

# Using Density Functional Theory Calculations to Estimate Radiative Forcing and Heat Capacity of $\text{CF}_3\text{OCHFCH}_3$

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## Abstract

This work used density functional theory and quantum chemistry along with a B3LYP/6-31g\* basis set in the Gaussian98 program to determine the radiative forcing and heat capacity of  $\text{CF}_3\text{OCHFCH}_3$ . This particular species comes from a class of compounds known as hydrofluoroethers (HFEs). This is an emerging class of compounds where almost no information is known about their environmental impact. All possible forms of the molecule were found and through a series of equations, radiative forcing and heat capacity were found. Radiative forcing constitutes half of the global warming potential equation and heat capacity deals with the efficiency of the species. Total radiative forcing was found to be  $0.37750536 \text{ W/m}^2\text{ppbv}$  and total heat capacity was found to be  $123.8592 \text{ J/(mol}\cdot\text{K)}$ . This procedure was repeated for a species where experimental data is known, showing excellent agreement. By finding the total global warming potential for species before they are manufactured, their environmental impact can be assessed and possible alternatives could be considered, leading to chemicals with the least environmental impact.