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Density Functional Theory Calculations for Chemical Reaction Mechanisms of C_4F_8

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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 saturated or unsaturated C_4F_8 species because of its high performance and reliability especially for van der Waals interactions. All the feasible isomerization and dissociation paths of C_4F_8 molecules were investigated at this theoretical level and rate constants of their chemical reactions were computed by using variational transition-state theory for a deep insight into C_4F_8 reaction mechanisms. Fates and roles of C4F8 molecules and their fragments in plasma phases could be clearly explained based on our computational results.

Keywords: C_4F_8, plasma molecule, DFT, reaction mechanism