Class 2: Bond Valence

Paulings electrostatic valence rule disregards distance between atoms. Distance is particularly important when there is more than one cation in the structure. Pauling's rules can be found in *J. Am. Chem. Soc.* **51** (1929) 1010.

Brown [The Chemical Bond in Inorganic Chemistry etc.] has (with others) suggested an extension of electrostatic valence by noting that the bond valence usually obeys a simple relation with distance:

$S_{ij} = \exp[(R_0 - R_{ij})/B]$ and $S_{ij} = (R_{ij}/R_0)^{-N}$

Where S_{ij} is the bond valence of the bond between i and j, and R_{ij} is the distance. B, R_0 and N are chosen from crystallographic data so that the bond valence sum is equal to the formal valence.

The Bond Valence Sum is simply the sum of all bond valences to an atom: $V_i = \Sigma_j S_{ij}$

Class 2: Bond Valence 2

In this class, we will examine the use of the bond valence calculator, *valence*, from I. D. Brown, and also SPuDs from Lufaso and Woodward.

We will also discuss a few publications on *ab-initio* structure prediction: Pannetier et al. *Nature* **346** (1990) 343; Schon and Jansen, *Angew. Chem. Int. Edn.* **35** (1996) 1304; Jansen, *Angew. Chem. Int. Edn.* 41 (2002) 3746.