THE NIST QUANTITATIVE INFRARED DATABASE

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With the recent developments in Fourier transform infrared (FT-IR) spectrometers it is becoming more feasible to place these instruments in field environments. As a result, there has been enormous increase in the use of FT-IR techniques for a variety of qualitative and quantitative chemical measurements. These methods offer the possibility of fully automated real-time quantitation of many analytes; therefore FT-IR has great potential as an analytical tool. Recently, the US Environmental Protection Agency (USEPA) has developed protocol methods for emissions monitoring using both extractive and open-path FT-IR measurements. Depending upon the analyte, the experimental conditions and the analyte matrix, approximately 100 of the hazardous air pollutants (HAPs) listed in the 1990 USEPA Clean Air Act amendment (CAAA) can be measured. The National Institute of Standards and Technology (NIST) has initiated a program to provide quality-assured infrared absorption coefficient data based on NIST prepared primary gas standards. Currently, absorption coefficient data has been acquired for approximately 20 of the HAPs. For each compound, the absorption coefficient spectrum was calculated using nine transmittance spectra at 0.12 cm^{-1} resolution and the Beer's law relationship. The uncertainties in the absorption coefficient data were estimated from the linear regressions of the absorbance data and considerations of other error sources such as the non-linear detector response. For absorption coefficient values greater than 1×10^{-4} (μmol/mol)$^{-1}$m^{-1}, the average relative expanded uncertainty is 2.2 %. This quantitative infrared database is currently an ongoing project at NIST. Additional spectra will be added to the database as they are acquired. Our current plans include continued data acquisition of the compounds listed in the CAAA, as well as the compounds that contribute to global warming and ozone depletion.