

Modified Model of the Inductive Effect. Refined Calculation of the Inductive Constants

Cherkasov A., Galkin V., Sibgatullin I., Cherkasov R.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The atomic inductive constants σ_A in terms of the previously proposed additivity model of the inductive effect were refined by multiparameter regression analysis of the whole array of available experimental Taft constants σ^* represented as a single matrix. A significant inductive effect of the hydrogen atom on a carbon reaction center was revealed, which was not taken into account in the previous version of the additivity model. The modified approach provides an appreciably higher accuracy in the calculation of substituent inductive constants.
