



Physics Colloquium

Friday March 26, 2021, 4:00 pm, PSC 3046

Claire MacDougall

Department of Physics, Saint Francis Xavier University

The Radiative Efficiency and Global Warming Potential of HFC-c-447ef.

Experimental absorption cross-section spectra of HFC-c-447ef ($\text{CF}_2\text{CF}_2\text{CF}_2\text{CHFCH}_2$) have been acquired at three different temperatures and a resolution of 0.1 cm^{-1} over the spectral range $550\text{-}3500 \text{ cm}^{-1}$. The absorption cross-section has been simulated over the $0\text{-}550 \text{ cm}^{-1}$ range with theoretical calculations using density functional theory methods at different levels of theory. A lifetime corrected radiative efficiency of $0.22 \text{ W}\cdot\text{m}^{-2}\cdot\text{ppb}^{-1}$ was obtained, leading to a 100-year time horizon global warming potential of 107 using an atmospheric lifetime of 2.8 years. Comparing the experimental and theoretical spectra reveals that computational methods can predict the integrated band strengths with good accuracy. The theoretical radiative efficiency depends on the level of theory chosen.

Keywords: HFC-c-447ef, 1,2,2,3,3,4,Heptafluorocyclopentane, Hydrofluorocarbon, Absorption cross-section, Infrared spectroscopy, Density functional theory, Radiative efficiency, Global warming potential



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Catherine Boisvert

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Swarm Relaxation: Optimizing the Attainment of Equilibrium in Simulations of Ice Nucleation

Monte Carlo computer simulations are often used to study systems at equilibrium. Normally, a single long run (SLR) is carried out to analyze the system observables and detect the attainment of equilibrium. However, such runs necessarily take a long time. Malek et al. recently showed that it is sometimes more efficient to run multiple, independently initialized runs in order to improve the sampling of independent microstates. We therefore run a large ensemble, a “swarm”, of M independent simulations and let them relax to equilibrium. Specifically, we look at the attainment of equilibrium of systems of $N=216$ and $N=1728$ molecules of water, where an ice nucleus is introduced. To confirm the attainment of equilibrium, we analyze the density, energy, and maximum nucleus size as a function of the number of Monte Carlo steps. Using the “swarm relaxation” method as described in Malek et al., we find that we can detect the attainment of equilibrium and dramatically decrease the wall-clock time required to do so. Our results serve as a starting point to understand more about the behaviour and anomalies exhibited by water.



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Mitchell Blacquiere

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Schlieren Imaging

Carl and I used an off-axis Schlieren Imaging technique to view how the refraction angle of light changes based on different temperatures of air a change in mediums such as helium and nitrogen. In the cases we observed, the index of refraction changes based on different temperature of air and/or the polarizability of the different mediums. Towards the end of collecting our data, we decided to test the system to fail by mixing a large amount of cold gas from a cup filled with liquid nitrogen with a flame from a candle; the results were successful, the index of refraction over the entire surface area of the mirror changed enough such that most of the light was refracted outside of the image causing most of the image to appear dark.