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Comparison of reactivity of fluoro- and chlorosubstituents of ethylene with ozone

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Abstract

DFT B2PLYP, *ab initio* CASSCF, MRMP2, coupled-cluster CCSD calculations were applied to reactivity of C=C bound of 1-monofluorethylene, 1-monochloroethylene, 1,1-difluorethylene, 1,1-dichloroethylene in reaction with ozone, aug-cc-pVDZ basis sets. Concerted and nonconcerted additions were investigated. It was shown that CCSD is better for modeling of reaction characteristics, MRMP2 results do not correspond to experiment in each case due to partial optimization. Once polar substituent is present, the role of nonconcerted mechanism becomes greater – about 50% in 1,1-difluorethylene, 98% in 1,1-dichloroethylene.