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Substituent effects on thermochemical properties of free radicals. New substituent scales for C-centered radicals

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Abstract

In this work, we have analyzed substituent effects on ionization potentials and electron affinities of C-centered radicals in terms of operational atomic contributions. The analysis was based on ionization potential data for 48 C-centered radicals and electron affinity data for 20 C-centered radicals. For both sets of data, the correlation between predicted numbers and experimental data was good (R = 0.98). Based on these operational atomic parameters, additive substituent constants have also been derived, and equations for prediction of ionization potentials and electron affinities of C-centered radicals are presented.