Research paper

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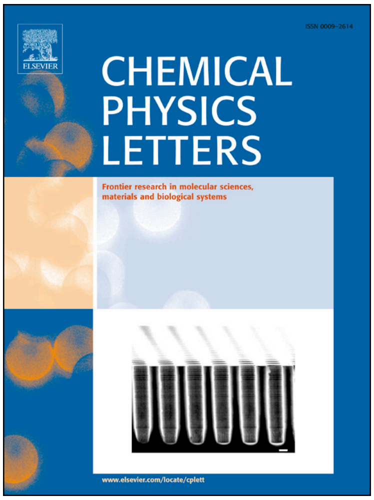

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Anomeric Effect Revisited: Perspective from Information-Theoretic Approach in Density Functional Reactivity Theory

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Abstract

In this work, we apply the quantities from the information-theoretic approach in density functional reactivity theory to examine the origin and nature of the anomeric effect, which is the preference of heteroatomic substituents within the cyclohexane ring to be in the *axial* orientation rather than the sterically less hindered *equatorial* position. Using α-D-glucopyranose as an example, we confirmed its complex stereoelectronic origin. With Shannon entropy, Fisher information, GBP entropy, information gain, Onicescu information energy, and relative Renyi entropy, we are able to accurately account for the axial-equatorial energy difference in general, with the anomeric effect included as a special case.

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