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Reaction Force Constant As a Descriptor of the Principle of Non-Perfect Synchronization

Reaction Force Constant As a Descriptor of the Principle of Non-Perfect Synchronization

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In this study, a small set of 1,3-dipolar cycloaddition reactions (see Scheme 1) that proceed at the same exothermicity is presented [1]. Our main objective was to extend the application of the reaction force constant concept [2] to gain an understanding of the reactivity principles. Inspired by a recent article where we show that the Bell-Evans-Polanyi principle is fulfilled under the condition of an equal degree of (a)synchronicity [3], here, we demonstrate that the reaction force constant (see Figure 1) is also a suitable descriptor to quantify the principle of non-perfect synchronization proposed by Bernasconi as a way to understand deviations from the Bell-Evans-Polanyi principle.

Scheme 1

Figure 1

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