Anhydrous Iron(III) Nitrate

Polar *ortho*-Substituent Constants

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IN a recent communication Liotta[1] introduced a new set of quantitative *ortho*-polar substituent effects based on earlier well known data.[2]

Apparently the values Liotta has reported were obtained by setting the ρ-value = 1 in a Hammett treatment of the reaction for *meta*- and *para*-substituted benzoic acid with 1,3-diphenylguanidine in benzene. However, these values are not scaled to the standard Hammett substituent constants and are therefore not applicable to or comparable with other reactions. For this purpose it is necessary to introduce the ρ-value for the reaction obtained from the data[2] for *meta*- and *para*-substituents; a linear regression analysis gives $\rho = 2{\cdot}079$ (correlation coefficient = 0·993), and the derived σ_o values are then: Me, −0·152; F, 0·250; Cl, 0·398; Br, 0·441; I, 0·464; NO_2, 1·051.

Charlton[4] has also reported *ortho*-polar substituent constants calculated from the same data. The values reported here and those of Charlton are comparable with those reported by Jones and Smith[5] and Taft[6] for different reactions.

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[1] C. L. Liotta, *Chem. Comm.*, 1968, 338.
[2] M. M. Davis and H. B. Hetzer, *J. Res. Nat. Bur. Stand. U.S.A.*, 1958, **60**, 569.
[3] M. Charlton, *J. Amer. Chem. Soc.*, 1964, **86**, 2033.
[4] D. A. K. Jones and G. G. Smith, *J. Org. Chem.*, 1964, **29**, 3521.
[5] R. W. Taft, jun., *J. Chem. Phys.*, 1960, **64**, 1805.