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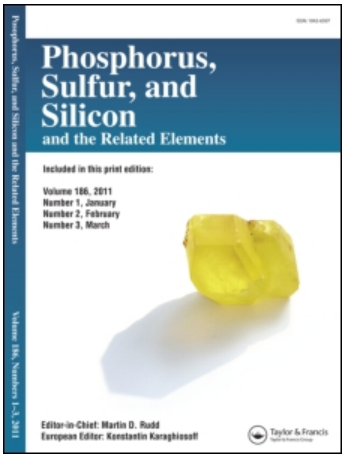

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3D Correlation Analysis in Organoelement Chemistry

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3D CORRELATION ANALYSIS IN ORGANOELEMENT CHEMISTRY

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On the basis of previously developed models of inductive and steric effects we have elaborated a new method for quantification of substituent effect, called "3D Correlation Analysis." The procedure of 3D Correlation Analysis allows the quantitative consideration of any free energy-related quantitative parameters in the framework of the following equation:

$$\Delta G = \Delta G^0 + \sum_{i \neq rc}^{N-1} \frac{g_i}{r_{rc-i}^2},$$

where N is the number of atoms in a molecule, *rc* is atom-reaction center, r_{rc-i} is the direct distance between i-th atom and the reaction center, and operational parameter *g* reflects the ability of this atom to contribute into intramolecular interactions determining the magnitude of $\Delta\Delta G$.

The adequacy of the developed approach has been tested on the example of various reaction series including those fundamental for correlation analysis (here we have considered pKa volumes of 827 different carboxylic acids and 802 protonated amines) and different reaction series concerning organoelement and organophosphorus reactivity.

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