**Hard and Soft Acids and Bases**

* 1965- Ralph Pearson introduced the hard-soft-acid-base (HSAB) principle.

***Hard acids prefer to coordinate the hard bases and soft acids to soft bases.***

* This very simple concept was used by Pearson to rationalize a variety of chemical information.
* 1983 the qualitative definition of HSAB was converted to a quantitative one by using the idea of polarizability.

**A less polarizable atom or ion is hard and a more easily polarized atom or ion is soft.**



* Actually, the electronegativity, X, of a neutral species-

X = (I.P. + E.A.) /2

The average of ionization potential and electron affinity.

* The Quantitative Definition of hardness:

N = (I.P. - E.A.)

* One can relate n (hardness) to the gap between the HOMO and LUMO:

N = (ELUMO - EHOMO) E (energy)



* HOMO and LUMO orbitals (molecules) or simply highest occupied and lowest unoccupied orbitals in atoms participate in the bonding more than any other levels.
* The lower the energy of the HOMO and the higher the energy of the LUMO, the more stable the species is thermodynamically.
* The greater the N value - the more hard the species is.
* basically, HSAB theory endeavours to help one decide if

AB + CD  AC + BD goes to the left or the right.

* Hard acid: High positive charge, Small size, Not easily polarizable.
* Hard base: Low polarizability, High electronegativity Not easily oxidized.
* Soft acid: Low positive charge, Large size; easily oxidized, Highly polarizable
* Soft base: High polarizability, Diffuse donor orbital, Low electronegativity, Easily oxidized.
* Hard acids prefer to bind to hard bases and soft acids prefer to bind to soft bases.
* This statement is neither an explanation nor a theory. It is simply a guideline that helps one to qualitatively predict the relative stability of acid-base adducts.
* Lewis acids: A+ Lewis bases: B: or B:-
* A+n the smaller and more highly charged, the harder it will be

B: or B:-n the larger the atom (or ion) the softer it will be.

**Classification of hard and soft acids**

* Important to remember that the listings in the tables do not have a sharp dividing line between them. These terms, “hard” & “soft”, are relative. Some are borderline and even though within the same category are not all of the same degree of “hardness” and “softness”.
* Although all alkali metals in ionic form M+ are “hard”, the larger, more polarizable, Cs+ ion is much softer than Li+.











