Atmospheric chemical behaviours of C4F7N by DFT method: The relationship between electronic structure and atmosphere lifetime

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Abstract

C4F7N with excellent insulation performance has been proposed to replace the traditional SF6 as a new insulating medium in power equipment. In the present study, the molecular structure and radiative efficiency (RE) of C4F7N are calculated and compared with SF6 based on DFT calculation. The decomposition of pure C4F7N and the basic interactions between C4F7N and hydroxyl radical in the constructed co-crystal of C4F7N-H2O have been simulated by applying Monte-Carlo calculation and Car-Parrinello molecular dynamics (CPMD) method, in order to obtain reasonable and full-scale atmospheric dissociation processes. Then the detailed decomposition pathways are learned with DFT method of M062X. The rate constants of different pathways are further applied for calculating the atmosphere lifetime of C4F7N, to evaluate the possibility of applying it as an alternative gas of SF6 in power equipment. All the atmospheric chemical behaviours are determined by electronic structure and reflected by the decomposition pathways of C4F7N with interacting with hydroxyl radicals. Rather than traditional hypothesizing reaction models, this study provides a reasonable and practicable method to evaluate more alternative protective gas for understand the greenhouse effect.

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