L. Pauling

\[ \Delta = a(\chi_A - \chi_B)^2 - \varepsilon(A - B) - \frac{\varepsilon(A - A) + \varepsilon(B - B)}{2} \]

\[ A_2 + B_2 \rightarrow AB \]

R. S. Mulliken

\[ X(g) \rightarrow X^+(g) + e^- \quad \Delta H_i^{0 \rightarrow i+}(X) \]

\[ Y(g)^+ + e^- \rightarrow Y^-(g) \quad -\Delta H_i^{1 \rightarrow 0}(Y) = \Delta H_i^{0 \rightarrow 1-}(Y) \]

\[ \therefore X(g) + Y(g) \rightarrow X^+Y^- \quad \Delta H_i^{0 \rightarrow 1+}(X) + \Delta H_i^{0 \rightarrow 1-}(Y) \]

同様にして

\[ X(g) + Y(g) \rightarrow X^-Y^+ \quad \Delta H_i^{0 \rightarrow 1-}(X) + \Delta H_i^{0 \rightarrow 1+}(Y) \]

\[ X^+Y^- < X^-Y^+ \quad \Delta H_i^{0 \rightarrow 1+}(X) + \Delta H_i^{0 \rightarrow 1-}(Y) < \Delta H_i^{0 \rightarrow 1-}(X) + \Delta H_i^{0 \rightarrow 1+}(Y) \]

\[ I(X) + Ae(X) < I(Y) + Ae(Y) \]

\[ \chi_M = \frac{I + Ae}{2} \]
電気陰性度の定義

- **Pauling**
  \[
  \Delta = a(\chi_p^a - \chi_p^b)^2 = \varepsilon(A - B) - \frac{\varepsilon(A - A) + \varepsilon(B - B)}{2}
  \]

- **Mulliken**
  \[
  \chi_M = \frac{I + A_e}{2}
  \]

- **Allred & Rochow**
  \[
  \chi_{AR} = 0.359 \frac{Z_{\text{eff}}}{r^2} \times 10^4 + 0.744
  \]

- **Sanderson**
  \[
  \chi_S = \frac{D}{D_i}
  \quad D = \frac{Z}{4\pi r^3}
  \]

種々の電気陰性度の比較
\[ \Delta \chi_s = \sqrt{\chi_s} \quad \text{(R.T. Sanderson)} \]
Sandersonによる電気陰性度と化学結合

KCl分子の生成

K
χ_S = 0.445
Δχ_S = 1.047
r = 231pm
r_1+ = 133pm

Cl
χ_S = 3.475
Δχ_S = 2.927
r = 99pm
r_1- = 181pm

電気陰性度の均等化

\[ \sqrt{\chi_A^S \cdot \chi_B^S} = \chi_S^{(eqli.)} \]
\[ = \sqrt{0.445 \cdot 3.475} \]
\[ = 1.244 \]

Kの\( \chi_S \)

0.445 → 1.244
Δχ_S = +0.799
+δ = \frac{0.799}{1.047} = 0.763

Clの\( \chi_S \)

3.475 → 1.244
Δχ_S = -2.231
-δ = \frac{-2.231}{2.927} = -0.762
Total Energy

Valence →

Energy

- -

Energy

+ +

Valence →

$\chi_A^+ = \chi_B^-$

$\chi_{-\delta}^A = \chi_{+\delta}^B$

電子親和力
イオン化エネルギー曲線
と
電気陰性度