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Influence of solvation on the mechanism of the hydroperoxide radicals' addition to the π-bonds of trans 1,2-and 1,4-diphenylbutadiyne-1,3

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The role of the effect of nonspecific solvation in the addition of hydroperoxide radicals to π-bonds of trans-1,2-diphenylethylene and trans, trans-1,4-diphenylbutadiene-1,3 in the medium of different polarity solvents was investigated via a set of kinetic methods (microvolumetry, method of inhibitors, rotating-sector method). When the medium polarity is varied, the logarithm of the rate constant of this reaction in the Kirkwood-Onsager equation coordinates shows a linear dependence. Quantum-chemical analysis (NWChem, DFT B3LYP/6-311G**) allows us to conclude that the influence of the polarity of the medium for nonspecific solvation on the rate of the considered reaction will depend on how much the solvation energies of the transition complex and the initial reaction complex differ. If the solvation energy of the transition complex is higher than the solvation energy of the initial reaction complex, the reaction rate should increase with increasing solvent polarity, otherwise it should decrease.

Biography

Roman Pliss has finished Yaroslavl State Technical University (Yaroslavl, Russia) in 1999. He has published more than 10 papers in reputed journals

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