Abstract Submitted
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Computational Study on Chemical Reaction Mechanisms of Octafluorocarbon Molecules[1] HEECHOL CHOI, MI-YOUNG SONG, JUNG-SIK YOON, Plasma Technology Research Center, National Fusion Research Institute (NFRI), PLASMA FUNDAMENTAL TECHNOLOGY RESEARCH TEAM — Saturated or unsaturated octafluorocarbons(OFCs) have been used extensively in dry etching processes due to their relatively low global warming potential and their high CF_2 radical levels in commercial plasma treatments. Many experimental and theoretical studies of these species have been performed for useful information about physical and chemical properties of OFCs. However, direct experimental studies of these chemicals are difficult because of their high reactivity in plasma state and high-level theoretical approaches such as G3(MP2) and CCSD(T)/CBS need huge computational cost. Recently, it has been shown that the ωB97X-D/aVTZ method is strongly recommended as the best practical density functional theory(DFT) for rigorous and extensive studies of OFCs because of its high performance and reliability for van der Waals interactions. All the feasible isomerization and dissociation paths of OFCs were investigated at ωB97X-D/aVTZ and rate constants of their chemical reactions were computed by using variational transition-state theory(VTST) for a deep insight into OFCs' reaction mechanisms. Fates and roles of OFCs and their fragments in plasma phases could be clearly explained based on the obtained reaction mechanisms.

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