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# Experimental and DFT study for the determination of the $g^3$ mixture ($C_4F_7N$-$CO_2$-$O_2$) byproducts and corresponding reaction pathways under the high electric ARC

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## Abstract

The main purpose of this research is to conduct a comprehensive study of the $g^3$ ($C_3F_7CN$ - $CO_2$ - $O_2$) mixture decomposition byproducts, produced under electric arc stress in the gas insulated circuit breaker (GIS) process. The insulated $g^3$ gas mixture is an alternative to $SF_6$ in high-voltage circuit breakers, which was identified as one of the six global warming potentials (GWP) in the Kyoto protocol of 1999. At extremely high temperatures (T = 40,000 K) and pressure conditions (P = 70 bar), arcing phenomena occur, leading to the conversion of the $g^3$ mixture into its respective decomposition by-products. Thermal Conductivity Detector - Gas Chromatography - Mass Spectrometry (TCD-GC-MS) analytical measurement reveals the main byproducts in $g^3$ polluted gas include $C_4F_7N$, $CO_2$, CO, $COF_2$, $CF_4$, $C_2F_6$, $C_3F_8$, $CF_3CN$, $C_2F_5CN$, and $(CN)_2$ in addition to the trace amount of $CH_3$-$SiF_3$, $SO_2$, $CF_3$-N+$SF_2$, $SiF(CH_3)_2$, $C_2F_4$, and amide. Theoretical studies are imperative to realize the degradation mechanism.

Density Functional Theory (DFT) modelling provides theoretical insights to understand the possible reaction pathway of $g^3$ ($C_3F_7CN$ - $CO_2$ - $O_2$) insulating gas mixture. In this research, a total of 32 possible chemical pathways were proposed, including eight recombination reactions.

Among the primarily dissociation reactions of the $C_4F_7NO$ molecule, two of them, $C_4F_7NO \rightarrow C_3F_3NO + CF_4$ and $C_4F_7NO \rightarrow C_2F_5CN + CF_2O$, are identified as the most favorable thermodynamically routes. The energy barriers for these two reactions are 91.7 kcal $mol^{-1}$ and 90.8 kcal $mol^{-1}$, respectively. Orbital energy gap ($E_a$) values reveal the highest value of $CF_4$ among all byproducts, and which refers to its contribution to the insulation strength along with the $g^3$ mixture. The variation in rate constant for the proposed reactions emphasizes the significance of reaction kinetics between 298.15 K and 3000 K.

**Keywords:** $SF_6$ alternatives, $C_3F_7CN$, Density Functional Theory, Chemical Reaction Mechanism, Reaction Kinetics