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Space Science & Technology Department	InHALE Data Format Specification Technical Note	Rev: 1	
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InHALE Data Format Specification



Technical Note

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1. Introduction

This technical note describes the format of data supplied by RAL Space Spectroscopy Group for measurements of far-infrared transmittance spectra of fluorocarbons for the InHALE project. Each measurement has two associated files. The first consists of metadata describing the instrumentation, sample nature and recording conditions. The second consists of the spectral transmittance data itself.

Each measurement is labelled according to the compound measured, its nominal partial and total pressures in Torr and the temperature in K according to the format '[Name]_[Partial pressure]_[Total pressure]_[Temperature]_'. The suffices 'Trans' or 'Meta' are added to distinguish the transmittance and metadata files followed by '.txt' file extension. Trade names are used to label the compounds, for example :

HFC-236fa_200_760_301_Trans.txt

HFC-236fa_200_760_301_Meta.txt

A separate data package is provided for each of the three compounds. The package folder structure segregates first by total pressure, and second by sample temperature.

2. Metadata

The metadata consist of the following :

Chemical name : IUPAC name, trade name, CAS no.

Physical properties : relative molecular mass, boiling point / °C

Supplier & stated purity :

Diluent : gas, supplier, product code, typical impurity levels

Temperature of sample : \pm / K

Total pressure : \pm / Torr

Sample partial pressure : \pm / Torr

Sample cell windows : HDPE, 1 mm thick, 4 mrad wedge, in-house

Absorption path length : \pm / cm

Instrument : Bruker IFS125 operated under vacuum (0.03 hPa)

Spectral range : 10 – 2000 cm^{-1}

Nominal resolution : 0.25 cm^{-1}

Maximum optical path difference : 3.6 cm


Apodisation function : Norton-Beer (medium)

ILS FWHM : 0.23 cm^{-1}

Zero-filling factor : 8

Spectral sampling interval : 0.015 cm^{-1}

Phase correction : Mertz, 1 cm^{-1}

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Beamsplitter : 6 μm Mylar

Source : Mid-infrared carbide glowbar

Scanner velocity : 5 kHz (HeNe crossing frequency)

No. of averages : 100

Detector : DTGS with CsI window

Nyquist frequency : 15798 cm^{-1}

3. Spectrum data

Transmittance spectra are written in tab-delimited ASCII format.

Header line : Wavenumber / cm^{-1} , Transmittance

N lines : $\bar{\nu}$, τ