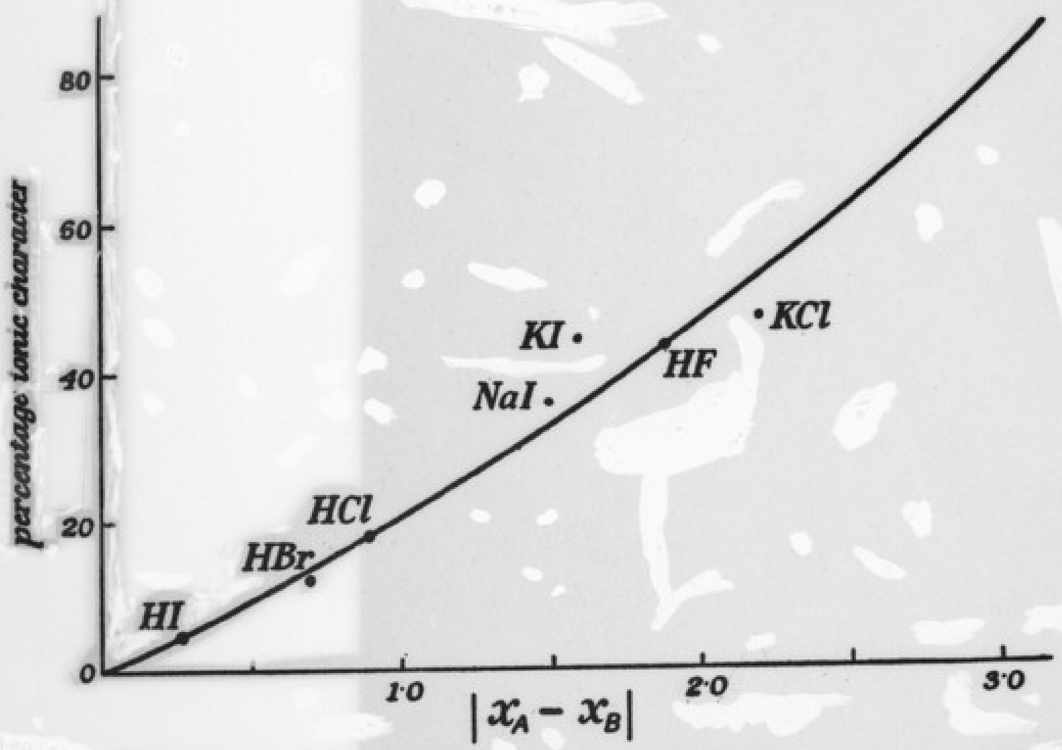
function (23) by the condition that $c_2 = c_3$. It is clear that in general this will involve $H_{22} = H_{33}$, where

$$H_{22} = \iint \psi_A(1)\psi_A(2)H\,\psi_A(1)\psi_A(2)\,d\tau_1\,d\tau_2 = \text{energy of structure } A^-B^+,$$

and H_{33} is the energy of A^+B^-. If we may neglect polarization and certain small differences in repulsive energies, this implies that, starting with two



Percentage ionic character in terms of electronegativity difference $|x_A - x_B|$, according to Hannay and Smyth's formula in equation (33). Experimental values shown by dots.

neutral atoms A and B, the same amount of energy is needed to create A^+B^- as A^-B^+, i.e.

$$I_A - E_B = I_B - E_A.$$

In other words, for a covalent bond

$$I_A + E_A = I_B + E_B.$$

For a polar bond we should expect that

$$(I_A - E_B) - (I_B - E_A) \propto x_A - x_B.$$

This implies that
$$x_A \propto (I_A + E_A),$$

as required in Mullik