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Density Functional Theory (DFT) Calculations for the Geometry, Energy, and Chemical Reaction Properties of C_4F_8

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Perfluorocarbons (PFCs) have been suggested as possible replacements for SF_6 and the fluorocarbons used in and emitted during technological plasma treatments because PFCs have significantly low greenhouse warming potentials. Of many PFCs, c-C_4F_8 and 2-C_4F_8 attract special attention because of their high CF_2 radicallevels in commercial plasma treatments. Accordingly, several experimental and theoretical studies of these C_4F_8 species have been conducted, although only the geometries at their stationary states and their adiabatic electron affinities (EAs) 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. Although the performance and reliability ofeach DFT functional have been examined carefully by the development team of each functional form with respect to the training and test data sets of well-known molecular systems, no PFC was included in the data sets. So a careful additional assessment of the reliability of DFT functionals for the study of PFC systems is highly required. 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.

Keywords: Plasma, Perfluorocarbon, DFT