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Influence of substitutors at double C=C bond on mechanism of addition of ozone

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Abstract

In this paper we report results of calculation of prime stage of reaction of ozone and double bond of ethylene, buten-2, chlorinated ethylene (C_2Cl_4, C_2Cl_3H etc.). Calculation was carried out with ab initio method MRMP2 and DFT-method B3LYP with 6-31+G/6-311+G basis sets involving diffuse functions and aug-cc-PVDZ. Kinetic dependences are studied for both concerted addition proceeding through symmetrical transition state (Kriegee) and nonconcerted addition proceeding through diradical transition state (Demore). Both of these mechanisms have successfully described in single-reference and multi-reference approach. Calculations confirmed the existence of both these paths for all reagents and gave sensible values for rate constants fitting experimental ones.