COMPARISON OF EXPERIMENTAL AND THEORETICAL ABSORPTION CROSS SECTIONS OF PFBAm

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We present a comparison of theoretical and experimental absorption cross sections of perfluorotributylamine (PFBAm). PFBAm is a fully-fluorinated liquid commonly used in electronic reliability and quality testing. PFBAm vapours can be considered potential greenhouse gases due being radiatively active in the mid-IR spectral region and having a long atmospheric lifetime.

Theoretical density functional theory (DFT) calculations are done using the B3LYP method and the 6-311G(d,p) basis set. The calculations have determined the optimized geometrical configuration and IR intensities and wavenumbers of the harmonic frequencies for both PFBAm (N(CF2CF2CF2CF3)3) and its congener (F3CN(CF2CF2CF2CF3)2).

Experimental cross sections are derived from Fourier transform spectroscopy performed from 600-1450 cm^{-1} at a resolution of 0.02 cm^{-1} for a temperature range of 273-296 K. These experimental results are compared to our theoretical calculations and both are compared to previous measurements of PFBAm made at room temperature by Young *et al*.