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Computational Study on Chemical Reaction Properties of C_4F_8 Plasma Molecules HEECHOL CHOI, National Fusion Research Institute (NFRI), YOUNG C. PARK, Korea Advanced Institute and Technology (KAIST), KYOUNG K. BAECK, Gangneung-Wonju National University (GWNU), YOON S. LEE, Korea Advanced Institute and Technology (KAIST), FUNDAMENTAL TECHNOLOGY RESEARCH DIVISION TEAM[1], DEP. OF CHEMISTRY TEAM[2], DEP. OF CHEMISTRY TEAM[3] — Of many perfluorocarbons(PFCs), C_4F_8 species attract special attention because of their potential for decreasing global warming gas emissions and their high CF_2 radical levels in commercial plasma treatments. Several experimental and theoretical studies of these species have been conducted, although only the geometries at their stationary states and their adiabatic electron affinities have been determined. However, this information is not sufficient for a deep understanding of all the possible fates and roles of C_4F_8 species and their fragments in plasma phases. So a careful additional assessment of the reliability of DFT functionals for the study of PFCs is highly required. First, in order to find a DFT method appropriate to PFCs, the geometry, energy, and chemical reaction properties of C_4F_8 were calculated and compared with reference data. Second, based on variational transition-state theory, the rate constants of dissociations and isomerizations of C_4F_8 species were computed for a deep insight into their mechanisms.

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