

$r =$ half the bond length of the Group IV element on the same row.

$$R = \frac{r_{\alpha} + r_{\beta}}{2}$$

$K_s =$ Thomas-Fermi free screening wave #

$$K_s^2 = \frac{4K_F}{\pi a_0}$$

$K_F =$ Fermi momentum with appropriate p

$$(K_F^3 = 3\pi^2 N)$$

Electronegativity scale:

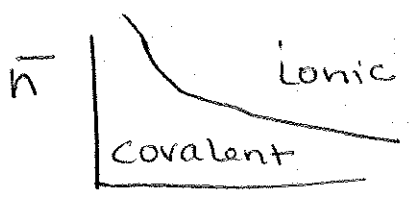
$$X_{\alpha} = 3.6 (Z_{\alpha}/r_{\alpha}) (0.9) \exp(-K_s r_{\alpha}) + 1/2$$

where 3.6 and 1/2 were chosen so that $X_{\alpha}(C) = 2.5$

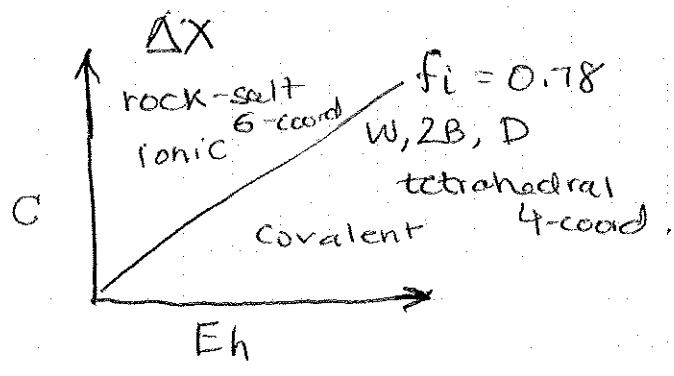
$$X_{\alpha}(CN) = 3.0$$

to agree with Pauling

1959 Mooser & Pearson



8 errors in 100 xtals



- much higher f_i needed for ionic transition of behavior though

i.e. MgO rock salt

refractive index decreases with hydrostatic pressure where alkali-halides \uparrow

* What else can you predict with these? (3)

Tetrahedral covalent radii
- not solely additive like Paulings

* Ionic radii
- b/c different from predicted
covalent radii

* Nonlinear optical susceptibilities

JC Phillips JA Van Vechten
Phys Rev (183) 709 1969

(charge
transfer
polarizability)

* Melting temperatures
JVV PRL (29) 769 1977

* Bandgap energies

VV Phys Rev (182) 891 1969

~~442~~

* Charge distribution & piezoelectric constants

P & VV PRL (23) 1115 1969

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Melting temperature scaling

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Optical susceptibilities

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Piezoelectric constants

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