PREPROCESS for all

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PREPROCESS for all

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

Introduction: One task of FRM4GHGII is to enable a processing compatible with COCCON requirements for a wider range of spectrometers. The COCCON processing chain has three steps:

- The pre-processing or L1-processing (performed by **PREPROCESS**): from raw OPUS interferograms to spectra. The resulting spectra are used for the quantitative trace gas analysis.
- The daily calculation of lookup tables with x-sections of gases for given atmospheric conditions (performed by **PCXS**)
- The trace gas retrievals (performed by **INVERS**)

In order to enable processing of observations with different spectrometers (Vertex70, Invenio, IRCube, IFS125HR in addition to EM27/SUN), mainly extensions of PREPROCESS are required (and some adaptions in INVERS + calculation of vertical sensitivities).

This talk describes the extended version of PREPROCESS.

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Contents:

- **Raw data / interferograms used for this work**
- **Single-sided interferograms and phase correction**
- **Analytical phase calculation**
- **Analytical phase calculation with blending option**

- **Recently added extension to PREPROCESS: instrument-specific background continuum**

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Raw data / interferograms (all in Bruker's OPUS format):

- EM27/SUN (Sodankyla, Karlsruhe)
- IFS125HR (Karlsruhe, Izana): Ka: NIR split in two subregions, Izana: broadband

Kindly provided by FRM4GHG partners:

- IRCube (Wollongong)
- Vertex70 (Sodankyla)
- Invenio (Uccle)

Issues noted on closer inspection of raw interferograms:

IRCube: Two channels stored in file – AC+DC from same detector? Uneven number of scans?

Invenio: DC quite variable - problems with tracker? (Poor weather?)

Vertex70 + Invenio: IFG centerbursts are nearly point symmetric around ZPD (instead of the expected axial symmetry)??

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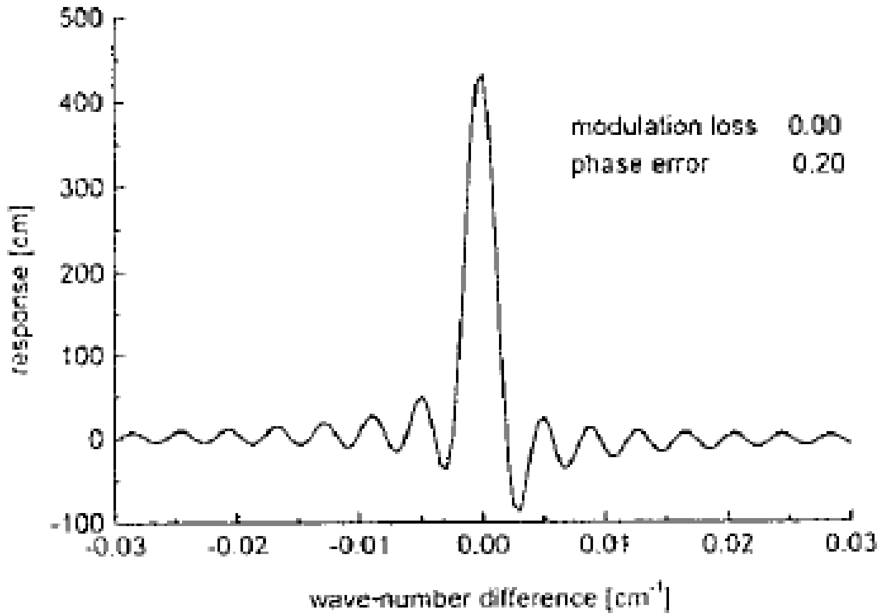
Single-sided interferograms and phase correction

- Note that SS interferograms are much more sensitive to phase errors
- Recording of DS interferograms is superior when aiming at high photometric accuracy!

e.g.: Richard C. M. Learner, Anne P. Thorne, Ian Wynne-Jones, James W. Brault, and Mark C. Abrams, "Phase correction of emission line Fourier transform spectra," J. Opt. Soc. Am. A 12, 2165-2171 (1995)



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Single-sided interferograms and phase correction

Therefore, accurate calculation of the phase spectrum is important especially in case of SS ifgs!

We expect that the phase spectrum is rather smooth, it is shaped by:

- Signal propagation delays (mismatch between laser and IR signal propagation delay, IR delay expected to depend on frequency)
- Optical effects: the BS is not fully symmetric when viewed from either interferometer arm (thickness mismatch of BS substrate + compensating plates, BS is a multilayer system with asymmetric refractive boundaries)

Standard approach: Construct the phase from a shorter DS-IFG (this needs careful numerical apodization!)

Residual problem: the phase spectrum might be still smoother than the phase resolution. But a further reduction of phase resolution will end up in a not well-defined interpolative performance (spectral sections with high signal just will dominate sections with low signal & the resulting phase spectrum is built on just a few IFG point in the direct vicinity of ZP).

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Single-sided interferograms and phase correction

Preferable would be a method which constructs a smooth analytical phase from a medium-resolution phase spectrum. In the fit procedure, each phase point is ascribed a weight according to the length of the spectral pointer, in addition, a low threshold for taking points into account for determining the fit can be introduced.

The new PREPROCESS offers an "analytical phase" option in addition to the standard approach. Procedure:

- The phase spectrum is developed out of the complex spectrum (as derived from the low-res DS IFG)
- The phase set by the orientation of the complex pointer at the spectral position with biggest complex amplitude acts as pivotal point for calculating the phase spectrum
- From this reference position, the phase is constructed towards higher and towards lower frequencies, using the cross product of two normalized complex vectors to determine the phase changes.
- A smooth curve (polynomial, 14 parms) is fitted to this phase spectrum, taking into account weights and clipping weights below a threshold (5% of max complex amplitude).
- Note when using this option: the analytical fit is restricted to the 3500 – 12300 cm-1 range!

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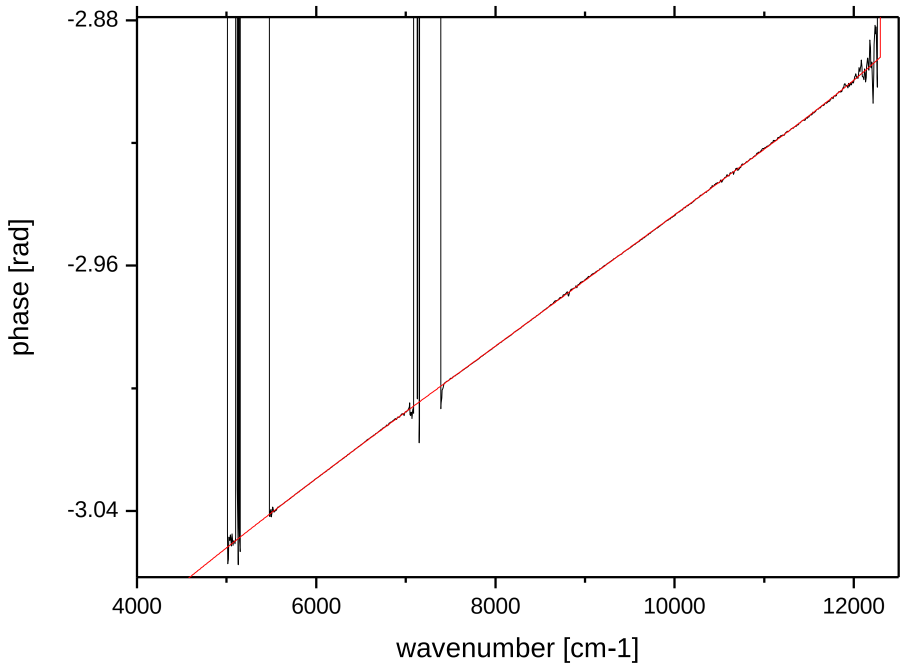
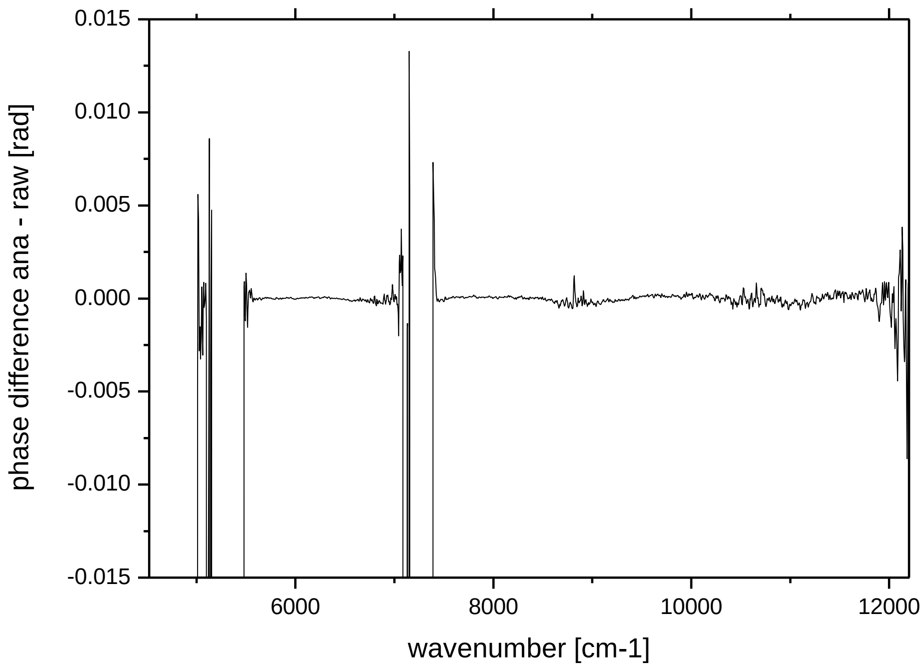
Single-sided interferograms and phase correction

Results for the EM27/SUN analytical phase:





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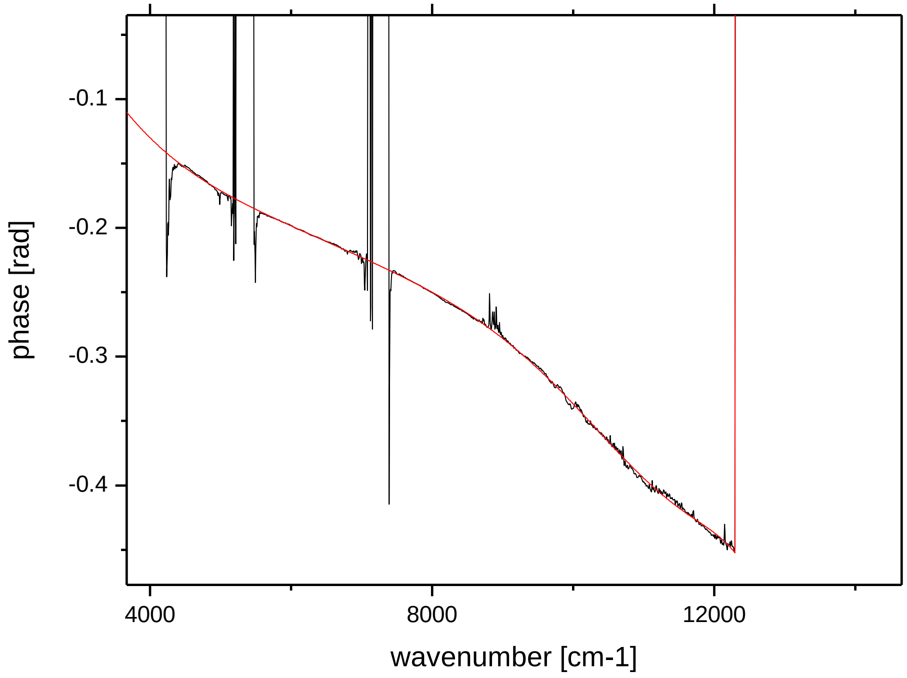
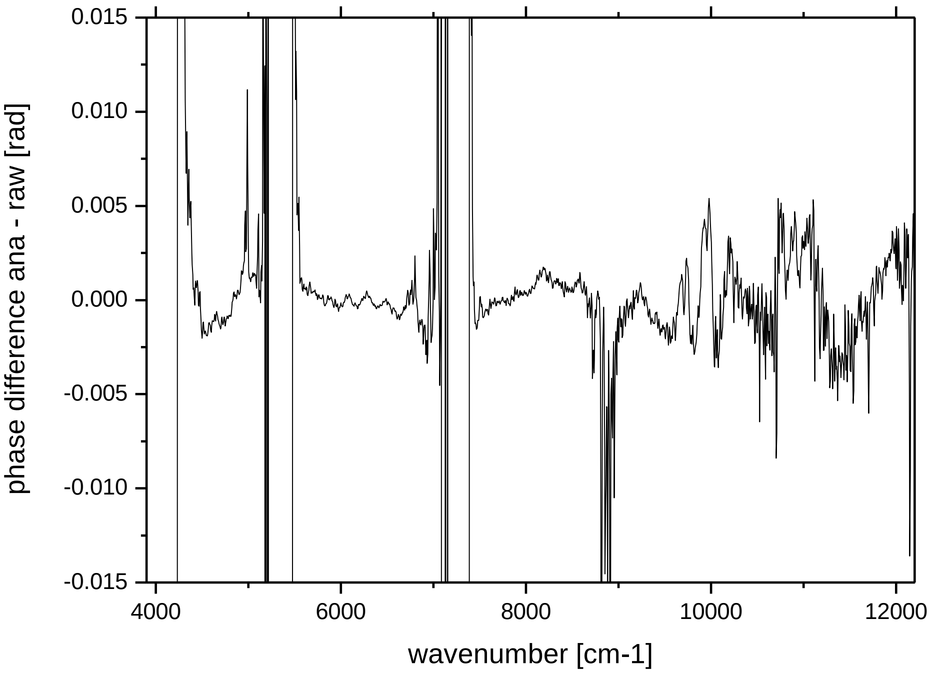
Single-sided interferograms and phase correction

Results for the IR Cube analytical phase:





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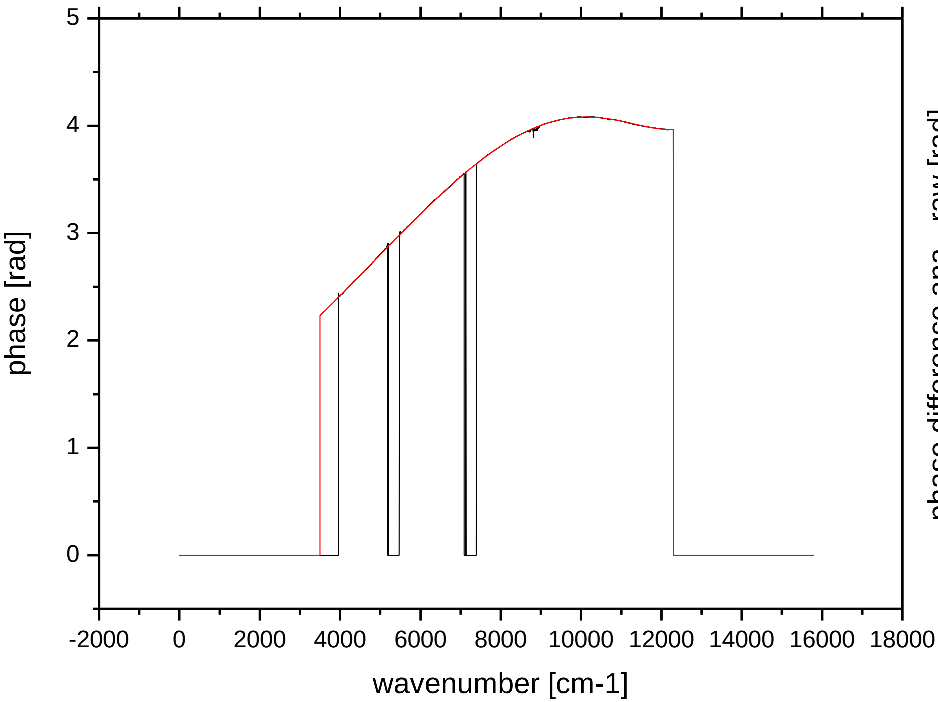
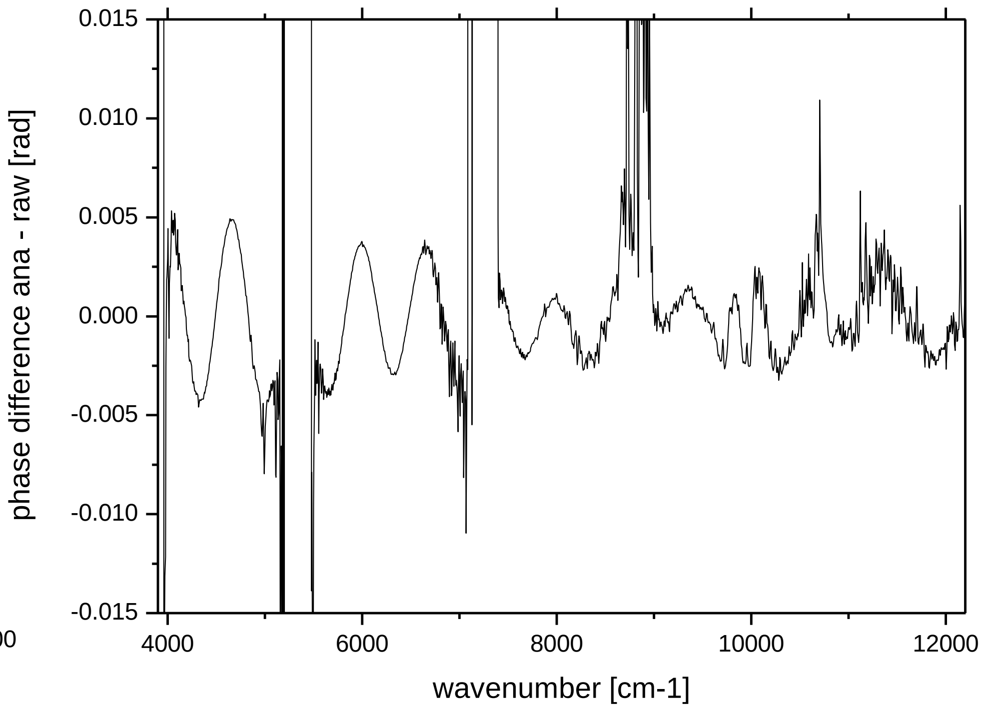
Single-sided interferograms and phase correction

Results for the Vertex70 analytical phase (the Invenio looks surprisingly similar, both contain a strange phase oscillation, ~ 400 … 500 cm-1 period):





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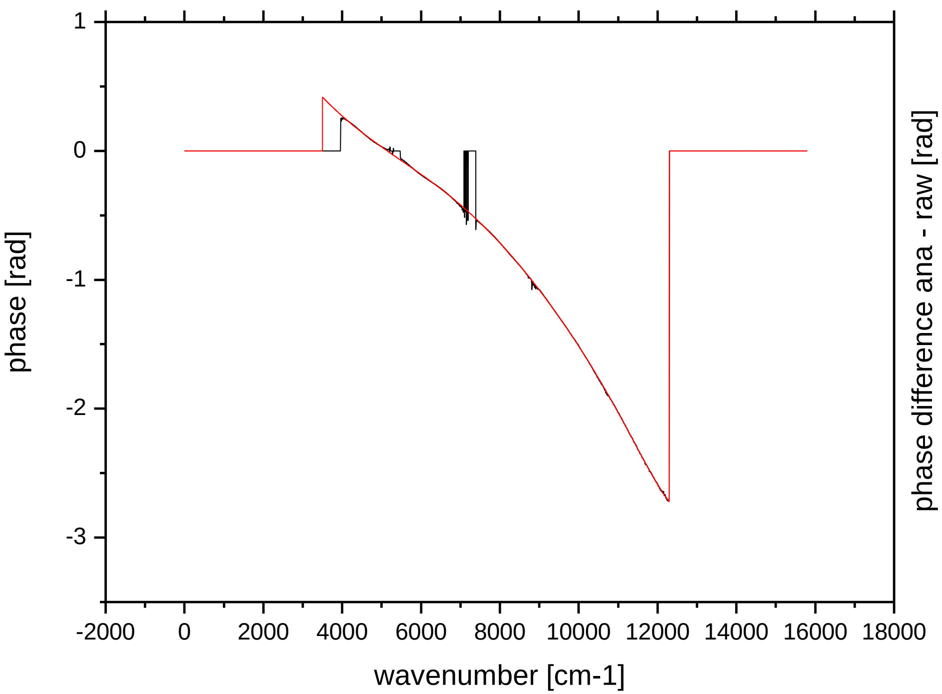
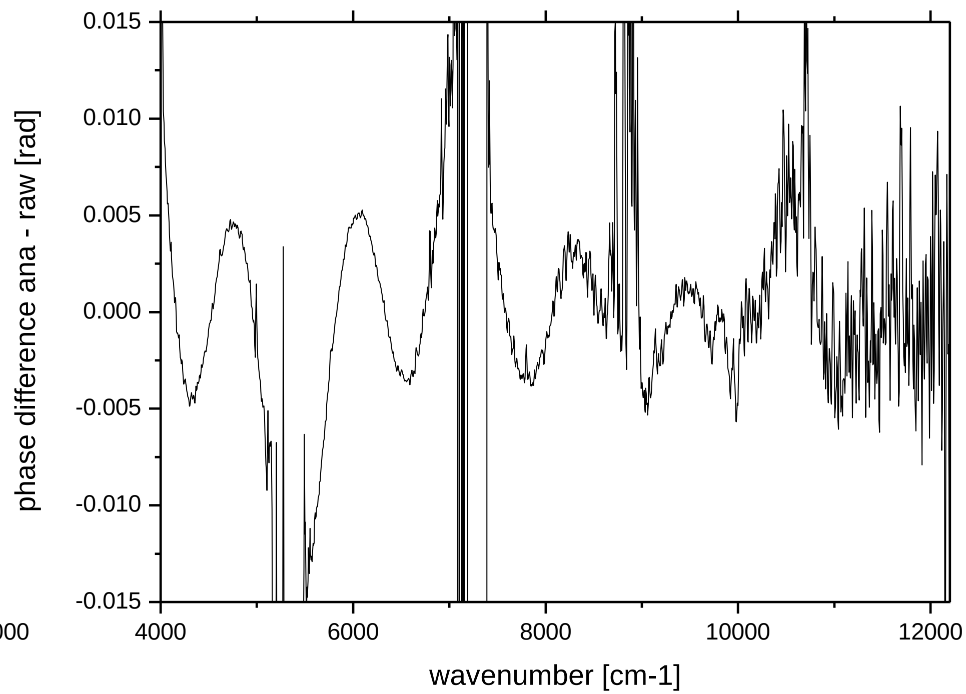
Single-sided interferograms and phase correction

Results for the Invenio analytical phase (similar oscillatory pattern as seen for Vertex70):





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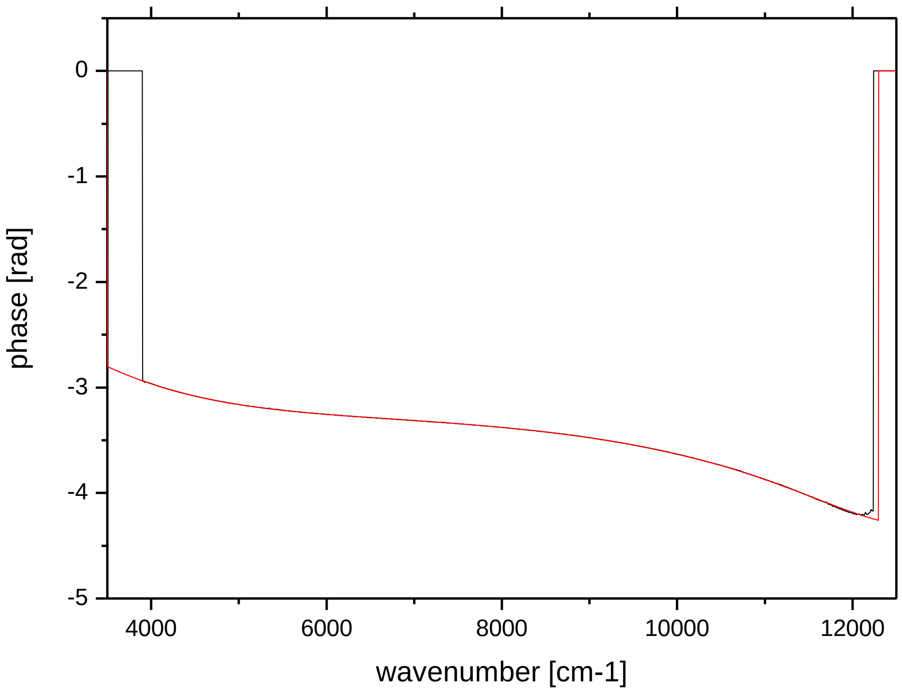
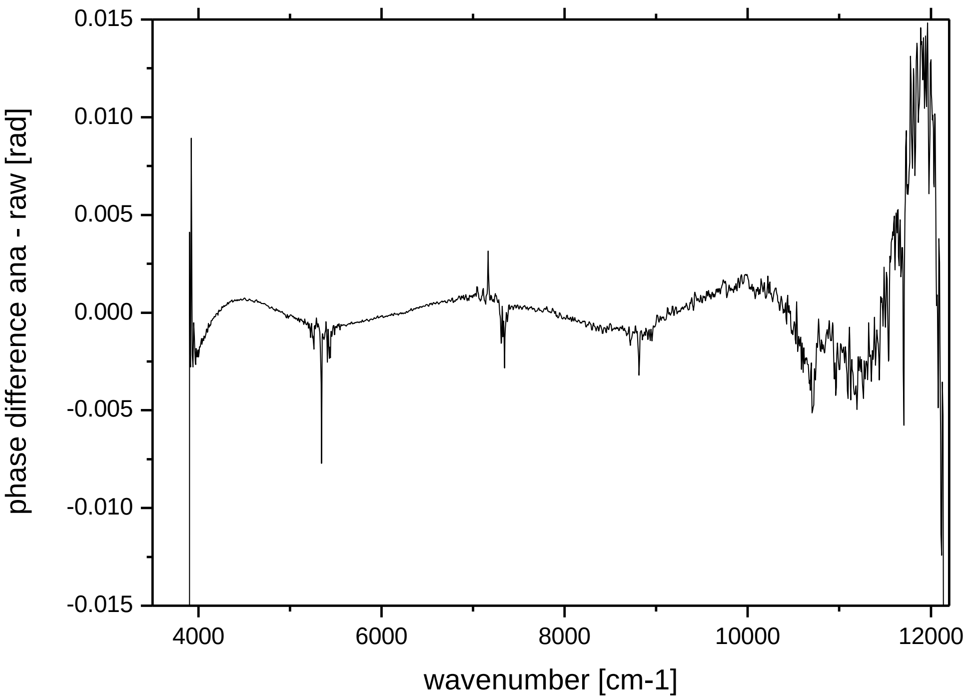
Single-sided interferograms and phase correction

TCCON example (125HR Izana, 2019):





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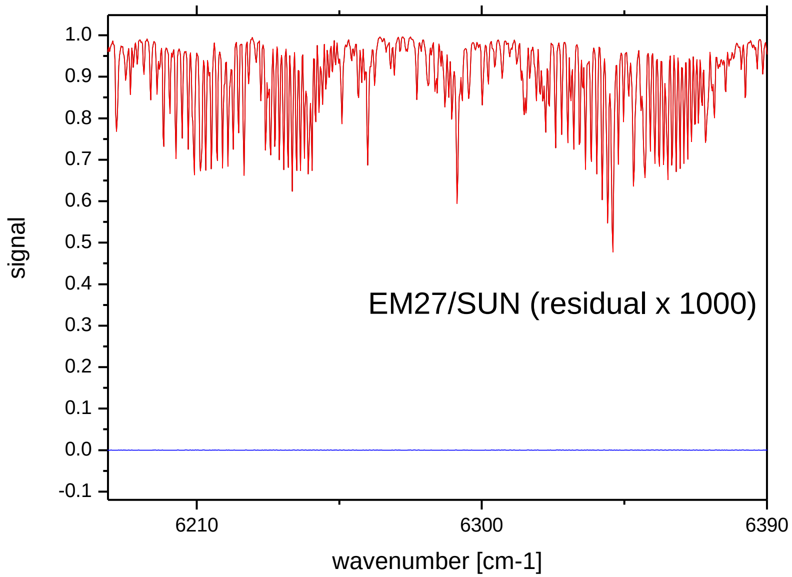
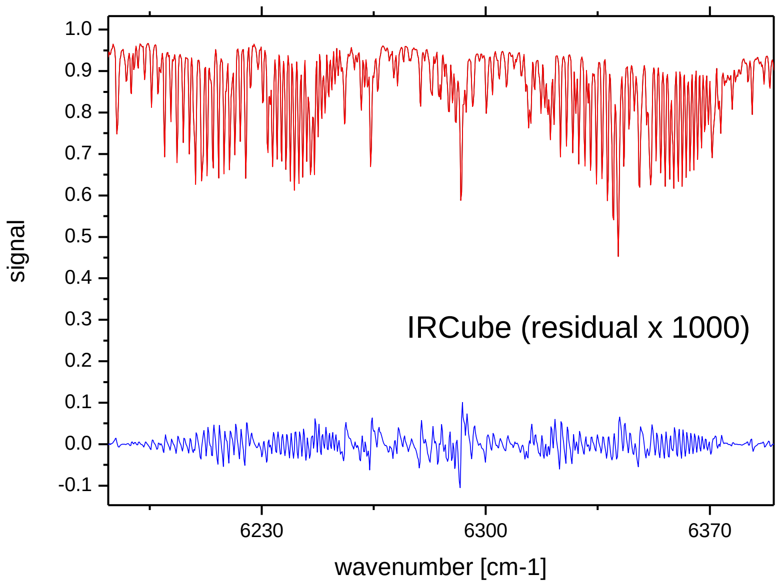
Single-sided interferograms and phase correction: intercomparison SS versus DS

These plots demonstrate the error propagation of phase errors into the spectrum for the SS and DS case (comparing spectra generated with the standard and analytical phase calculation schemes)





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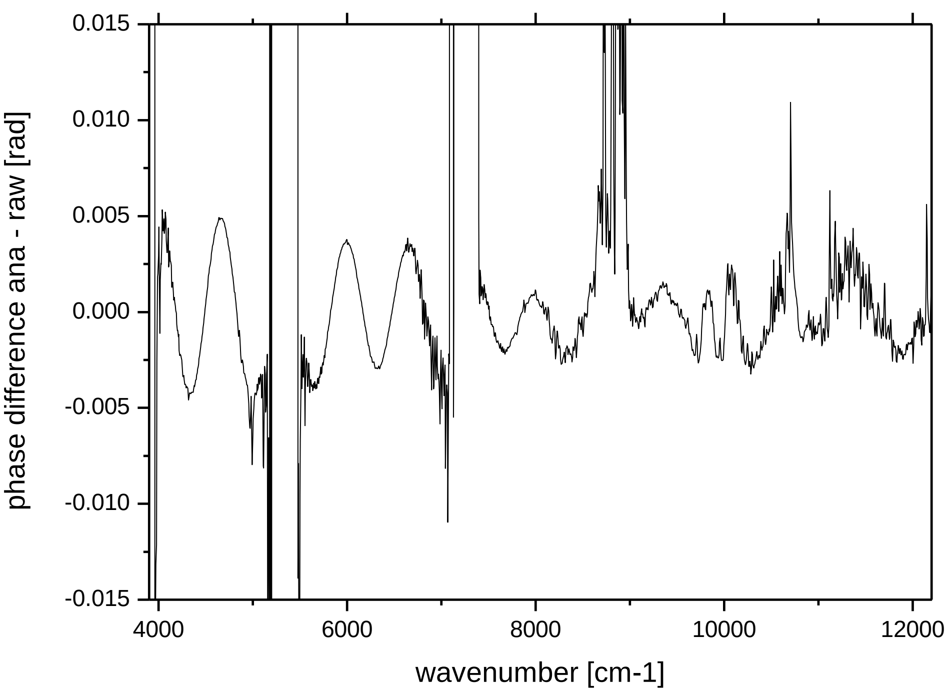
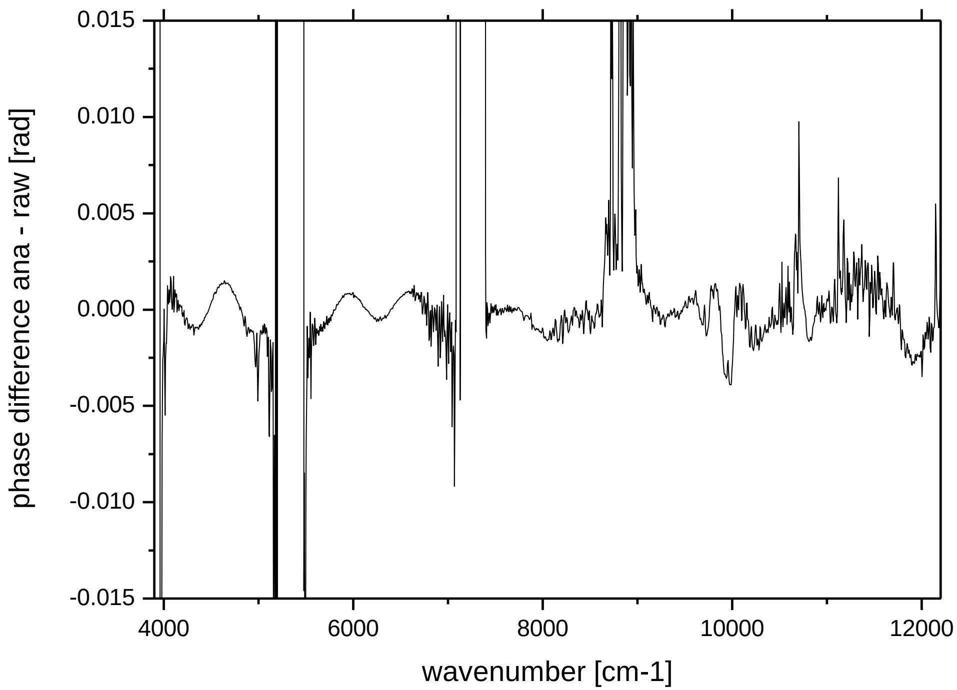
Single-sided interferograms and phase correction – phase blending option

Idea: feed in additional information on permanent phase structures too narrow to be resolved by the smooth analytical phase – ideally from additional, e.g. lamp measurements. (The blending option is activated by adding a table named “refphase.inp”.)

No blending



use blending



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Single-sided interferograms and phase correction

Conclusions on analytical phase method:

- The analytical phase fitting seems to work well, with blending option approaching an optimal reconstruction of the actual phase spectrum.
- The EM27/SUN ironically has outstanding phase quality - note: nearly linear, no dispersion! (Exactly here, it's of lesser importance…)
- The IR-Cube phase looks ok, insertion of a long pass filter for limiting the signal below ~ 12000 cm-1 might be recommendable (significant signal level at HFL!)
- The Vertex70 / Invenio phase is very unusual (oscillating phase, pp variation ~ 5 mrad) – instrumental issue?
- The tested TCCON Izana spectrum looks reasonable, but also some detectable variations superimposed on smooth phase (pp variation < 3 mrad), larger variations beyond > 10 000 cm-1.

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Instrument-specific background continuum

Paul: "Which instrumental problem limits the accuracy of the EM27/SUN"?

Still unsure about the shortwave region. For the longwave detector, the presence of residual channeling is a problem, dominated by an 8 cm^{-1} channeling generated in the detector substrate (we accept pp $< 0.05\%$). CO window very crowded, fit in atmospheric spectra not reliable.

B. Baier: inconsistent XCO SBS results: we noted a tiny absorption dip in EM27/SUN SN42, evolved over time, located in CO window.

Omaira, Oscar, Africa: use of the EM27/SUN for deriving AOD.

Note: channeling and long-wavelength cut-off of detector element are T-dependent (other artefacts might be temperature dependent).

Current implementation: EM27/SUN T-sensor is evaluated by PREPROCESS, the user can provide a table of transmissions as function of T (0 … 56 C, in 2 C steps).

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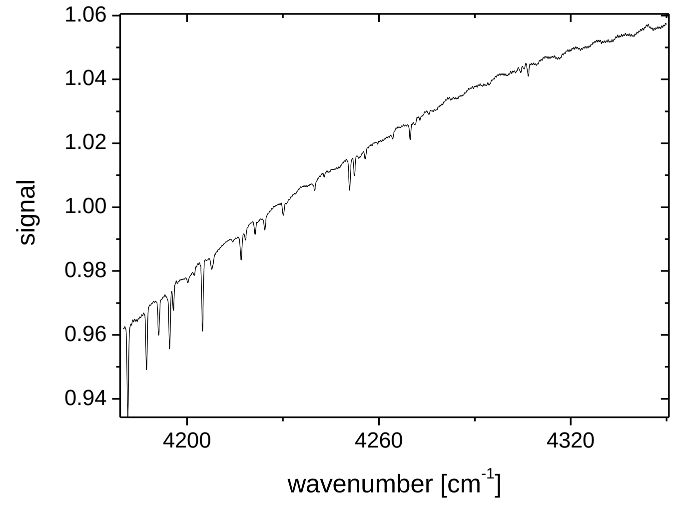
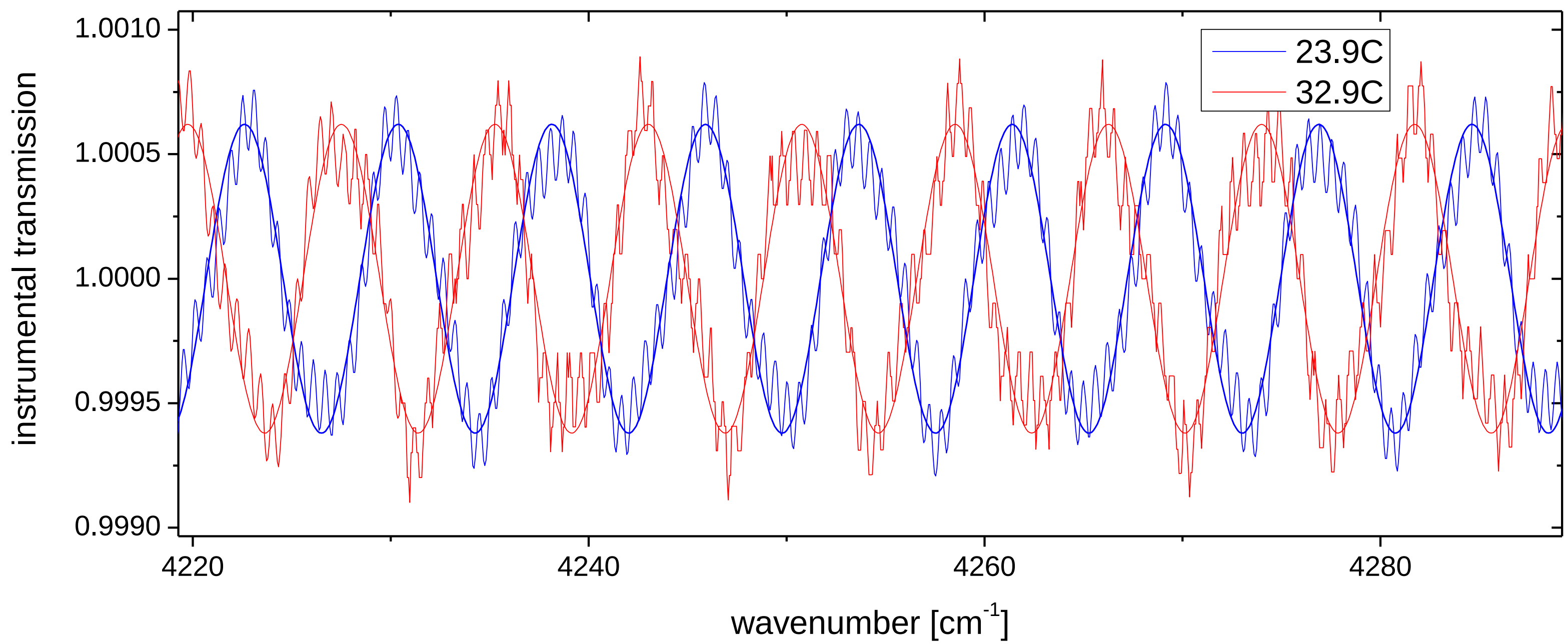
Instrument-specific background continuum

Channeling of SN191 as delivered to KIT, violates the acceptance threshold …





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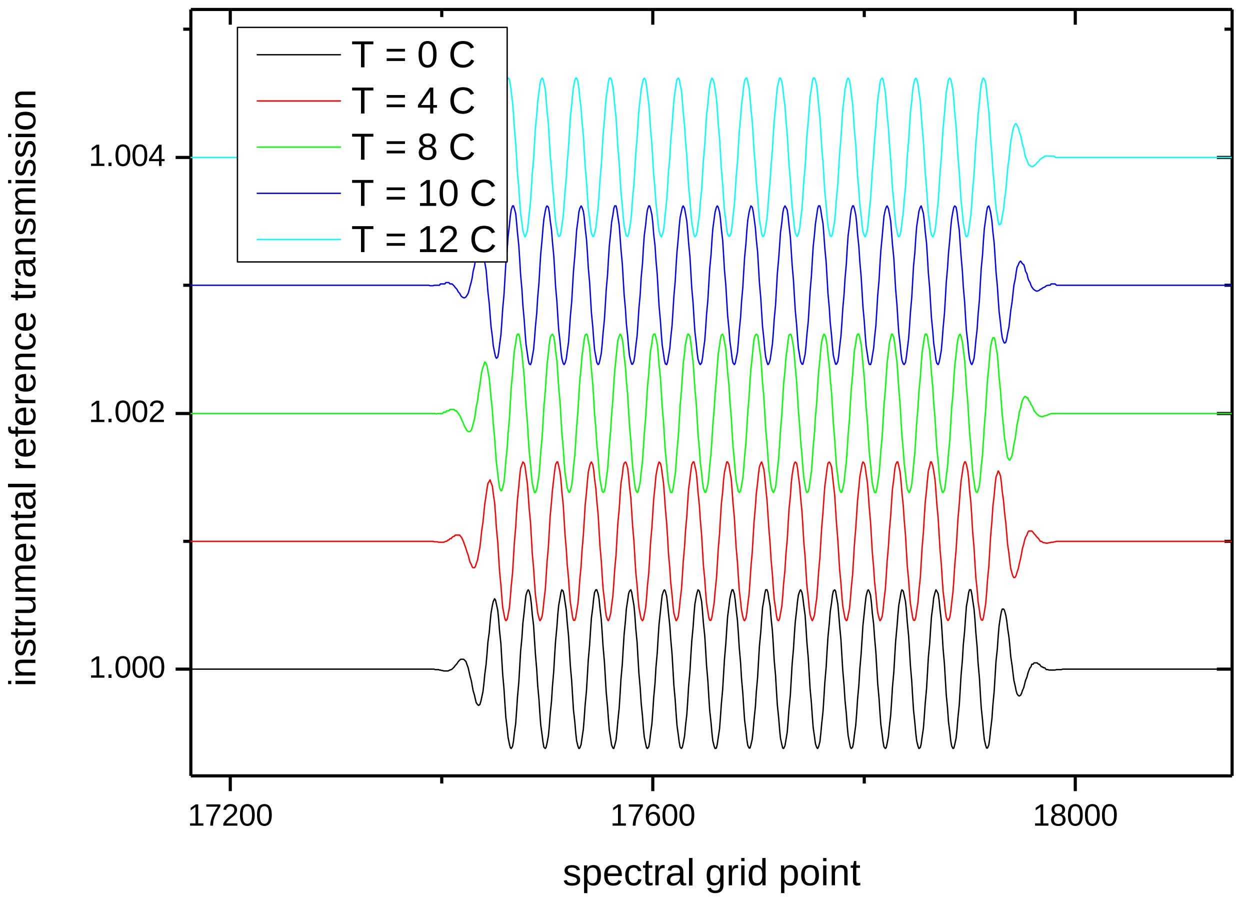
Instrument-specific background continuum



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Conclusions on instrument-specific background continuum

- Basically, now supported by the new PREPROCESS, but requires careful lab characterisation and advanced user to actually bring this option to life.

- We plan to test the effects for a selected spectrometer with noticeable channeling (SN191, cover wider T range for calibrating the channeling model).

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Required technical adaptions:

So far, interferograms to be processed were all of the same kind:

- The EM27/SUN collects data from two detector channels: SN + SM
- Two IFGs in OPUS file: first IFG block: SN, second IFG block: SM)
- All EM27/SUNs have the same FOV
- All EM27/SUNs record double-sided IFGs with RES = 0.5 cm-1

So we need

- Wideband detector used: derive SN+SM from one broadband channel
- The channels might be swapped (IFS125HR Ka) or the broadband channel to be used might be associated with the second IFG block.
- User specification of semiFOV in PREPROCESS input file required (reported in *.bin file header)
- Enable different choices for spectral resolution (user-selectable, support clipping of IFGs)
- Support processing of SS IFG recording

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Required technical adaptions: New extended input file (1)

Generate ASCII output for testing
mpowFFT (17 for EM27/SUN and IR Cube: 1.8 cm MPD, 181/182: 2.5 cm /3.0 cm MPD, 19 for VERTEX / INVENIO: 4.5 cm MPD, 20 for 125HR: 16.2 cm MPD)
DCmin
DCvar
$
.false. ←For operational work, please select F – otherwise, your HDD will be filled up with
17
0.05
0.10

ILS parameter: apo + phase error
primary channel
secondary channel
semiFOV [rad]
$
0.9825 -0.001
0.9825 -0.001
2.36e-3

…

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Required technical adaptions: New extended input file (2)

…

Quiet execution (no user requests)
Output path diagnosis
Output path bin spectra
Dual IFG recording (T/F)
Swap channels (applies for dual IFG recording: 1st channel SN, second channel SM - otherwise choose swap = true)
use analytical phase (T/F)
band selection (0: only generate SN from first channel, 1: generate SN from first and SM from second channel, 2: generate SN + SM from first channel)
$
.true.
standard
standard
.true.
.false.
.false.
1