doi:10.1351/goldbook.H02732

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*-XC_6H_4Y. k or K is the rate or equilibrium constant, respectively, for the given reaction of *m*- or *p*-XC_6H_4Y; k_0 or K_0 refers to the reaction of C_6H_5Y, i.e. X = H; is the substituent constant characteristic of *m*- or *p*-X: 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

