Название публикации:

Influence of haloid substitution and conjugation on ozone-olefine reaction

Авторы:

Mamin, E.A.a,b, Krisyuk, B.E.c, Mayorov, A.V.b,d, Ovchinnikov, V.A.a,b, Tyubaeva, P.M.a,b, Popov, A.A.a,b

a) Plekhanov Russian University of Economics, Moscow, 117997, Russian Federation
b) Emanuel Institute of Biochemical Physics RAS, Moscow, 119334, Russian Federation
c) Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow obl., 142432, Russian Federation
d) National Institute of Standards and Technology, Gaithersburg, MD 20899, United States

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Аннотация:

Primary stage of ozone-olefine reaction was investigated using quantum-chemical methods. The reaction can proceed through different transition states - concerted and nonconcerted mechanisms. The presence of a halogen substitutor at the double bond and the conjugation can influence the rate constant and ratio of rate constants of different reaction mechanisms. This influence can be estimated in terms of quantum chemical methods B3LYP, B2PLYP, CCSD and CASSCF which allow to find stationary points at potential energy surface of the reaction and estimate Ea and k. © 2018 Author(s).

Ключевые слова:

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