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Quantum chemical calculation of reactions in the plasma molecules important for the operation of the RPC system

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The current operation of the Resistive Plate Chamber (RPC) system within the CMS experiment involves tetrafluoroethane (C2H2F4, TFE) and SF6. However, in response to climate change concerns, the European Union has instituted a ban on these molecules due to their high Global Warming Potential (GWP).

As a result, researchers have been dedicated to investigating novel ecological gas mixtures based on tetrafluoropropene (C3H2F4, HFO-1234ze) and NOVEC 4710 to ensure sustainable functionality of RPCs. This study focuses on ab initio and density functional theory (DFT) calculations of electron impact ionization, electron impact excitation, and electron attachment reactions in plasma for these molecules using Gaussian 16 and ORCA quantum chemical packages. We calculate vertical and adiabatic transition energies, the values of thermodynamic functions for these reactions, and investigate the stability of the produced species during these reactions. Based on this calculation, we can draw conclusions about the behavior of these new species, compare their behavior with the molecules in use, and assess their potential as replacements. This study will help us in the systematic search for new eco-friendly gaseous alternatives.

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