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Calculations of activation energy of cycloaddition reaction in solution

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Abstract

With the method, principally different from the quantum ones, there has been performed the calculation of activation energies of 20 cycloaddition reactions in solutions. The objects under examination included: non-catalyzed reactions of diene synthesis, reactions of 1,3-dipolar cycloaddition, reactions of polar [2+2]-cycloaddition. Calculation results have been compared with the experimental data. The comparison testifies in favor of closeness of calculated values and experimental data.