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ACCEPTED MANUSCRIPT

Computational study of the 1,3-dipolar cycloaddition between methyl 2trifluorobutynoate and substituted azides in terms of reactivity indices and activation parameters

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Running Title: Computational study of the 1,3-dipolar cycloaddition

Key words: 1,3-dipolar cycloaddition; phenyl azide; methyl 2-trifluorobutynoate; DFT-based reactivity indices; activation energy; transition states.

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