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Quantum chemical study of the addition of ozone to acetylene

Авторы:
Krisyuk, BE [1,2] ; Maiorov, AV [3] ; Mamin, EA [3] ; Popov, AA [2,3]

[1] Russian Acad Sci, Inst Problems Chem Phys, Chernogolovka 142432, Moscow Oblast, Russia
[2] Plekhanov Russian Univ Econ, Moscow 117997, Russia
[3] Russian Acad Sci, Emanuel Inst Biochem Phys, Moscow 119334, Russia

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Аннотация:
The primary step of acetylene ozonation was studied by the B1LYP, PBE0, CASSCF, MRMP2, and CCSD methods using the 6-31+G**, aug-cc-pVDZ, cc-pVTZ, and aug-cc-pVTZ basis sets. The study confirmed the earlier B3LYP-based conclusions that the intermediate complex, as well as the transition states of the concerted addition (Criegee's mechanism) and unconcerted addition (DeMore's mechanism), are involved in this reaction event. The activation enthalpy and entropy and rate constants of the reaction were calculated. Criegee's mechanism was shown to dominate in the reaction with acetylene, but the contribution from DeMore's mechanism is also noticeable, being 1-8%.

Ключевые слова:
Molecular-structure; ethylene; energetics; complexes; mechanism; kinetics