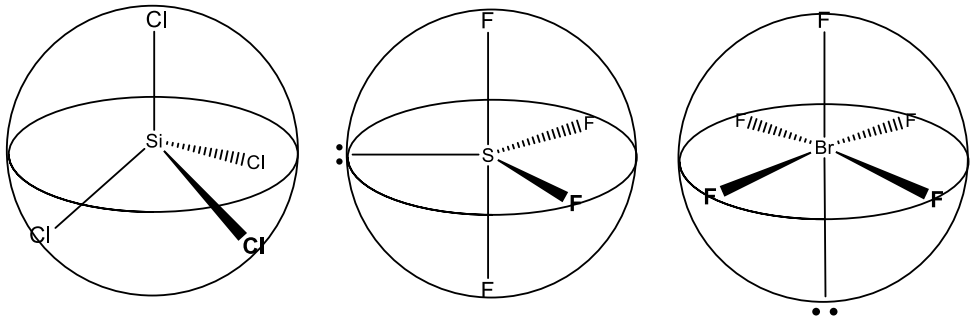
The electrons are arranged in pairs that are either bonding (shared) pairs [X] or non bonding (unshared) pairs [E]. In the usual σ - π treatment this usually means ignoring the π bonds temporarily since they will follow the σ bonds and therefore the two bonding pairs of a double bond or three bonding pairs of a triple bond are all primarily considered as a single point on the sphere.

e.g. **H_2O** **AX_2E_2** 2 bonding pairs and 2 lone pairs on Oxygen as central atom

$O{=}PCl_3$ **AX_4** **4 bonding pairs** π bond ignored with phosphorus as central atom

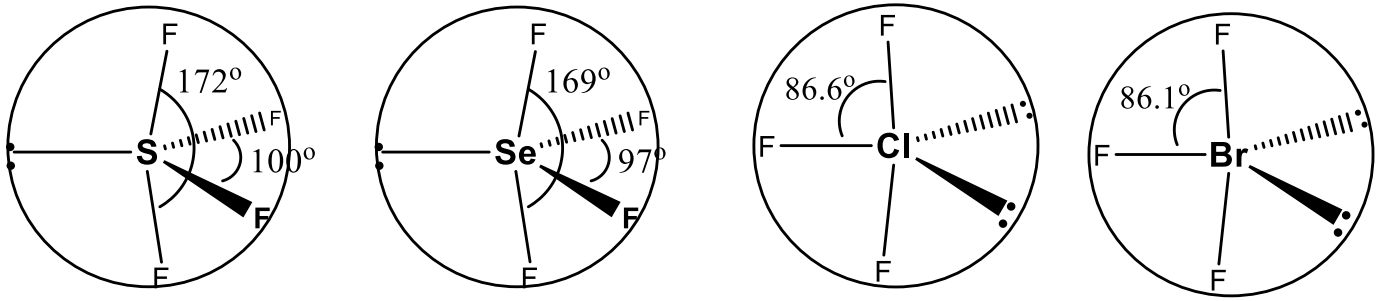
The rules

The pairs of electrons in the valence shell adopt that arrangement which maximizes their distances apart. This in other words means that the bonding and non bonding electron pairs are arranged as far apart from each other as possible on the surface of a sphere with the atom A at the centre of the sphere.

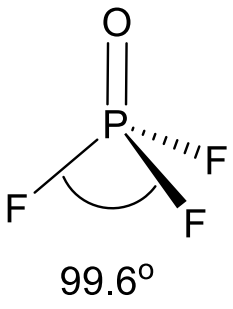


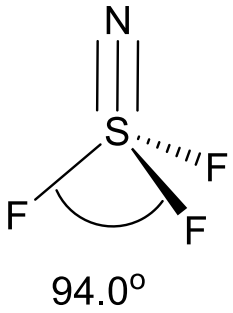
Rules which take care of the deviations observed from the ideal geometry

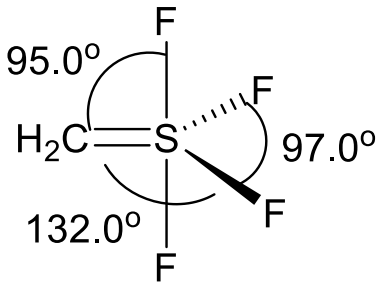
Rule 1: A non bonding lone pair [E] occupies more space on the surface of the central atom than a bonding pair [X]. In other words, lone pair- lone pair repulsion is greater than lone pair- bond pair repulsion which is greater than bond pair-bond pair repulsion. Lone pairs choose the largest site, e.g., **equatorial in trigonal bipyramid and axial in pentagonal bipyramid.** If all sites are equal, lone pairs will be better placed trans to each other.

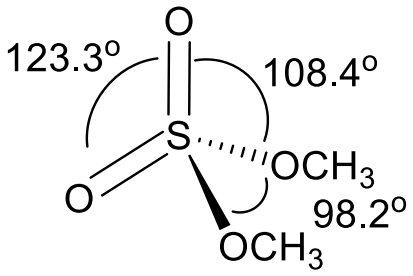


Rule 2: The strengths of the repulsions between bonds of different multiplicity decreases in the order: triple–double > double– double > double–single > single–single.



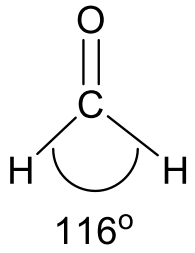


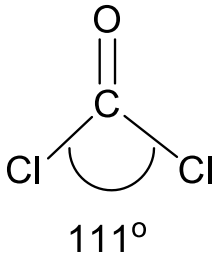


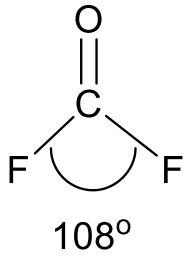


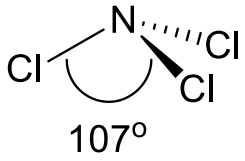
Rule 3: Bonding pairs to electronegative substituents occupy less space than those to more electropositive substituents. Therefore angles between the single bonds, decrease with increasing electronegativity of the substituent.

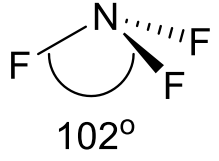
This decrease in domain size with increasing electronegativity of the substituent happens as more of the bonding electron density is shifted to the electronegative substituent. In other words, the repulsion between single bonds decreases with increasing electronegativity of the substituent and/or decreasing electronegativity of the central atom.











VSEPR stands the test of time and is still valid

JOURNAL OF CHEMICAL EDUCATION

COMMENTARY

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Is It Time To Retire the Hybrid Atomic Orbital?

Published: March 11, 2011

Alexander Grushow*

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ABSTRACT: A rationale for the removal of the hybrid atomic orbital from the chemistry curriculum is examined. Although the hybrid atomic orbital model does not accurately predict spectroscopic energies, many chemical educators continue to use and teach the model despite the confusion it can cause for students. Three arguments for retaining the model in the chemical curriculum are presented. These arguments are then refuted and methods for teaching chemistry without invoking the hybrid atomic orbital model are presented to show how the model can be removed from the chemistry curriculum with little negative effect.

structure. The beauty of VSEPR is that it does not require any orbitals at all. It simply answers the question, how can these electron domains be moved as far away from each other as possible? Although it does seem that this commentary is designed to refute the localized electron model, Lewis structures do more good than harm in helping students understand chemical bonding, whereas I would argue that the hybrid atomic orbital model does more harm than good. In the study of bonding of

Shapes of compounds having odd number of electrons

The odd electron also has an influence on the molecular geometry similar to a normal lone pair but of relatively lesser strength. As a result, the geometry will be midway between the molecule with a full electron pair and the molecule with one less electron pair on the central atom.

Nitrogen dioxide (NO_2) ($AX_2E_{0.5}$) bent shape with an ONO angle **134°**.

NO_2^- which is AX_2E is also bent but has an ONO angle approximately of **120°**

while NO_2^+ (AX_2) is linear .

Similarly ClO_2 ($AX_2E_{1.5}$) with a lone pair and an unpaired electron has OClO angle of **117.6°**
while ClO_2^- with two lone pairs (AX_2E_2) has a OClO angle of **111°**.

Exceptions to the VSEPR rules

1. Metal complexes and organometallic compounds based on transition elements

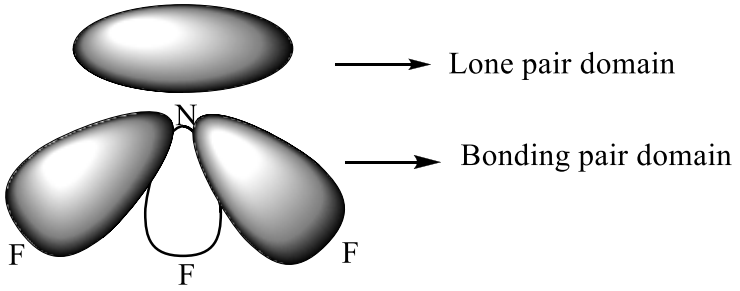
2. Many **triatomic alkaline earth metal dihalides**, although expected to be linear have been found to be bent (approximate X-M-X angles: CaF_2, 145°; SrF_2, 120°; BaF_2, 108°; $SrCl_2$, 130°; $BaCl_2$, 115°; $BaBr_2$, 115° and BaI_2, 105°). Gillespie has proposed that the reason for the same is due *to loss of spherical symmetry of the inner shell of the metal atom due to polarising effect of the relatively electronegative halide substituent's*.
Li_2O also is linear although it is expected to be bent and this has been ascribed to the bonding being more ionic resulting in repulsion between the lithium atoms.

3. The **silyl ether $O(SiH_3)_2$** has a relatively larger Si-O-Si angle (144.1°), while similar bond angles of Cl_2O (110.9°) and $(CH_3)_2O$ (111.7°) are in the expected range.

Gillespie's rationalization for this observation is that the localization of the lone pairs, and therefore their ability to repel other electron pairs, is greatest when **the ligand has an electronegativity similar to or greater than, that of the central atom.** When the central atom is more electronegative, as in $O(SiH_3)_2$, the lone pairs are **less well-localised** and have therefore a weaker repulsive effect.

4. Some molecules in which the central atom is from periods 3 and 4 and in which the ligands are **less electronegative**, do not have sufficient space in their valence shell to accommodate six bonding domains and a large lone pair domain. In such molecules the **lone pair is squeezed into a spherical domain surrounding the core** and inside the bonding domains (**stereochemically inactive s orbital**) which therefore have an octahedral arrangement. Thus some AX_6E molecule such as $SeCl_6^{2-}$ and $TeBr_6^{2-}$ have a regular octahedral shape but with longer than normal bonds.

Some new developments



The electron pair domain model

proposed by Gillespie and Harigittai in 1991 followed by Gillespie and Robinson in 1996. This model was based not on pairs of electrons but on a region in space where there is more probability of finding an electron pair (bonding or lone pair).

An electron pair domain is a region in space where there is an enhanced probability of finding an electron pair.

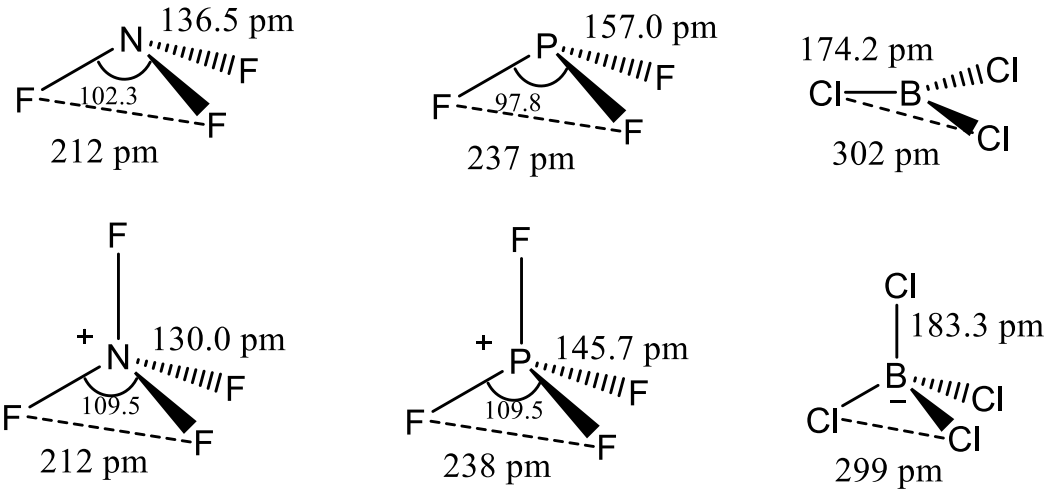
An electron pair domain extends around the most probable position of finding an electron pair as determined by the Pauli principle and the probability decreases on increasing the distance from the most probable position.

A lone pair domain can in general be thought of as more spread out and larger than a bonding pair domain as the electrons of a lone pair are subject to the attraction of only one atomic nucleus while those of a bonding air are subject to the attraction of two nuclei taking part in the bond formation.

A bonding pair domain therefore taken up less space around a nucleus compared to a lone pair domain because the former is stretched out more towards the ligand/ substituent of the central atom. Why a lone pair occupies more space than a bonding pair is well explained by the domain concept.

Ligand close packing model

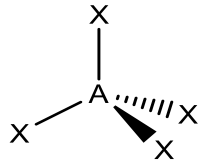
The basis of this model is that the bond **angles** are determined by the packing of the ligands or substituents around a central atom. Irrespective of having lone pairs or not, the distance maintained between the substituents on a central atom will be almost same while the bond lengths and bond angles will be different as shown in the following examples.

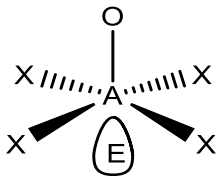


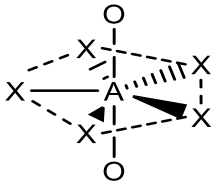
Arrive at the shape of the following compounds using VSEPR theory

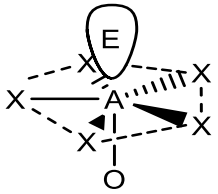
NSF_3 IOF_4^- $IO_2F_5^{2-}$ $XeOF_5^-$ $XeOF_3^-$

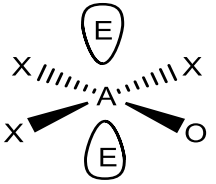
Td Sq. Py PBP Pent Pyr Sq.Pl









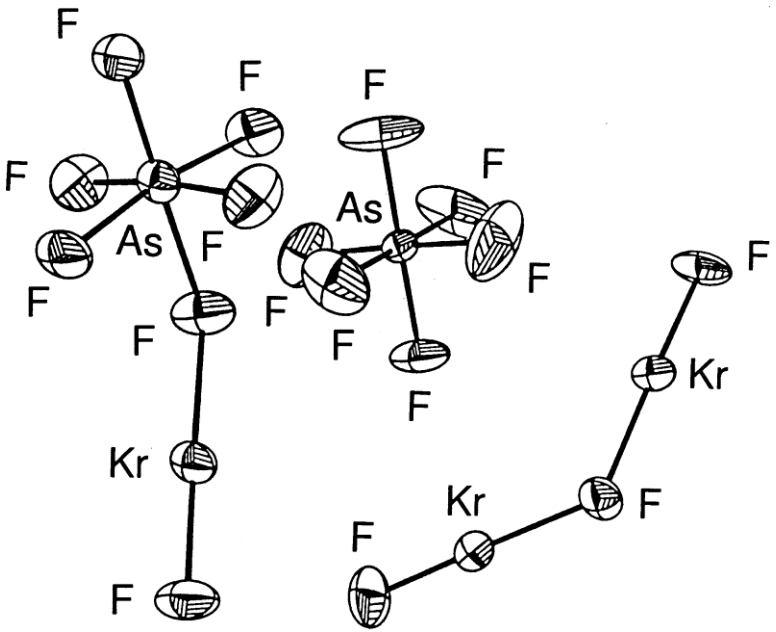


ICl_2^+, ICl_2^- IF_4^+, IF_4^- XeF_5^+, XeF_5^-

bent Lin. See saw Sq. PL Sq. Pyr Pent.Pl

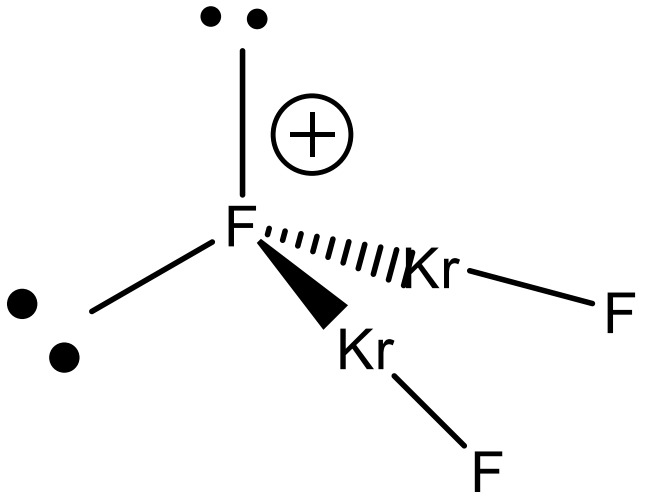
IO_3^- IF_5^{2-} BiF_7^{2-} $Kr_2F_3^+$

Tr.Pyr Pent.Pl PBP



$[Kr_2F_3][AsF_6]\cdot[KrF][AsF_6]$

$Kr_2F_3^+$



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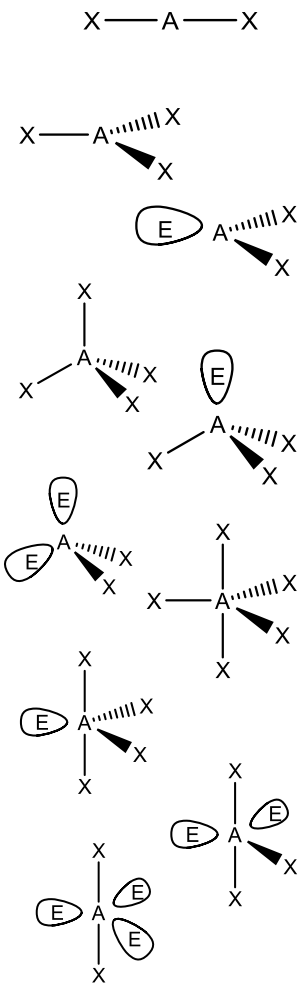
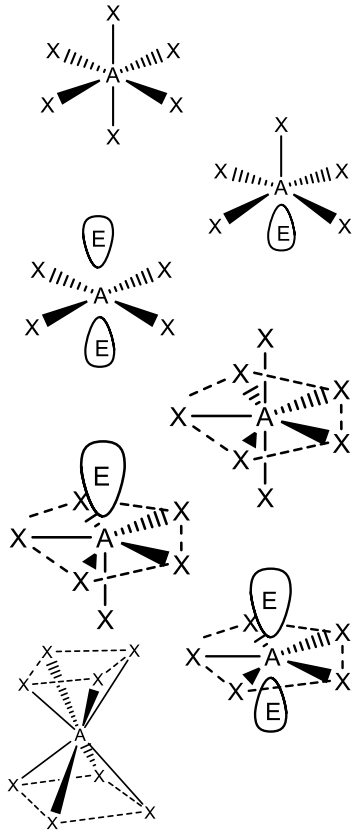
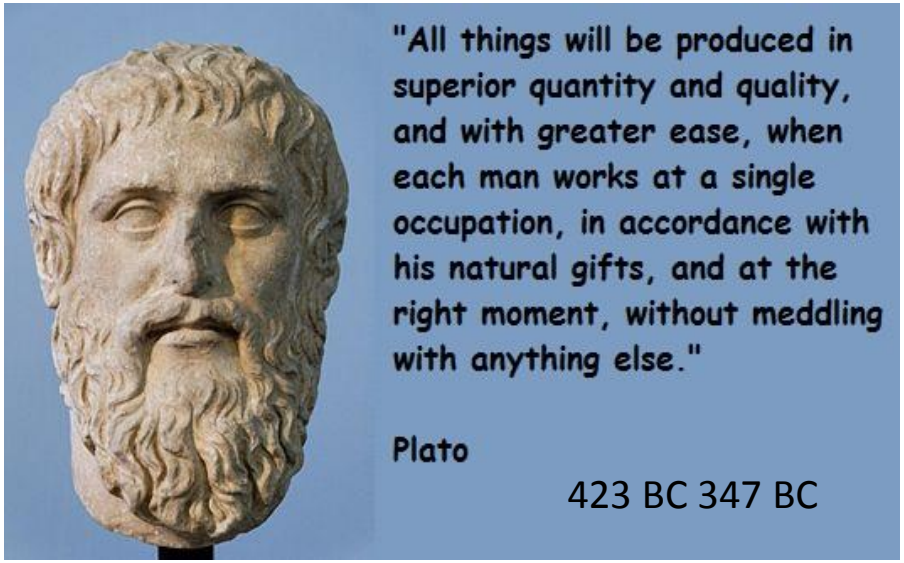
Around central F : Td
Around Krypton : TBP

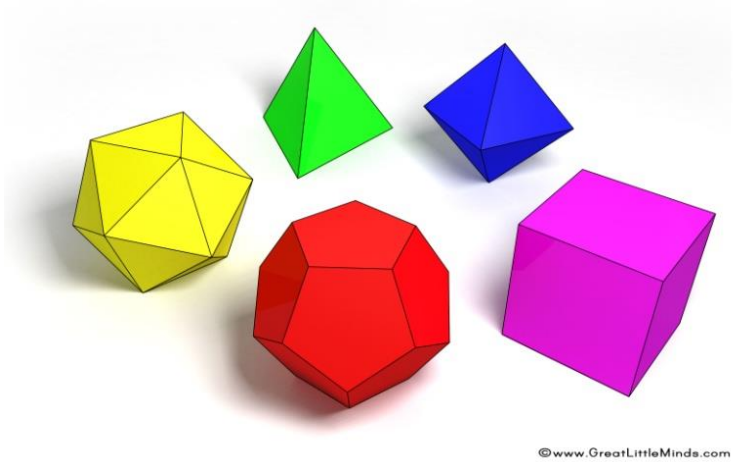
Arrangement	Bonding pairs X	Lone pairs E	Occupancy/ Steric number	Shape of the molecule	Examples
Linear	2	0	2	Linear AX_2	CO_2, CS_2, HCN, $BeCl_2$, N_2O, NO_2^+, NCF, NCBr
Triangular	3	0	3	Triangular planar AX_3	SO_3, BF_3, $COCl_2$, NO_3^-, CO_3^{2-}, BO_3^{3-}
	2	1	3	Bent (V shape) AX_2E	SO_2, O_3, NOCl, $SnCl_2$, PbF_2, NOF
Tetrahedral	4	0	4	Tetrahedral AX_4	CH_4, $SiCl_4$, SO_2Cl_2, $POCl_3$, XeO_4, NSF_3, ClO_4^-, PO_4^{3-}
	3	1	4	Triangular Pyramidal AX_3E	NH_3, PCl_3, $SOCl_2$, IO_3^-
	2	2	4	Bent AX_2E_2	H_2O, SCl_2, NSF, ICl_2^+, $SeCl_2$, $[I(C_6H_5)_2]^+$, $Kr_2F_3^+$
Trigonal bipyramid	5	0	5	Trigonal Bipyramidal AX_5	PF_5, SF_4O
	4	1	5	See saw AX_4E	SF_4, XeO_2F_2, IF_4^+, IOF_3, $IO_2F_2^-$
	3	2	5	Bent T shape AX_3E_2	ClF_3, BrF_3, $XeOF_2$, $I(Ph)[(CF_3C(O)O)]_2$
	2	3	5	Linear AX_2E_3	XeF_2, I_3^-, ICl_2^-, BrF_2^-. $(C_6F_5)_2Xe$



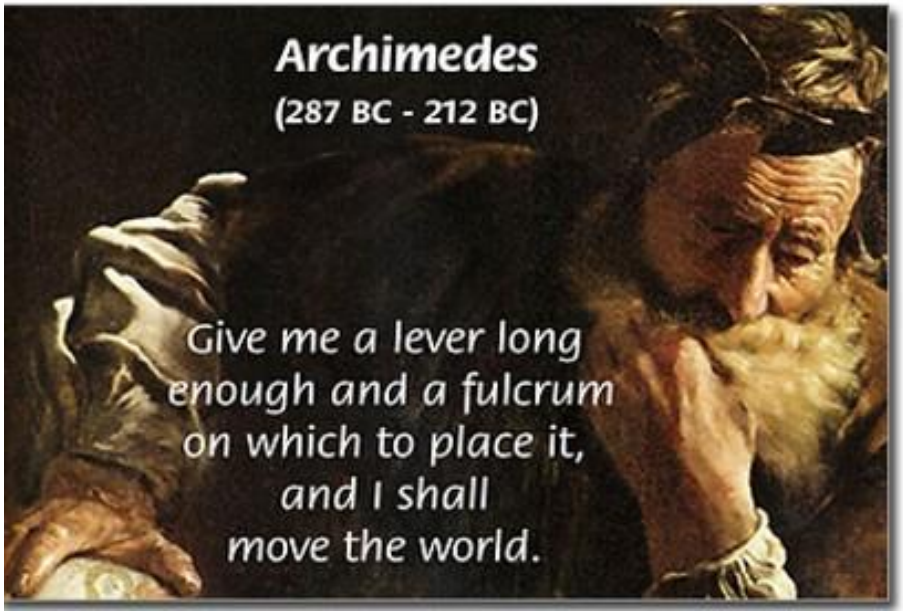
Arrangement	Bonding pairs X	Lone pairs E	Occupancy / Steric number	Shape of the molecule	Examples
Octahedral	6	0	6	Octahedral AX_6	SF_6, PF_6^-, SiF_6^{2-}, AlF_6^{3-}, IF_6^+
	5	1	6	Square pyramidal AX_5E	BrF_5, XeF_5^+, IOF_4^-, TeF_5^-, SbF_5^{2-} $[C_6H_4C(O)O]$ $I(OAc)_3$
	4	2	6	Square planar AX_4E_2	XeF_4, IF_4^-, $XeOF_3^-$
Pentagonal bipyramid	7	0	7	Pentagonal bipyramid AX_7	IF_7, $IO_2F_5^{2-}$ IOF_6^-, TeF_7^-, $CH_3OTeF_6^-$, $(CH_3O)_2TeF_5^-$ BiF_7^{2-}, SbF_7^{2-}
	6	1	7	Pentagonal Pyramid AX_6E	$XeOF_5^-$, IOF_5^{2-} $[IF_5(C_6H_5)]^-$ XeF_6 (-monocapped octahedron)
	5	2	7	Pentagonal planar AX_5E_2	XeF_5^-, IF_5^{2-}
Square antiprism	8	0	0	Square antiprism AX_8	IF_8^-, ~~XeF_8~~, XeF_8^{2-} (AX_8E)

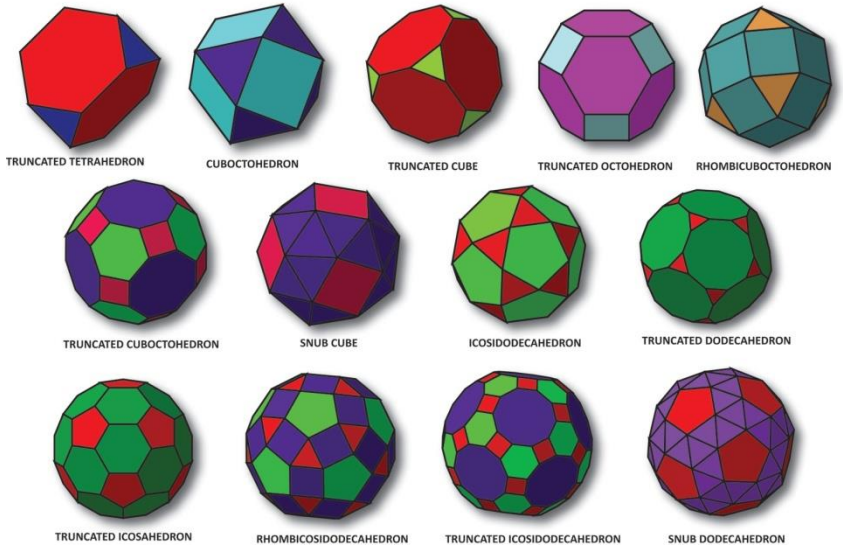






Platonic Solids





Archimedian Solids