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ATOM exam reviw

# chemical periodicity

Four aspects need to be known, atom radius, Ionization energy, electron affinity, electronegativity.

## Atomic radius

### Atomic radius decreases within a period since Z\_eff increases and valence electron are more tightly bound to nucleus.

### Atomic radius increases within a group: n increase (more orbitals) so atomic radius increase. Due to the shielding effects, Z\_eff only increases slightly.

## Ionization energy

### Definition: the amount of energy needed to remove an electron from the gaseous atom E in its ground state. (All electrons occupy the lowest energetic levels)

### I\_1 increases within a period due to the contracting atomic radius (radius decreases, more energy needs to ionize) and the stronger attraction of the valence electrons (nucleus mass increases doesn’t lead to more orbitals, so it attracts the valence electrons at the same level more effectively).

### I\_1 decreases down as a column. Since the orbital is more far away from the nucleus, less energy is needed to ionize.

### Exceptions needs to notice: a small jump from all filled up s-shell or p-shell partial filled up with single electron. (after, the ionization energy become a little bit less).

### Transition metal: 4s is effectively shielded by 3d, 4p shielded by 3d.

## Electron affinity

### Definition: the energy change after the energy if an electron added to E

### EA becomes more negative due to the Z\_eff increased.

### EA of the main group elements become less negative down a group due to the distance to the nucleus increases.

## Electronegativity

### Definition: A chemical property that describes the tendency of an atom to attract electron density towards itself in a molecule or a compound.

### X = I + |EA|/2

### General trends: EN increases across a period, Fc increases because of increasing Z\_eff. EN decreases down a group due to the increasing r\_atom. EN increases with the oxidation state. The oxidation state increase means the element loses more electrons, so that it has stronger tendency to attract electrons.

# Notation of an atom

## There are three methods: orbital diagram (skip), spdf notation, noble gas notation.

### spdf: 1s^2, 2s^2, 2p^6.

### noble gas notation: [Ar (noble gas)] 4s^2 3d^3 (notation from noble gas)

# Chemical bond

## Large difference in EN => ionic bond

### Valence electrons are transferred to more electronegative elements so that both elements can reach noble gas configuration.

### The ionic compounds tend to form crystalline solids. Size and stability, radius ratio.

### Lattice energy: the energy that keeps the shape of the crystal. A balance between Coulomb attraction and Born repulsion. High lattice energy corresponds to high melting points, high hardness, and low solubility in water.

## Large values of EN and small difference in EN => covalent bonding

### Valence electrons are shared between both atoms to reach a noble gas configuration.

### Detail in 4.

## Small values of EN and small difference in EN => metallic bonding

### Both elements give away the valence electrons to reach noble gas configuration and form an electron cloud.

# COvalent bond

## LEWIS (skip)

## VSEPR Model

### This is the actual arrangement of atoms in space. The most stable arrangement of valence electron pairs around a nucleus is the one that minimizes the electron-electron repulsions.

### A diagram of a triangle Description automatically generated with medium confidence

### A screenshot of a computer Description automatically generated

### The order of bonding pairs and lone pairs repel each other electrostatically in bond angles is BP – BP < LP – BP < LP – LP

### Space occupations: LP > TP > DB > SB

## Valence bond theory

### Hybridization: the linear combination of different wave functions of the same atom to generate new hybrid wave functions. Or simply say, the more overlap, better separation of bonding pairs and hence more stable molecules.

### Principle: hybridization includes s-, p- and d-orbitals: sp: s + p, sp^2: s + 2p. Only **non-equivalent orbital can hybridize then form a new orbital**. (promotion of the electron from ground state first and then hybridize).

### Sigma bond is overlap of orbitals from end-to-end fashion. Pi bonds are the sideways overlap of two p-orbitals.

### Double bond configuration: a strong sigma-bond, a weaker pi-bond. Easy possibility of the pi-bond to open and form new bonds in a chemical reaction.

### Triple bond configuration: one sigma-bond, two pi-bonds.

## MO theory

### Bonding and anti-bonding: constructive interference and destructive interference.

### Bond order = (bonding electrons – antibonding electrons)/2

### Sigma 2pz is dropping from Li2 to F2. After O2, the sigma 2pz bond will drop below the pi2px, pi2py level.

### In heteroatomic MOs, bonding and anti-bonding MOs will be energetically closer to one of the AOs. (Worth to notice: H’s orbital even higher than 3px, 3py and 3pz. And H will interact with 3pz and form bonding and anti-bonding for sigma 3pz.)

### Variation Principle: The best LACO c coefficients can be obtained by minimize the value of the energy E.

### Symmetry: only AOs of the same symmetry will be combined, for the anti-bonding and bonding are not necessary the same just with different sign.

### Ligand field: Delta is the crystal field splitting energy, one is going to eg orbital and the other is t2g orbital. (vertical charge is located at vertices of an octahedron not he full sphere). D1-d3 are three successive filling of the degenerated t2g orbitals. D4-d7 two possibilities depending on delta. D8-d10 successive filling of eg orbitals.

# Effective charge

## Penetration and shielding

### Refers to the extent to which a given orbital lies inside other filled orbitals.

### The node is the position that doesn’t have radial distribution of the electrons. Means these points have less electron penetrations. So 2s orbitals provides less shielding than 1s orbital.

### Electron shielding refers to the weakening of the attraction between an electron and the atomic nucleus due to the presence of more penetrating.

## Effective charge

### For the many-electron atoms, we neglect electron-electron repulsion. The total wavefunction will be considered as the product of single electron wave function.

### The repulsion can be reintroduced via an effective charge of the nucleus with the equation E = Z\_eff^2/n^2

### Z\_eff = Z – S via four rules: electrons with higher n don’t contribute to the shielding S, the shielding S through the other electron on s-orbital is 0.3, all other electrons on the same shell contribute 0.35. Shielding from electrons on the next lower shell contribute to shielding with 0.85 for s and p. n-2 provide 1 to the shielding.

## The Hartree-Fock method

### This set of wavefunction is used to determine an averaged charge density of the electrons and calculate for each electron the repulsion between this electron and the averaged charge density of the others.

### This gives energetic levels of the orbitals within a shell for different electron numbers.