Towards Universal Substituent Constants: Interpreting QTAIM Substituent Properties with Multivariate Data Analysis

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The properties of substituents are routinely interpreted using proxies to the substituent effect, measured by the substituent's effect elsewhere in the moleculem [1,2]. The Quantum Theory of Atoms in Molecules provides a means to directly assess substituent properties [3]. Here, using Partial Least Squares and Principal Components Analysis, QTAIM intrinsic substituent properties are related to empirical proxies and are shown to be able to describe the same information, but from a more foundational perspective [4,5]. This work presents a step to moving beyond proxies in describing substituent effects.

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