

Hammett equation (Hammett relation)

The equation in the form:

$$\log_{10}\left(\frac{k}{k_0}\right) = \rho \sigma$$

or

$$\log_{10}\left(\frac{K}{K_0}\right) = \rho \sigma$$

applied to the influence of *meta*- or *para*-substituents X on the reactivity of the functional group Y in the benzene derivative *m*- or *p*-XC₆H₄Y. *k* or *K* is the rate or equilibrium constant, respectively, for the given reaction of *m*- or *p*-XC₆H₄Y; *k*₀ or *K*₀ refers to the reaction of C₆H₅Y, i.e. X = H; ρ is the substituent constant characteristic of *m*- or *p*-X; σ is the reaction constant characteristic of the given reaction of Y. The equation is often encountered in a form with $\log_{10}k_0$ or $\log_{10}K_0$ written as a separate term on the right hand side, e.g.

$$\log_{10}k = \rho \sigma + \log_{10}k_0$$

or

$$\log_{10}K = \rho \sigma + \log_{10}K_0$$

It then signifies the intercept corresponding to X = H in a regression of $\log_{10}k$ or $\log_{10}K$ on σ .

See also: ρ -value, σ -constant, Taft equation, Yukawa-Tsuno equation

Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1119