

Theoretical study of the gas-phase reactions of CHF<sub>2</sub>OCHF<sub>2</sub> (HFE-134) with Cl atoms

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**Abstract:** Theoretical studies have been carried out on the mechanism, kinetics and thermochemistry of the gas-phase reactions between CHF<sub>2</sub>OCHF<sub>2</sub> (HFE-134) and Cl atom using the high-level ab initio G2(MP2) and hybrid density functional model MPWB1K methods. Two conformers relatively close in energy have been identified for CHF<sub>2</sub>OCHF<sub>2</sub>, both of them are likely to be important in the temperature range of our study. The hydrogen abstraction pathway for the reactions of the two lower energy conformers with the Cl atom has been studied and the rate constants determined in a wide temperature range of 250-1000 K. The G2(MP2) calculated total rate constant value of  $5.9 \times 10^{-16}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296 K is found to be in good agreement with the recent experimental value of  $(5.7 \pm 1.5) \times 10^{-16}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296  $\pm$  1 K. The rate constant value obtained from the MPWB1K method ( $8.6 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>) is found to be somewhat lower than the available experimental result. The heats of formation for the CHF<sub>2</sub>OCHF<sub>2</sub> molecule and the CHF<sub>2</sub>OCHF<sub>2</sub> radical and the atmospheric lifetime of CHF<sub>2</sub>OCHF<sub>2</sub> are also reported.

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