Dissociative electron attachment to SF_5CF_3 leading to a stable combination of anionic SF_4 and neutral CF_4: Ab initio molecular dynamics study

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Since the first claim of its potential global warming effect of SF_5CF_3, almost two decades ago,[1] numerous experimental and theoretical studies were carried out to provide deeper understanding about its fate in the earth's atmosphere, as reviewed in a book chapter.[2] Among all possible removal processes of SF_5CF_3 from atmospheric environment, its reaction with low-energy electrons in the mesosphere is regarded to be the most probable pathway. Several research groups have made related experimental and theoretical studies,[3-6] and confirmed the production of the anionic product (SF_5^-) and radical (CF_3). So far, the fragment anion, SF_5^-, is assumed not recycled by its subsequent reaction with other chemical species. The energetic property of the product combination, neither the combination of anionic product (SF_5^-) and radical (CF_3) nor their dipole bound complex anion,[5] however, is not stable enough to be considered as an ultimately stable stage of the dissociative electron attachment. According to our theoretical study, as shown in this work,[7] there exists an additional pathway leading to the more stable combination of anionic SF_4 and neutral CF_4 by the recombination of the initial fragments, the anionic product (SF_5^-) and radical (CF_3), produced in the first stage of the electron attachment to SF_5CF_3. Ab initio calculations and subsequent classical molecular dynamics studies were carried out in the present work to support our new claim.

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