Russian Journal of Physical Chemistry A 2014 vol.88 N5, pages 890-892

Enthalpy and entropy of activation and the heat effect of the ene reaction between 4-phenyl-1,2,4-triazoline-3,5-dione and 2,3-dimethyl-2-butene in solution

Kiselev V., Kornilov D., Potapova L., Kashaeva H., Konovalov A.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The rate of the fastest ene reaction between 4-phenyl-1,2,4-triazoline-3,5- dione (1) and 2,3-dimethyl-2-butene (2) is studied by means of stopped flow in solutions of benzene (k 2 = 55.6 ± 0.5 and 90.5 ± 1.3 L mol-1 s-1 at 23.3 and 40°C) and 1,2-dichloroethane (335 ± 9 L mol-1 s-1 at 23.5°C). The enthalpy of reaction (-139.2 ± 0.6 kJ/mol in toluene and -150.2 ± 1.4 kJ/mol in 1,2-dichloroethane) and the enthalpy (20.0 ± 0.5 kJ/mol) and entropy (144 ± 2 J mol-1 K-1) of activation are determined. A clear correlation is observed between the reaction rate and ionization potential in a series of ene reactions of 4-phenyl-1,2,4-tri-azoline- 3,5-dione with acyclic alkenes.

http://dx.doi.org/10.1134/S0036024414050136

Keywords

2,3-dimethyl-2-butene, 4-phenyl-1,2,4-triazoline-3,5-dione, ene synthesis, kinetics, thermochemistry