Odin/SMR

Level2 processing configuration

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Contents

Chapter 1 | Introduction

1.1 Aim and scope of this document

Odin/SMR performs passive limb measurements of the atmosphere, mainly at wavelengths and frequencies around 0.6 mm and 500 GHz, respectively. From these measurements, profiles of O_3, ClO, N_2O, HNO_3, H_2O, CO, and isotopologues of H_2O, and O_3, that are species that are of interest for studying stratospheric and mesospheric chemistry and dynamics, can be derived. Odin/SMR has been in operation for approximately 18 years, and thus, the Level2 dataset can potentially be applied for scientifically interesting trend analysis.

A new Odin/SMR Level2 product dataset has been generated, and in Murtagh et al. (2020) the new Odin/SMR Level2 products (v3.0.0) are compared to correlative measurements from other instruments, as well as with the Level2 data from the older 2.0/2.1 versions of the Odin/SMR processing chain. A general description of the Odin/SMR retrieval process is described in Eriksson (2020), including the basic configuration of the forward model deployed, the optimal estimation method implementation, and the retrieval variables for the Odin/SMR processing. In practise, the exact configuration of the Odin/SMR level2 processing is product or frequency mode specific, and all detailed settings are not reported in Eriksson (2020).

The aim of this report is mainly to document the configuration of Odin/SMR Level2 processing in details. The information has been collected from the QSMR-Data repository (`https://github.com/Odin-SMR/qsmr-data`), that is actually used by the Odin/SMR Level2 processing system. The information presented in this document is relevant for future processing and validation studies, as it for example should allow for a reproduction of the results.

1.2 Document structure

Chapter 2 defines the configuration of the Odin/SMR Level2 processing, the actual setting deployed for the various frequency modes, and the source and modifications of applied spectroscopic data and absorption continua models.

Chapter 2 | Level2 processing configuration

2.1 Configuration by frequency mode

The Odin/SMR Level2 processing is controlled by a tailored matlab software package. The retrieval settings for the various modes of Odin/SMR are defined by two matlab functions:

Q_STND handles frequency mode 1, 2, 8, and 17

Q_MESO handles frequency mode 13, 14, 19, 21, 22, and 24.

A description of the configuration parameters are found in Sect. 2.1.1, and the actual values of the parameters for the standard and mesospheric modes are described in Sect. 2.1.2 and Sect. 2.1.3, respectively.

2.1.1 Configuration description

This section contains a brief description of the settings considered by the Qsmr retrieval system. These settings are packed into a structure denoted as Q. This structure must contain an exact set of fields; all fields must be present and no additional ones are allowed. The defined fields are described below, in alphabetical order.

Qsmr operates also with two other structures. For the various pre-calculations a structure denoted as P is used. The fields of P are defined and are shortly described in the file p_std.m. The structure R works as repository for internal variables and data. That is, no fields of R are set by the user.

Most fields of Q are of simple types such scalar value, vector or string, but some fields are structures. This more complex type is only used for retrieval quantities, in order to allow simple communication with some functions copied from Qarts.

All fields listed affect the inversions, either in the pre-calculation phase or when doing the actual inversion. The settings are applied by various functions and if you are using individual functions of Qsmr you need to figure out what settings that have an effect or not. For example, the fields TB_SCALING_FAC and TB_CONTRAST_FAC are not applied directly when loading the data, but are applied on the L1B data by a special function.

ABS_P_INTERP_ORDER An integer. The polynomial order to apply for pressure interpolation of the absorption look-up table. See further the ARTS workspace variable with the same name.

ABS_SPECIES An array of structures. Each array element provides settings for a gas species. The fields of the structure are as follows. TAG: Definition of the species following the ARTS format, e.g. O3-*-501e9-503e9. SOURCE: A string describing from where temperature a priori shall be taken. Handled options are 'WebApi' and 'Bdx'. RETRIEVE: A boolean, flagging if the species shall be retrieved or not. All fields below are ignored if RETRIEVE is false. L2: A boolean, flagging if the species is part of the L2 data of the frequency mode. GRID: Retrieval grid to use for the species. UNC_REL and UNC_ABS: Minimum relative and absolute uncertainty (1 std dev), respectively. The absolute and relative values are compared using the a priori profile and the largest of the two is selected (but not exceeding 1e3 in relative value). CORRLEN: Correlation length, in meter, to use when creating Sx. LOG_ON: Set to true to impose a positive constrain for the species. L2NAME: A string. The name to give the retrieved product. ISOFAC: A scalar. The isotopologue fraction assumed in ARTS. If the complete species VMR is the output, this field shall be set to 1.

Note that when creating L2 data the outermost points of GRID are removed.

ABS_T_INTERP_ORDER An integer. The polynomial order to apply for temperature interpolation of the absorption look-up table. See further the ARTS workspace variable with the same name.

ARTS A string. Name or path of the ARTS executable to use.

BACKEND_NR An integer. Index of expected backend. Index coding described in L1B ATBD.

BACKEND_FILE Empty or a string. If empty, the name of file to read is generated automatically following the channel seperation. If you don't want to use these default files, you put the name of the alternative file in this field.

BASELINE A structure. Definition of baseline off-set retrieval. The fields of the structure are as follows. RETRIEVE: A boolean, flagging if baseline off-set shall be retrieved or not. UNC: A priori uncertainty (1 std dev). MODEL: A string. If set to 'common' a single off-set is retrieved for each spectrum. If set to 'module' an off-set for each active AC module is retrieved, i.e. up to four off-set per spectrum are derived. If set to 'adaptive' then all modules contributing with more than 125 channels are grouped and a common off-set for these modules is retrieved, while separate off-sets are retrieved for remaining modules (<= 125 channels).

DZA_GRID_EDGES A vector. Complements DZA_MAX_IN_CORE in the specification of the angular grid used for pencil beam calculations. The vector specifies the values to add outside the lower and upper boresight direction. These are relative angles (in degrees), where 0 shall not be included.

DZA_MAX_IN_CORE A scalar value. Determines the maximum spacing (in degrees) of the angular grid used for pencil beam calculations. This value sets the spacing between the lower and upper boresight direction.

FOLDER_ABSLOOKUP A string. Full path to folder containing the different versions of absorption look-up tables. That is, this folder is expected to contain folders. The exact folder specification is a result of this field and ABSLOOKUP_OPTION.

FOLDER_ANTENNA A string. Full path to folder containing antenna pattern response files.

FOLDER_BACKEND A string. Full path to folder containing backend channel response files.

FOLDER_BDX A string. Full path to folder containing files of the Bordeaux a priori database. Files having .mat format are expected.

FOLDER_FGRID A string. Full path to folder containing frequency grid files.

FOLDER_MSIS90 A string. Full path to folder holding the MSIS90 climatology (version taken from arts-xml-data). Only needed of temperature data taken from MSIS90, which is the case for some pre-calculations.

FOLDER_WORK A string. Full path to a folder where temporary files and/or folders can be placed. If this field is set to '/tmp', a temporary folder is created and all files are placed in this folder, and the folder is removed when the calculations are done. Otherwise, temporary files are placed directly in the specified folder, and these are left when the calculations are done. This option is useful for debugging, but note that just a single Qsmr process can use a folder for debugging. If several Qsmr processes are given the same debugging folder, files will be overwritten and the calculations will crash or be incorrect.

FREQMODE An integer. The frequency mode. See L1B ATBD for definition of existing frequency modes.

FREQUENCY A structure. Definition of frequency off-set retrieval. The fields of the structure are as follows. RETRIEVE: A boolean, flagging if frequency off-set shall be retrieved or not. UNC: A priori uncertainty (1 std dev). NPOLY: The polynomial order to apply for frequency fit. For example, 0 means that a constant off-set is retrived and 1 means that the varies is assumed to vary linearly with zenith angle. The value -1 has a special meaning. With -1, an off-set for each tangent altitude is retrieved. The a priori uncertainty is set to following UNC for all polynomial coefficients, or for each off-set of NPOLY is -1.

FRONTEND_NR An integer. Index of expected frontend. Index coding described in L1B ATBD.

F_RANGES A matrix, having two columns. This matrix specifies the frequency ranges to include in the retrieval, where the first and second column give the lower and upper frequency limit, respectively. Each row specifies a new frequency range to include.

F_GRID_NFILL An integer. If set to > 0, the sensor response matrix will include a cubic frequency interpolation of the spectra, with F_GRID_NFILL points added between existing grid points. See further the ARTS workspace method sensor_responseFillFgrid. If set to 0, no such interpolation is made.

F_LO_NOMINAL A scalar value. Nominal value of the LO frequency.

GA_FACTOR_NOT_OK A scalar value. The factor with which the Marquardt-Levenberg factor is increased when not a lower cost value is obtained. This starts a new sub-iteration. This value must be > 1.

GA_FACTOR_OK	A scalar value. The factor with which the Marquardt-Levenberg factor is decreased after a lower cost values has been reached. This value must be > 1.
GA_MAX	A scalar value. Maximum value for gamma factor for the Marquardt-Levenberg method. The inversion is halted and flagged as unsuccessful if this value is reached. This value must be > 0.
GA_START	A scalar value. Start value for gamma factor for the Marquardt-Levenberg method. See the L2 ATBD for a definition of the gamma factor. This value must be $>= 0$.
INVEMODE	A string. A short string naming the inversion set-up used.
LO_COMMON	A boolean. If true, the initial value of LO frequencies are set to be constant over the scan. This value is set following LO_ZREF. If false, the L1B value for each altitude is used.
LO_ZREF	A scalar value. Reference altitude for LO frequency. When performing frequency cropping, frequencies are taken from the spectra with the closest altitude. Further, if LO_COMMON is set to true, the LO frequency is taken from the L1B data of the spectrum closest to this altitude.
MIN_N_FREQS	A scalar value. The required number of frequencies (i.e. channels) of spectra to start an inversion. This number refers to the number of spectra after frequency cropping and quality filtering.
MIN_N_SPECTRA	A scalar value. The required number of spectra of a scan to start an inversion. This number refers to the number of spectra after altitude cropping and quality filtering.
NOISE_CORRMODEL	A string. Model of correlations inside Se. Only correlation between adjacent channels of each spectrum is modelled. The options are as follows. 'none': this generates a pure diagonal Se. 'empi': Uses empirically derived values making Se a five-diagonal matrix. 'expo': Exponentially decreasing correlation, approximating the empirically derived values.
POINTING	A structure. Definition of pointing off-set retrieval. The fields of the structure are as follows. RETRIEVE: A boolean, flagging if pointing off-set shall be retrieved or not. UNC: A priori uncertainty (1 std dev).
PPATH_LMAX	A scalar value. The maximum distance between points of the propagation path. See further the ARTS workspace variable with the same name.
PPATH_LRAYTRACE	A scalar value. The length to apply for ray tracing to consider the effect of refraction. See further the ARTS workspace variable with the same name.
P_GRID	A vector. The pressure grid to be used. See further the ARTS workspace variable with the same name. Note that this setting is also used when pre-calculating absorption lookup tables.
QFILT_FCORR	A logical. So far only used for CO modes. Set to true to remove data were the frequency correction failed or is uncertain.

QFILT_LAG0MAX A logical. Sets the maximum allowed value of ZeroLagVar. This quality filtering operates on AC sub-bands.

QFILT_MOON A logical. Determines if data shall be filtered based on the MOON quality flag. This quality filtering operates on tangent altitudes.

QFILT_NOISE A logical. Determines if data shall be filtered based on the NOISE quality flag. This quality filtering operates on tangent altitudes.

QFILT_REF1 A logical. Determines if data shall be filtered based on the REF1 quality flag. This quality filtering operates on tangent altitudes.

QFILT_REF2 A logical. Determines if data shall be filtered based on the REF2 quality flag. This quality filtering operates on tangent altitudes.

QFILT_SCANNING A logical. Determines if data shall be filtered based on the SCANNING quality flag. This quality filtering operates on tangent altitudes.

QFILT_SPECTRA A logical. Determines if data shall be filtered based on the SPECTRA quality flag. This quality filtering operates on tangent altitudes.

QFILT_TBRANGE A logical. Determines if data shall be filtered based on the TB range quality flag. This quality filtering operates on tangent altitudes.

QFILT_TINT A logical. Determines if data shall be filtered based on the TINT quality flag. This quality filtering operates on tangent altitudes.

QFILT_TREC A logical. Determines if data shall be filtered based on the TREC quality flag. This quality filtering operates on tangent altitudes.

QFILT_TSPILL A logical. Determines if data shall be filtered based on the TSPILL quality flag. This quality filtering operates on tangent altitudes.

SIDEBAND_LEAKAGE A scalar or 'model'. If a scalar value, this is taken as the sideband leakage. This leakage is assumed to be flat over the (main) frequency band. If set to 'model', the sideband response is set according a model based on Tcal and SBPATH.

STOP_DX OEM stop criterion. The iteration is halted when the change in x is < stop_dx. Eq. 5.29 in the book by Rodgers is followed, but a normalisation with the length of x is applied. This means that STOP_DX should in general be in the order of 0.01 (and not change with the length of the state vector).

REFRACTION_DO A boolean. Determines if refraction is considered or not by the forward model. Set to true to include refraction.

T A structure. Definition of atmospheric temperature profile. The fields of the structure are as follows. SOURCE: A string describing from where temperature a priori shall be taken. Handled options are 'WebApi' and 'MSIS90'. RETRIEVE: A boolean, flagging if temperature shall be retrieved or not. All fields below are ignored if RETRIEVE is false. L2: A boolean, flagging if temperature is part of L2 data of the frequency mode. GRID: Retrieval grid to use for temperature. UNC: A vector of length 5, with a priori uncertainty (1 std dev) at 100, 10, 1, 0.1 and 0.01 hPa (roughly 16, 32, 48, 64 and 80 km). CORRLEN: Correlation length, in meter, to use when creating Sx. LIMITS: A vector of length 2, specifying allowed limits for retrieved temperatures. The first and second value is the lower and upper limit, respectively. L2NAME: A string. Will be used as L2.Product.

TB_CONTRAST_FAC A scalar value. This factor modifies the contrast of each spectrum part. If this factor is denoted as c, the scaling is: Tb_new = c * (Tb -Tb_min) + Tb_min, where Tb_min as an estimate of the noise-free minimum value of each spectrum part. This scaling is applied after TB_SCALING_FAC. This contrast scaling is applied on each AC module separately. That is, the complete spectrum is divided into four individual parts when performing this scaling. To leave the data unchanged, set this field to [] or 1.

TB_SCALING_FAC A scalar value. The L1B brightness temperature data are scaled with this factor. If this factor is denoted as c, the scaling is Tb_new = c * Tb. For example setting this field to 1.005 will convert an original Tb-value of 200 K to 201 K. To leave the data unchanged, set this field to [] or 1.

VERSION_ARTS A string. This string shall match the version string provided by the expected version of ARTS. For example: 'arts-2.3.562'

VERSION_QSMR A string. This string shall match the version string found at the top of Qsmr's ChangeLOg file. The version is expcted to be placed on line 3 and be proceeded with a '*'.

ZTAN_LIMIT_BOT A vector of length 4. The lower limit for tangent altitudes to include in the inversion. That is, this setting determines the lower limit when cropping the scan range. The four values give the tangent altitude limit at 0, +-30, +-60 and +-90 degrees in latitude. That is, the tangent altitude mask is assumed to be symmetric around the equator.

ZTAN_LIMIT_TOP A scalar value. The upper limit for tangent altitudes to include in the inversion. That is, this setting determines the upper limit when cropping the scan range.

ZTAN_MIN_RANGE A vector of length two. This field specifies the minimum altitude coverage of a scan to start an inversion. The order between lower and upper limit is free. The scan must have at least one tangent altude below and above the given limits. This check is done after applying ZTAN_LIMIT_BOT/TOP.

2.1.2 Q standard

```
% Q_STND   Settings for standard inversion mode
%
%   This function contains the settings used for operational "standard"
%   inversions. That is, don't modify without careful consideration.
%
%   The Q-fields are set according to selected frequency mode. The returned
%   Q is complete besides that all fields related to paths. These fields
%   should be set by *q_paths*.
%
% FORMAT   Q = q_stnd(freqmode)
%
% OUT   Q          A Q-structure (lacking path and version settings)
%  IN   freqmode   Frequency mode number


function Q = q_stnd(freqmode)


%---------------------------------------------------------------------------
%--- Frequency and inversion modes
%---------------------------------------------------------------------------

Q.FREQMODE           = freqmode;
Q.INVEMODE           = 'stnd';


%---------------------------------------------------------------------------
%--- Absorption tables
%---------------------------------------------------------------------------

Q.F_GRID_NFILL       = 0;
Q.ABS_P_INTERP_ORDER = 1;
Q.ABS_T_INTERP_ORDER = 3;


%---------------------------------------------------------------------------
%--- RT and sensor
%---------------------------------------------------------------------------

Q.REFRACTION_DO      = true;
Q.PPATH_LMAX         = 15e3;
Q.PPATH_LRAYTRACE    = 20e3;

Q.DZA_MAX_IN_CORE    = 0.01;
Q.DZA_GRID_EDGES     = [ Q.DZA_MAX_IN_CORE*[1:3 5 8 12 21] ];

Q.LO_COMMON          = true;
Q.LO_ZREF            = 60e3;

Q.BACKEND_FILE       = [];

Q.TB_SCALING_FAC     = 1.0025;
Q.TB_CONTRAST_FAC    = [];
```

```
%--------------------------------------------------------------------------
%--- OEM settings
%--------------------------------------------------------------------------

Q.STOP_DX           = 0.5;
Q.GA_START          = 1;
Q.GA_FACTOR_NOT_OK  = 10;
Q.GA_FACTOR_OK      = 10;
Q.GA_MAX            = 1e4;


%--------------------------------------------------------------------------
%--- Common retrieval settings
%--------------------------------------------------------------------------

Q.NOISE_CORRMODEL    = 'expo';  % 'none', 'empi' 'expo'

Q.ZTAN_LIMIT_BOT     = [ 19e3 19e3 14e3 10e3 ];

Q.BASELINE.RETRIEVE  = true;
Q.BASELINE.MODEL     = 'adaptive';  % 'common', 'module', 'adaptive'
Q.BASELINE.UNC       = 2;

Q.POINTING.RETRIEVE  = true;
Q.POINTING.UNC       = 0.01;

Q.FREQUENCY.RETRIEVE = true;
Q.FREQUENCY.NPOLY    = 0;
Q.FREQUENCY.UNC      = 1e6;

Q.T.SOURCE           = 'WebApi';
Q.T.RETRIEVE         = true;
Q.T.UNC              = [ 3 3 9 15 15 ];
Q.T.CORRLEN          = 8e3;
Q.T.LIMITS           = [100 350];


%--------------------------------------------------------------------------
%--- Quality criteria
%--------------------------------------------------------------------------

Q.QFILT_TSPILL       = true;
Q.QFILT_TREC         = true;
Q.QFILT_NOISE        = true;
Q.QFILT_SCANNING     = true;
Q.QFILT_SPECTRA      = true;
Q.QFILT_TBRANGE      = true;
Q.QFILT_TINT         = true;
Q.QFILT_REF1         = true;
Q.QFILT_REF2         = false;
Q.QFILT_MOON         = true;
Q.QFILT_FCORR        = true;
Q.QFILT_LAGOMAX      = 2.5;

Q.MIN_N_SPECTRA      = 8;
```

```
Q.MIN_N_FREQS        = 200;



%--------------------------------------------------------------------------
%--- Band specific
%--------------------------------------------------------------------------

switch freqmode

 case 1
  %
  Q.BACKEND_NR               = 2;
  Q.FRONTEND_NR              = 2;
  Q.F_LO_NOMINAL             = 497.885e9;
  Q.SIDEBAND_LEAKAGE         = 'model';
  Q.BASELINE.MODEL           = 'module'; % Added 2017-11-02 for testing
  %
  Q.P_GRID                   = q2_pgrid( [], 70e3 );
  %
  Q.F_RANGES                 = [ 501.16e9 501.60e9; 501.96e9 502.40e9 ];
  Q.ZTAN_LIMIT_TOP           = 60e3;
  Q.ZTAN_MIN_RANGE           = [ 25e3 40e3 ];
  %
  Q.T.L2                     = false;
  Q.T.GRID                   = q2_pgrid( 10e3, 65e3, 4 );
  %
  Q.ABS_SPECIES(1).TAG{1}    = 'ClO-*-498e9-505e9';
  Q.ABS_SPECIES(1).RETRIEVE  = true;
  Q.ABS_SPECIES(1).L2        = true;
  Q.ABS_SPECIES(1).L2NAME    = 'ClO / 501 GHz / 20 to 55 km';
  Q.ABS_SPECIES(1).GRID      = q2_pgrid( 10e3, 70e3, 4 );
  Q.ABS_SPECIES(1).UNC_REL   = 0.5;
  Q.ABS_SPECIES(1).UNC_ABS   = 2.5e-10;
  Q.ABS_SPECIES(1).CORRLEN   = 5e3;
  Q.ABS_SPECIES(1).LOG_ON    = false;
  %
  Q.ABS_SPECIES(2).TAG{1}    = 'N2O-*-491e9-512e9';
  Q.ABS_SPECIES(2).RETRIEVE  = true;
  Q.ABS_SPECIES(2).L2        = true;
  Q.ABS_SPECIES(2).L2NAME    = 'N2O / 502 GHz / 15 to 50 km';
  Q.ABS_SPECIES(2).GRID      = q2_pgrid( 10e3, 70e3, 8 );
  Q.ABS_SPECIES(2).UNC_REL   = 0.25;
  Q.ABS_SPECIES(2).UNC_ABS   = 20e-9;
  Q.ABS_SPECIES(2).CORRLEN   = 5e3;
  Q.ABS_SPECIES(2).LOG_ON    = false;
  %
  Q.ABS_SPECIES(3).TAG{1}    = 'O3-666-491e9-512e9';
  Q.ABS_SPECIES(3).RETRIEVE  = true;
  Q.ABS_SPECIES(3).L2        = true;
  Q.ABS_SPECIES(3).GRID      = q2_pgrid( 10e3, 70e3, 8 );
  Q.ABS_SPECIES(3).L2NAME    = 'O3 / 501 GHz / 20 to 50 km';
  Q.ABS_SPECIES(3).UNC_REL   = 0.5;
  Q.ABS_SPECIES(3).UNC_ABS   = 1e-6;
  Q.ABS_SPECIES(3).CORRLEN   = 5e3;
  Q.ABS_SPECIES(3).LOG_ON    = false;
```

```
%
Q.ABS_SPECIES(4).TAG{1}    = 'O3-668-498e9-505e9';
Q.ABS_SPECIES(4).RETRIEVE  = true;
Q.ABS_SPECIES(4).L2        = false;
Q.ABS_SPECIES(4).GRID      = q2_pgrid( 10e3, 70e3, 4 );
Q.ABS_SPECIES(4).L2NAME    = 'O3-dummy / 501 GHz';
Q.ABS_SPECIES(4).UNC_REL   = 0.5;
Q.ABS_SPECIES(4).UNC_ABS   = 0.5e-6;
Q.ABS_SPECIES(4).CORRLEN   = 10e3;
Q.ABS_SPECIES(4).LOG_ON    = true;
%
Q.ABS_SPECIES(5).TAG{1}    = 'O3-667-498e9-505e9';
Q.ABS_SPECIES(5).RETRIEVE  = true;
Q.ABS_SPECIES(5).L2        = false;
Q.ABS_SPECIES(5).GRID      = q2_pgrid( 10e3, 70e3, 4 );
Q.ABS_SPECIES(5).L2NAME    = 'O3-dummy / 501 GHz';
Q.ABS_SPECIES(5).UNC_REL   = 0.5;
Q.ABS_SPECIES(5).UNC_ABS   = 0.5e-6;
Q.ABS_SPECIES(5).CORRLEN   = 10e3;
Q.ABS_SPECIES(5).LOG_ON    = true;
%
Q.ABS_SPECIES(6).TAG{1}    = 'H2O-*-400e9-650e9';
Q.ABS_SPECIES(6).TAG{2}    = 'H2O-ForeignContStandardType';
Q.ABS_SPECIES(6).TAG{3}    = 'H2O-SelfContStandardType';
Q.ABS_SPECIES(6).RETRIEVE  = true;
Q.ABS_SPECIES(6).L2        = false;
Q.ABS_SPECIES(6).GRID      = q2_pgrid( 10e3, 30e3, 4 );
Q.ABS_SPECIES(6).L2NAME    = 'H2O-dummy / 501 GHz';
Q.ABS_SPECIES(6).UNC_REL   = 0.5;
Q.ABS_SPECIES(6).UNC_ABS   = 2e-6;
Q.ABS_SPECIES(6).CORRLEN   = 10e3;
Q.ABS_SPECIES(6).LOG_ON    = true;
%
Q.ABS_SPECIES(7).TAG{1}    = 'N2-SelfContMPM93';
Q.ABS_SPECIES(7).RETRIEVE  = false;
%
Q.ABS_SPECIES(8).TAG{1}    = 'O2-*-400e9-650e9';
Q.ABS_SPECIES(8).RETRIEVE  = false;
%
Q.ABS_SPECIES(9).TAG{1}    = 'HNO3-*-498e9-505e9';
Q.ABS_SPECIES(9).RETRIEVE  = false;
%
Q.ABS_SPECIES(10).TAG{1}   = 'CH3Cl-*-498e9-505e9';
Q.ABS_SPECIES(10).RETRIEVE = false;
%
Q.ABS_SPECIES(11).TAG{1}   = 'H2O2-*-498e9-505e9';
Q.ABS_SPECIES(11).RETRIEVE = false;
%
[Q.ABS_SPECIES.ISOFAC]     = deal( 1 );
[Q.ABS_SPECIES.SOURCE]     = deal( 'WebApi' );
%-------------------------------------------------------------------------


case 2
 %
 Q.BACKEND_NR              = 1;
```

```
Q.FRONTEND_NR              = 4;
Q.F_LO_NOMINAL             = 548.500e9;
%Q.SIDEBAND_LEAKAGE         = 0.05;   % Used for VDS-STD6
Q.SIDEBAND_LEAKAGE         = 'model'; % So far just for testing
%
Q.P_GRID                   = q2_pgrid( [], 120e3 );
%
Q.F_RANGES                 = [544.3e9 544.9e9];
Q.ZTAN_LIMIT_TOP           = 100e3;
Q.ZTAN_MIN_RANGE           = [ 25e3 40e3 ];
%
Q.T.L2                     = true;
Q.T.RETRIEVE               = true;
Q.T.L2NAME                 = 'Temperature / 545 GHz / 15 to 65 km';
Q.T.GRID                   = q2_pgrid( 10e3, 100e3, 8 );
%
Q.ABS_SPECIES(1).TAG{1}    = 'O3-666-534e9-556e9';
Q.ABS_SPECIES(1).RETRIEVE  = true;
Q.ABS_SPECIES(1).L2        = true;
Q.ABS_SPECIES(1).L2NAME    = 'O3 / 545 GHz / 20 to 85 km';
Q.ABS_SPECIES(1).GRID      = q2_pgrid( 10e3, 110e3, 8 );
Q.ABS_SPECIES(1).UNC_REL   = 0.5;
Q.ABS_SPECIES(1).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(1).CORRLEN   = 6e3;
Q.ABS_SPECIES(1).LOG_ON    = false;
Q.ABS_SPECIES(1).ISOFAC    = 1;
%
Q.ABS_SPECIES(2).TAG{1}    = 'HNO3-*-534e9-554e9';
Q.ABS_SPECIES(2).RETRIEVE  = true;
Q.ABS_SPECIES(2).L2        = true;
Q.ABS_SPECIES(2).L2NAME    = 'HNO3 / 545 GHz / 20 to 50 km';
Q.ABS_SPECIES(2).GRID      = q2_pgrid( 10e3, 70e3, 4 );
Q.ABS_SPECIES(2).UNC_REL   = 0.5;
Q.ABS_SPECIES(2).UNC_ABS   = 1e-9;
Q.ABS_SPECIES(2).CORRLEN   = 10e3;
Q.ABS_SPECIES(2).LOG_ON    = false;
Q.ABS_SPECIES(2).ISOFAC    = 1;
%
Q.ABS_SPECIES(3).TAG{1}    = 'O3-668-534e9-556e9';
Q.ABS_SPECIES(3).RETRIEVE  = true;
Q.ABS_SPECIES(3).L2        = true;
Q.ABS_SPECIES(3).L2NAME    = 'O3-668 / 545 GHz / 25 to 45 km';
Q.ABS_SPECIES(3).GRID      = q2_pgrid( 10e3, 70e3, 4 );
Q.ABS_SPECIES(3).UNC_REL   = 0.5;
Q.ABS_SPECIES(3).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(3).CORRLEN   = 6e3;
Q.ABS_SPECIES(3).LOG_ON    = false;
Q.ABS_SPECIES(3).ISOFAC    = 3.98194e-03;
%
Q.ABS_SPECIES(4).TAG{1}    = 'H2O-*-444e9-646e9';
Q.ABS_SPECIES(4).TAG{2}    = 'H2O-ForeignContStandardType';
Q.ABS_SPECIES(4).TAG{3}    = 'H2O-SelfContStandardType';
Q.ABS_SPECIES(4).RETRIEVE  = true;
Q.ABS_SPECIES(4).L2        = true;
Q.ABS_SPECIES(4).L2NAME    = 'H2O / 545 GHz / 15 to 30 km';
Q.ABS_SPECIES(4).GRID      = q2_pgrid( 10e3, 40e3, 4 );
```

```
    Q.ABS_SPECIES(4).UNC_REL   = 0.5;
    Q.ABS_SPECIES(4).UNC_ABS   = 1e-6;
    Q.ABS_SPECIES(4).CORRLEN   = 10e3;
    Q.ABS_SPECIES(4).LOG_ON    = false;
    Q.ABS_SPECIES(4).ISOFAC    = 1;
    %
    Q.ABS_SPECIES(5).TAG{1}    = 'N2-SelfContMPM93';
    Q.ABS_SPECIES(5).RETRIEVE  = false;
    %
    Q.ABS_SPECIES(6).TAG{1}    = 'O2-*-444e9-644e9';
    Q.ABS_SPECIES(6).RETRIEVE  = false;
    %
    Q.ABS_SPECIES(7).TAG{1}    = 'O3-*-534e9-554e9';
    Q.ABS_SPECIES(7).RETRIEVE  = false;
    %
    Q.ABS_SPECIES(8).TAG{1}    = 'N2O-*-534e9-554e9';
    Q.ABS_SPECIES(8).RETRIEVE  = false;
    %
    Q.ABS_SPECIES(9).TAG{1}    = 'H2O2-*-534e9-554e9';
    Q.ABS_SPECIES(9).RETRIEVE  = false;
    %
    [Q.ABS_SPECIES.SOURCE]     = deal( 'WebApi' );
    %-----------------------------------------------------------------------


   case 8
    %
    Q.BACKEND_NR               = 2;
    Q.FRONTEND_NR              = 2;
    Q.F_LO_NOMINAL             = 492.750e9;
    Q.SIDEBAND_LEAKAGE         = 'model';
    %
    Q.P_GRID                   = q2_pgrid( [], 100e3 );
    %
    Q.F_RANGES                 = [ 488.350e9 488.750e9; 488.950e9 489.35e9 ];
    Q.ZTAN_LIMIT_TOP           = 90e3;
    Q.ZTAN_MIN_RANGE           = [ 30e3 55e3 ];
    %
    Q.GA_START                 = 90;
    %
    Q.T.L2                     = false;
    Q.T.GRID                   = q2_pgrid( 10e3, 100e3, 4 );
    %
    Q.ABS_SPECIES(1).TAG{1}    = 'H2O-161-488.3e9-489.4e9';
    Q.ABS_SPECIES(1).RETRIEVE  = true;
    Q.ABS_SPECIES(1).L2        = true;
    Q.ABS_SPECIES(1).L2NAME    = 'H2O / 488 GHz / 20 to 70 km';
    Q.ABS_SPECIES(1).GRID      = q2_pgrid( 10e3, 95e3, 8 );
    Q.ABS_SPECIES(1).UNC_REL   = 0.5;
    Q.ABS_SPECIES(1).UNC_ABS   = 1e-6;
    Q.ABS_SPECIES(1).CORRLEN   = 10e3;
    Q.ABS_SPECIES(1).LOG_ON    = false;
    Q.ABS_SPECIES(1).ISOFAC    = 1;
    %
    Q.ABS_SPECIES(2).TAG{1}    = 'H2O-181-488.3e9-489.4e9';
    Q.ABS_SPECIES(2).RETRIEVE  = true;
```

```
Q.ABS_SPECIES(2).L2        = true;
Q.ABS_SPECIES(2).L2NAME    = 'H2O-181 / 488 GHz / 20 to 60 km';
Q.ABS_SPECIES(2).GRID      = q2_pgrid( 10e3, 95e3, 4 );
Q.ABS_SPECIES(2).UNC_REL   = 0.5;
Q.ABS_SPECIES(2).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(2).CORRLEN   = 10e3;
Q.ABS_SPECIES(2).LOG_ON    = false;
Q.ABS_SPECIES(2).ISOFAC    = 1.99983E-03;
%
Q.ABS_SPECIES(3).TAG{1}    = 'H2O-*-360e9-620e9';
Q.ABS_SPECIES(3).TAG{2}    = 'H2O-ForeignContStandardType';
Q.ABS_SPECIES(3).TAG{3}    = 'H2O-SelfContStandardType';
Q.ABS_SPECIES(3).RETRIEVE  = true;
Q.ABS_SPECIES(3).L2        = false;
Q.ABS_SPECIES(3).GRID      = q2_pgrid( 10e3, 40e3, 4 );
Q.ABS_SPECIES(3).L2NAME    = 'H2O-dummy / 488 GHz';
Q.ABS_SPECIES(3).UNC_REL   = 0.5;
Q.ABS_SPECIES(3).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(3).CORRLEN   = 10e3;
Q.ABS_SPECIES(3).LOG_ON    = true;
Q.ABS_SPECIES(3).ISOFAC    = 1;
%
Q.ABS_SPECIES(4).TAG{1}    = 'O3';
Q.ABS_SPECIES(4).RETRIEVE  = true;
Q.ABS_SPECIES(4).L2        = true;
Q.ABS_SPECIES(4).GRID      = q2_pgrid( 10e3, 95e3, 8 );
Q.ABS_SPECIES(4).L2NAME    = 'O3 / 488 GHz / 20 to 60 km';
Q.ABS_SPECIES(4).UNC_REL   = 0.5;
Q.ABS_SPECIES(4).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(4).CORRLEN   = 10e3;
Q.ABS_SPECIES(4).LOG_ON    = false;
Q.ABS_SPECIES(4).ISOFAC    = 1;
%
Q.ABS_SPECIES(5).TAG{1}    = 'CH3Cl';
Q.ABS_SPECIES(5).RETRIEVE  = false;
%Q.ABS_SPECIES(5).L2        = true;
%Q.ABS_SPECIES(5).GRID      = q2_pgrid( 10e3, 40e3, 4 );
%Q.ABS_SPECIES(5).L2NAME    = 'CH3Cl / 488 GHz / 20 to 30 km';
%Q.ABS_SPECIES(5).UNC_REL   = 0.5;
%Q.ABS_SPECIES(5).UNC_ABS   = 1e-10;
%Q.ABS_SPECIES(5).CORRLEN   = 5e3;
%Q.ABS_SPECIES(5).LOG_ON    = true;
%Q.ABS_SPECIES(5).ISOFAC    = 1;
%
Q.ABS_SPECIES(6).TAG{1}    = 'N2-SelfContMPM93';
Q.ABS_SPECIES(6).RETRIEVE  = false;
%
Q.ABS_SPECIES(7).TAG{1}    = 'O2-*-360e9-620e9';
Q.ABS_SPECIES(7).RETRIEVE  = false;
%
Q.ABS_SPECIES(8).TAG{1}    = 'HNO3-*-484e9-494e9';
Q.ABS_SPECIES(8).RETRIEVE  = false;
%
Q.ABS_SPECIES(9).TAG{1}   = 'HO2-*-484e9-494e9';
Q.ABS_SPECIES(9).RETRIEVE = false;
%
```

```
 Q.ABS_SPECIES(10).TAG{1}   = 'H2O2-*-484e9-494e9';
 Q.ABS_SPECIES(10).RETRIEVE = false;
 %
 [Q.ABS_SPECIES.SOURCE]     = deal( 'WebApi' );
 %-----------------------------------------------------------------------


case 17
 %
 Q.BACKEND_NR               = 2;
 Q.FRONTEND_NR              = 2;
 Q.F_LO_NOMINAL             = 494.250e9;
 Q.SIDEBAND_LEAKAGE         = 'model';
 %
 Q.P_GRID                   = q2_pgrid( [], 100e3 );
 %
 Q.F_RANGES                 = [ 489.950e9 490.750e9 ];
 Q.ZTAN_LIMIT_TOP           = 90e3;
 Q.ZTAN_MIN_RANGE           = [ 30e3 55e3 ];
 %
 Q.GA_START                 = 90;
 %
 Q.T.L2                     = false;
 Q.T.GRID                   = q2_pgrid( 10e3, 100e3, 4 );
 %
 Q.ABS_SPECIES(1).TAG{1}    = 'H2O-162-489.9e9-490.8e9';
 Q.ABS_SPECIES(1).RETRIEVE  = true;
 Q.ABS_SPECIES(1).L2        = true;
 Q.ABS_SPECIES(1).L2NAME    = 'HDO / 489 GHz / 20 to 60 km';
 Q.ABS_SPECIES(1).GRID      = q2_pgrid( 10e3, 95e3, 4 );
 Q.ABS_SPECIES(1).UNC_REL   = 0.5;
 Q.ABS_SPECIES(1).UNC_ABS   = 1e-6;
 Q.ABS_SPECIES(1).CORRLEN   = 10e3;
 Q.ABS_SPECIES(1).LOG_ON    = false;
 Q.ABS_SPECIES(1).ISOFAC    = 3.10693E-04;
 %
 Q.ABS_SPECIES(2).TAG{1}    = 'H2O-*-360e9-620e9';
 Q.ABS_SPECIES(2).TAG{2}    = 'H2O-ForeignContStandardType';
 Q.ABS_SPECIES(2).TAG{3}    = 'H2O-SelfContStandardType';
 Q.ABS_SPECIES(2).RETRIEVE  = true;
 Q.ABS_SPECIES(2).L2        = false;
 Q.ABS_SPECIES(2).GRID      = q2_pgrid( 10e3, 40e3, 4 );
 Q.ABS_SPECIES(2).L2NAME    = 'H2O-dummy / 489 GHz';
 Q.ABS_SPECIES(2).UNC_REL   = 0.5;
 Q.ABS_SPECIES(2).UNC_ABS   = 1e-6;
 Q.ABS_SPECIES(2).CORRLEN   = 10e3;
 Q.ABS_SPECIES(2).LOG_ON    = true;
 Q.ABS_SPECIES(2).ISOFAC    = 1;
 %
 Q.ABS_SPECIES(3).TAG{1}    = 'O3-668-489.9e9-490.8e9';
 Q.ABS_SPECIES(3).RETRIEVE  = true;
 Q.ABS_SPECIES(3).L2        = true;
 Q.ABS_SPECIES(3).L2NAME    = 'O3-668 / 489 GHz / 20 to 60 km';
 Q.ABS_SPECIES(3).GRID      = q2_pgrid( 10e3, 95e3, 4 );
 Q.ABS_SPECIES(3).UNC_REL   = 0.5;
 Q.ABS_SPECIES(3).UNC_ABS   = 1e-6;
```

```
Q.ABS_SPECIES(3).CORRLEN   = 10e3;
Q.ABS_SPECIES(3).LOG_ON    = false;
Q.ABS_SPECIES(3).ISOFAC    = 3.98194E-03;
%
Q.ABS_SPECIES(4).TAG{1}    = 'O3-686-489.9e9-490.8e9';
Q.ABS_SPECIES(4).RETRIEVE  = true;
Q.ABS_SPECIES(4).L2        = true;
Q.ABS_SPECIES(4).L2NAME    = 'O3-686 / 489 GHz / 20 to 60 km';
Q.ABS_SPECIES(4).GRID      = q2_pgrid( 10e3, 95e3, 4 );
Q.ABS_SPECIES(4).UNC_REL   = 0.5;
Q.ABS_SPECIES(4).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(4).CORRLEN   = 10e3;
Q.ABS_SPECIES(4).LOG_ON    = false;
Q.ABS_SPECIES(4).ISOFAC    = 1.99097E-03;
%
Q.ABS_SPECIES(5).TAG{1}    = 'O3-667-489.9e9-490.8e9';
Q.ABS_SPECIES(5).RETRIEVE  = true;
Q.ABS_SPECIES(5).L2        = true;
Q.ABS_SPECIES(5).L2NAME    = 'O3-667 / 489 GHz / 20 to 60 km';
Q.ABS_SPECIES(5).GRID      = q2_pgrid( 10e3, 95e3, 4 );
Q.ABS_SPECIES(5).UNC_REL   = 0.5;
Q.ABS_SPECIES(5).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(5).CORRLEN   = 10e3;
Q.ABS_SPECIES(5).LOG_ON    = false;
Q.ABS_SPECIES(5).ISOFAC    = 7.40475E-04;
%
Q.ABS_SPECIES(6).TAG{1}    = 'O3-*-479e9-509e9';
Q.ABS_SPECIES(6).RETRIEVE  = true;
Q.ABS_SPECIES(6).L2        = false;
Q.ABS_SPECIES(6).GRID      = q2_pgrid( 10e3, 40e3, 4 );
Q.ABS_SPECIES(6).L2NAME    = 'O3-dummy / 489 GHz';
Q.ABS_SPECIES(6).UNC_REL   = 0.5;
Q.ABS_SPECIES(6).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(6).CORRLEN   = 10e3;
Q.ABS_SPECIES(6).LOG_ON    = true;
Q.ABS_SPECIES(6).ISOFAC    = 1;
%
Q.ABS_SPECIES(7).TAG{1}    = 'N2-SelfContMPM93';
Q.ABS_SPECIES(7).RETRIEVE  = false;
%
Q.ABS_SPECIES(8).TAG{1}    = 'O2-*-360e9-620e9';
Q.ABS_SPECIES(8).RETRIEVE  = false;
%
Q.ABS_SPECIES(9).TAG{1}    = 'HNO3-*-485e9-500e9';
Q.ABS_SPECIES(9).RETRIEVE  = false;
%
Q.ABS_SPECIES(10).TAG{1}   = 'HO2-*-484e9-494e9';
Q.ABS_SPECIES(10).RETRIEVE = false;
%
Q.ABS_SPECIES(11).TAG{1}   = 'H2O2-*-484e9-494e9';
Q.ABS_SPECIES(11).RETRIEVE = false;
%
[Q.ABS_SPECIES.SOURCE]     = deal( 'WebApi' );
%-------------------------------------------------------------------------
```

```
 otherwise
  error( 'Frequency band %d is not yet handled.', freqmode );
end
```

2.1.3 Q meso

```
% Q_MESO   Settings for mesospheric inversion mode
%
%   This function contains the settings used for operational "mesospheric"
%   inversions. That is, don't modify without careful consideration.
%
%   The Q-fields are set according to selected frequency mode. The returned
%   Q is complete besides that all fields related to paths. These fields
%   should be set by *q_paths*.
%
% FORMAT   Q = q_meso(freqmode)
%
% OUT   Q          A Q-structure (lacking path and version settings)
%  IN   freqmode   Frequency mode number


function Q = q_meso(freqmode)


%---------------------------------------------------------------------------
%--- Frequency and inversion modes
%---------------------------------------------------------------------------

Q.FREQMODE           = freqmode;
Q.INVEMODE           = 'meso';


%---------------------------------------------------------------------------
%--- Absorption tables
%---------------------------------------------------------------------------

Q.F_GRID_NFILL       = 0;
Q.ABS_P_INTERP_ORDER = 1;
Q.ABS_T_INTERP_ORDER = 3;


%---------------------------------------------------------------------------
%--- RT and sensor
%---------------------------------------------------------------------------

Q.REFRACTION_DO      = false;
Q.PPATH_LMAX         = 15e3;
Q.PPATH_LRAYTRACE    = 20e3;

Q.DZA_MAX_IN_CORE    = 0.01;
Q.DZA_GRID_EDGES     = [ Q.DZA_MAX_IN_CORE*[1:3 5 8 12 21] ];

Q.LO_COMMON          = true;
Q.LO_ZREF            = 60e3;

Q.BACKEND_FILE       = [];

Q.TB_SCALING_FAC     = 1.0025;
Q.TB_CONTRAST_FAC    = [];
```

```
%--------------------------------------------------------------------------
%--- OEM settings
%--------------------------------------------------------------------------

Q.STOP_DX            = 0.5;
Q.GA_START           = 10;
Q.GA_FACTOR_NOT_OK   = 10;
Q.GA_FACTOR_OK       = 10;
Q.GA_MAX             = 1e4;


%--------------------------------------------------------------------------
%--- Common retrieval settings
%--------------------------------------------------------------------------

Q.NOISE_CORRMODEL    = 'expo';  % 'none', 'empi' 'expo'

Q.BASELINE.RETRIEVE  = true;
Q.BASELINE.MODEL     = 'adaptive';  % 'common', 'module', 'adaptive'
Q.BASELINE.UNC       = 2;

Q.POINTING.RETRIEVE  = true;
Q.POINTING.UNC       = 0.01;

Q.FREQUENCY.RETRIEVE = true;
Q.FREQUENCY.NPOLY    = 0;
Q.FREQUENCY.UNC      = 1e6;

Q.T.SOURCE           = 'WebApi';
Q.T.RETRIEVE         = true;
Q.T.UNC              = [ 3 3 9 15 15 ];
Q.T.CORRLEN          = 8e3;
Q.T.LIMITS           = [100 350];


%--------------------------------------------------------------------------
%--- Quality criteria
%--------------------------------------------------------------------------

Q.QFILT_TSPILL       = true;
Q.QFILT_TREC         = true;
Q.QFILT_NOISE        = true;
Q.QFILT_SCANNING     = true;
Q.QFILT_SPECTRA      = true;
Q.QFILT_TBRANGE      = true;
Q.QFILT_TINT         = true;
Q.QFILT_REF1         = true;
Q.QFILT_REF2         = false;
Q.QFILT_MOON         = true;
Q.QFILT_FCORR        = true;
Q.QFILT_LAGOMAX      = 2.5;

Q.MIN_N_SPECTRA      = 8;
Q.MIN_N_FREQS        = 100;
```

```
%------------------------------------------------------------------------------
%--- Band specific
%------------------------------------------------------------------------------

switch freqmode

 case 13
  %
  Q.BACKEND_NR              = 1;
  Q.FRONTEND_NR             = 1;
  Q.F_LO_NOMINAL            = 553.300e9;
  %
  Q.SIDEBAND_LEAKAGE        = 'model'; % So far just for testing
  %
  Q.GA_START                = 1000;
  Q.GA_FACTOR_OK            = sqrt(10);
  %
  Q.P_GRID                  = q2_pgrid( [], 140e3 );
  %
  Q.F_RANGES                = [ 556.6e9 557.2e9; ];
  Q.ZTAN_LIMIT_TOP          = 140e3;
  Q.ZTAN_LIMIT_BOT          = [ 45e3 45e3 45e3 45e3 ];
  Q.ZTAN_MIN_RANGE          = [ 60e3 80e3 ];
  %
  Q.T.L2                    = true;
  Q.T.L2NAME                = 'Temperature - 557 (Fmode 13) - 45 to 90 km';
  Q.T.GRID                  = q2_pgrid( 40e3, 130e3, 4 );
  Q.T.UNC                   = [ 3 3 5 5 5 ];
  %
  Q.ABS_SPECIES(1).TAG{1}    = 'H2O-*-556e9-558e9';
  Q.ABS_SPECIES(1).RETRIEVE  = true;
  Q.ABS_SPECIES(1).L2        = true;
  Q.ABS_SPECIES(1).L2NAME    = 'H2O - 557 GHz - 45 to 100 km';
  Q.ABS_SPECIES(1).GRID      = q2_pgrid( 40e3, 140e3, 4 );
  Q.ABS_SPECIES(1).UNC_REL   = 0.5;
  Q.ABS_SPECIES(1).UNC_ABS   = 1e-6;
  Q.ABS_SPECIES(1).CORRLEN   = 10e3;
  Q.ABS_SPECIES(1).LOG_ON    = true;
  %
  Q.ABS_SPECIES(2).TAG{1}    = 'O3-*-548e9-558e9';
  Q.ABS_SPECIES(2).RETRIEVE  = true;
  Q.ABS_SPECIES(2).L2        = true;
  Q.ABS_SPECIES(2).GRID      = q2_pgrid( 40e3, 130e3, 4 );
  Q.ABS_SPECIES(2).L2NAME    = 'O3 - 557 GHz - 45 to 90 km';
  Q.ABS_SPECIES(2).UNC_REL   = 0.5;
  Q.ABS_SPECIES(2).UNC_ABS   = 1e-6;
  Q.ABS_SPECIES(2).CORRLEN   = 10e3;
  Q.ABS_SPECIES(2).LOG_ON    = false;
  %
  [Q.ABS_SPECIES.ISOFAC]     = deal( 1 );
  [Q.ABS_SPECIES.SOURCE]     = deal( 'WebApi' );
  %---------------------------------------------------------------------------

 case 14
```

```
 %
 Q.BACKEND_NR              = 2;
 Q.BACKEND_FILE            = 'backend_df1000kHz_withHan_PLLdisf.xml';
 Q.FRONTEND_NR             = 3;
 Q.F_LO_NOMINAL            = 572.762e9;
 Q.LO_COMMON               = false;
 Q.FREQUENCY.NPOLY         = -1;
 Q.SIDEBAND_LEAKAGE        = 0.05;
 %
 %Q.GA_START                = 100;
 %
 Q.P_GRID                  = q2_pgrid( [], 140e3 );
 %
 Q.F_RANGES                = [ 576.118e9 576.418e9 ];
 %Q.F_RANGES                = [ 576.168e9 576.615e9 ];
 Q.ZTAN_LIMIT_TOP          = 100e3;
 Q.ZTAN_LIMIT_BOT          = [ 40e3 40e3 40e3 40e3 ];
 Q.ZTAN_MIN_RANGE          = [ 65e3 80e3 ];
 %
 Q.T.RETRIEVE              = false;
 Q.T.L2                    = true;
 Q.T.L2NAME                = 'Temperature - 576 GHz';
 Q.T.GRID                  = q2_pgrid( 40e3, 140e3, 4 );
 %
 Q.ABS_SPECIES(1).TAG{1}    = 'CO-*-575e9-578e9';
 Q.ABS_SPECIES(1).RETRIEVE  = true;
 Q.ABS_SPECIES(1).L2        = true;
 Q.ABS_SPECIES(1).GRID      = q2_pgrid( 40e3, 140e3, 4 );
 Q.ABS_SPECIES(1).L2NAME    = 'CO - 576 GHz';
 Q.ABS_SPECIES(1).UNC_REL   = 1;
 Q.ABS_SPECIES(1).UNC_ABS   = 1e-8;
 Q.ABS_SPECIES(1).CORRLEN   = 10e3;
 Q.ABS_SPECIES(1).LOG_ON    = true;
 Q.ABS_SPECIES(1).SOURCE    = 'MIPAS';
 %
 Q.ABS_SPECIES(2).TAG{1}    = 'O3-*-575e9-578e9';
 Q.ABS_SPECIES(2).RETRIEVE  = false;
 Q.ABS_SPECIES(2).L2        = true;
 Q.ABS_SPECIES(2).GRID      = q2_pgrid( 40e3, 110e3, 4 );
 Q.ABS_SPECIES(2).L2NAME    = 'O3 - 576 GHz';
 Q.ABS_SPECIES(2).UNC_REL   = 0.5;
 Q.ABS_SPECIES(2).UNC_ABS   = 1e-6;
 Q.ABS_SPECIES(2).CORRLEN   = 10e3;
 Q.ABS_SPECIES(2).LOG_ON    = false;
 Q.ABS_SPECIES(2).SOURCE    = 'WebApi';
 %
 [Q.ABS_SPECIES.ISOFAC]     = deal( 1 );
 %-------------------------------------------------------------------------


case 19
 %
 Q.BACKEND_NR              = 1;
 Q.FRONTEND_NR             = 4;
 Q.F_LO_NOMINAL            = 553.05e9;
 Q.SIDEBAND_LEAKAGE        = 'model'; % So far just for testing
```

```
 %
 Q.GA_START                 = 1000;
 Q.GA_FACTOR_OK             = sqrt(10);
 %
 Q.P_GRID                   = q2_pgrid( [], 140e3 );
 %
 Q.F_RANGES                 = [ 556.6e9 557.2e9; ];
 Q.ZTAN_LIMIT_TOP           = 140e3;
 Q.ZTAN_LIMIT_BOT           = [ 40e3 40e3 40e3 40e3 ];
 Q.ZTAN_MIN_RANGE           = [ 45e3 80e3 ];
 %
 Q.T.L2                     = true;
 Q.T.L2NAME                 = 'Temperature - 557 (Fmode 19) - 45 to 90 km';
 Q.T.GRID                   = q2_pgrid( 40e3, 130e3, 4 );
 Q.T.UNC                    = [ 3 3 5 5 5 ];
 %
 Q.ABS_SPECIES(1).TAG{1}    = 'H2O-*-556e9-558e9';
 Q.ABS_SPECIES(1).RETRIEVE  = true;
 Q.ABS_SPECIES(1).L2        = true;
 Q.ABS_SPECIES(1).L2NAME    = 'H2O - 557 GHz - 45 to 100 km';
 Q.ABS_SPECIES(1).GRID      = q2_pgrid( 40e3, 140e3, 4 );
 Q.ABS_SPECIES(1).UNC_REL   = 0.5;
 Q.ABS_SPECIES(1).UNC_ABS   = 1e-6;
 Q.ABS_SPECIES(1).CORRLEN   = 10e3;
 Q.ABS_SPECIES(1).LOG_ON    = false;
 %
 Q.ABS_SPECIES(2).TAG{1}    = 'O3-*-548e9-558e9';
 Q.ABS_SPECIES(2).RETRIEVE  = true;
 Q.ABS_SPECIES(2).L2        = true;
 Q.ABS_SPECIES(2).GRID      = q2_pgrid( 40e3, 130e3, 4 );
 Q.ABS_SPECIES(2).L2NAME    = 'O3 - 557 GHz - 45 to 90 km';
 Q.ABS_SPECIES(2).UNC_REL   = 0.5;
 Q.ABS_SPECIES(2).UNC_ABS   = 1e-6;
 Q.ABS_SPECIES(2).CORRLEN   = 10e3;
 Q.ABS_SPECIES(2).LOG_ON    = false;
 %
 [Q.ABS_SPECIES.ISOFAC]     = deal( 1 );
 [Q.ABS_SPECIES.SOURCE]     = deal( 'WebApi' );
 %-------------------------------------------------------------------------


case 21
 %
 Q.BACKEND_NR               = 1;
 Q.FRONTEND_NR              = 4;
 Q.F_LO_NOMINAL             = 547.753e9;
 Q.SIDEBAND_LEAKAGE         = 0.05;
 %
 Q.P_GRID                   = q2_pgrid( [], 140e3 );
 %
 Q.F_RANGES                 = [ 551.13e9 551.58e9; ];
 Q.ZTAN_LIMIT_TOP           = 140e3;
 Q.ZTAN_LIMIT_BOT           = [ 40e3 40e3 40e3 40e3 ];
 Q.ZTAN_MIN_RANGE           = [ 60e3 80e3 ];
 %
 Q.T.L2                     = true;
```

```
 Q.T.LIMITS                  = [100 1000];
 Q.T.L2NAME                  = 'Temperature - 551 GHz - 45 to 65 km';
 Q.T.GRID                    = q2_pgrid( 40e3, 140e3, 4 );
 %
 Q.ABS_SPECIES(1).TAG{1}     = 'NO-*-541e9-562e9';
 Q.ABS_SPECIES(1).RETRIEVE   = true;
 Q.ABS_SPECIES(1).L2         = true;
 Q.ABS_SPECIES(1).L2NAME     = 'NO - 551 GHz - 45 to 115 km';
 Q.ABS_SPECIES(1).GRID       = q2_pgrid( 40e3, 140e3, 4 );
 Q.ABS_SPECIES(1).UNC_REL    = 1;
 Q.ABS_SPECIES(1).UNC_ABS    = 1e-8;
 Q.ABS_SPECIES(1).CORRLEN    = 6e3;
 Q.ABS_SPECIES(1).LOG_ON     = true;
 %
 Q.ABS_SPECIES(2).TAG{1}     = 'O3-*-541e9-562e9';
 Q.ABS_SPECIES(2).RETRIEVE   = true;
 Q.ABS_SPECIES(2).L2         = true;
 Q.ABS_SPECIES(2).GRID       = q2_pgrid( 40e3, 110e3, 4 );
 Q.ABS_SPECIES(2).L2NAME     = 'O3 - 551 GHz - 45 to 90 km';
 Q.ABS_SPECIES(2).UNC_REL    = 0.5;
 Q.ABS_SPECIES(2).UNC_ABS    = 1e-6;
 Q.ABS_SPECIES(2).CORRLEN    = 10e3;
 Q.ABS_SPECIES(2).LOG_ON     = false;
 %
 [Q.ABS_SPECIES.ISOFAC]      = deal( 1 );
 [Q.ABS_SPECIES.SOURCE]      = deal( 'WebApi' );
 %-------------------------------------------------------------------------

case 22
 %
 Q.BACKEND_NR                = 2;
 Q.BACKEND_FILE              = 'backend_df1000kHz_withHan_PLLdisf.xml';
 Q.FRONTEND_NR               = 3;
 Q.F_LO_NOMINAL              = 572.964e9;
 Q.LO_COMMON                 = false;
 Q.FREQUENCY.NPOLY           = -1;
 Q.SIDEBAND_LEAKAGE          = 0.05;
 %
 %Q.GA_START                  = 100;
 %
 Q.P_GRID                    = q2_pgrid( [], 140e3 );
 %
 Q.F_RANGES                  = [ 576.118e9 576.418e9 ];
%Q.F_RANGES                   = [ 576.168e9 576.615e9 ];
 Q.ZTAN_LIMIT_TOP            = 100e3;
 Q.ZTAN_LIMIT_BOT            = [ 40e3 40e3 40e3 40e3 ];
 Q.ZTAN_MIN_RANGE            = [ 65e3 80e3 ];
 %
 Q.T.RETRIEVE                = false;
 Q.T.L2                      = true;
 Q.T.L2NAME                  = 'Temperature - 576 GHz';
 Q.T.GRID                    = q2_pgrid( 40e3, 140e3, 4 );
 %
 Q.ABS_SPECIES(1).TAG{1}     = 'CO-*-575e9-578e9';
 Q.ABS_SPECIES(1).RETRIEVE   = true;
 Q.ABS_SPECIES(1).L2         = true;
```

```
Q.ABS_SPECIES(1).GRID      = q2_pgrid( 40e3, 140e3, 4 );
Q.ABS_SPECIES(1).L2NAME    = 'CO - 576 GHz';
Q.ABS_SPECIES(1).UNC_REL   = 1;
Q.ABS_SPECIES(1).UNC_ABS   = 1e-8;
Q.ABS_SPECIES(1).CORRLEN   = 10e3;
Q.ABS_SPECIES(1).LOG_ON    = true;
Q.ABS_SPECIES(1).SOURCE    = 'MIPAS';
%
Q.ABS_SPECIES(2).TAG{1}    = 'O3-*-575e9-578e9';
Q.ABS_SPECIES(2).RETRIEVE  = false;
Q.ABS_SPECIES(2).L2        = true;
Q.ABS_SPECIES(2).GRID      = q2_pgrid( 40e3, 110e3, 4 );
Q.ABS_SPECIES(2).L2NAME    = 'O3 - 576 GHz';
Q.ABS_SPECIES(2).UNC_REL   = 0.5;
Q.ABS_SPECIES(2).UNC_ABS   = 1e-6;
Q.ABS_SPECIES(2).CORRLEN   = 10e3;
Q.ABS_SPECIES(2).LOG_ON    = false;
Q.ABS_SPECIES(2).SOURCE    = 'WebApi';
%
[Q.ABS_SPECIES.ISOFAC]     = deal( 1 );
%-------------------------------------------------------------------------

case 24
 %
 Q.BACKEND_NR               = 1;
 Q.BACKEND_FILE             = 'backend_df1000kHz_withHan_PLLdisf.xml';
 Q.FRONTEND_NR              = 3;
 Q.F_LO_NOMINAL             = 572.762e9;
 Q.LO_COMMON                = false;
 Q.FREQUENCY.NPOLY          = -1;
 Q.SIDEBAND_LEAKAGE         = 0.05;
 %
 %Q.GA_START                 = 100;
 %
 Q.P_GRID                   = q2_pgrid( [], 140e3 );
 %
 Q.F_RANGES                 = [ 576.118e9 576.418e9 ];
 %Q.F_RANGES                 = [ 576.168e9 576.615e9 ];
 Q.ZTAN_LIMIT_TOP           = 100e3;
 Q.ZTAN_LIMIT_BOT           = [ 40e3 40e3 40e3 40e3 ];
 Q.ZTAN_MIN_RANGE           = [ 65e3 80e3 ];
 %
 Q.T.RETRIEVE               = false;
 Q.T.L2                     = true;
 Q.T.L2NAME                 = 'Temperature - 576 GHz';
 Q.T.GRID                   = q2_pgrid( 40e3, 140e3, 4 );
 %
 Q.ABS_SPECIES(1).TAG{1}    = 'CO-*-575e9-578e9';
 Q.ABS_SPECIES(1).RETRIEVE  = true;
 Q.ABS_SPECIES(1).L2        = true;
 Q.ABS_SPECIES(1).GRID      = q2_pgrid( 40e3, 140e3, 4 );
 Q.ABS_SPECIES(1).L2NAME    = 'CO - 576 GHz';
 Q.ABS_SPECIES(1).UNC_REL   = 1;
 Q.ABS_SPECIES(1).UNC_ABS   = 1e-8;
 Q.ABS_SPECIES(1).CORRLEN   = 10e3;
 Q.ABS_SPECIES(1).LOG_ON    = true;
```

```
    Q.ABS_SPECIES(1).SOURCE    = 'MIPAS';
    %
    Q.ABS_SPECIES(2).TAG{1}    = 'O3-*-575e9-578e9';
    Q.ABS_SPECIES(2).RETRIEVE  = false;
    Q.ABS_SPECIES(2).L2        = true;
    Q.ABS_SPECIES(2).GRID      = q2_pgrid( 40e3, 120e3, 4 );
    Q.ABS_SPECIES(2).L2NAME    = 'O3 - 576 GHz';
    Q.ABS_SPECIES(2).UNC_REL   = 0.5;
    Q.ABS_SPECIES(2).UNC_ABS   = 1e-6;
    Q.ABS_SPECIES(2).CORRLEN   = 10e3;
    Q.ABS_SPECIES(2).LOG_ON    = false;
    Q.ABS_SPECIES(2).SOURCE    = 'WebApi';
    %
    [Q.ABS_SPECIES.ISOFAC]     = deal( 1 );

  otherwise
   error( 'Frequency band %d is not yet handled.', freqmode );
end
return
```

2.2 Spectroscopic data and absorption continua

The bulk of the data are taken from the latest HITRAN (high-resolution transmission molecular absorption) database (HITRAN2016). For the most important transitions for Odin/SMR some hand-picked data are used to replace the corresponding value in HITRAN, and this is described in Sect. 2.2.2. Nitrogen and water vapour continua models applied are described in Sect. 2.2.1.

2.2.1 Nitrogen and water vapour continua

```
# Common part of ARTS setup files for simulations of Odin-SMR measurements.

Arts2 {

# ----- Absorption models used for Odin-SMR -------------------------------

abs_cont_descriptionInit

# ----- H2O continuum ------------------------------------

# Present values are taken from Podobedov et al., JQSRT, 2008 (Table 3,
# experiment b).

abs_cont_descriptionAppend( abs_cont_names, abs_cont_models, abs_cont_parameters,
  "H2O-SelfContStandardType",
  "user",
  [ 9.21e-34, 5.50 ]
)

abs_cont_descriptionAppend( abs_cont_names, abs_cont_models, abs_cont_parameters,
  "H2O-ForeignContStandardType",
  "user",
  [ 5.32e-35, 1.80 ]
)



# ----- N2 continuum -------------------------------------
#
# the reference for the scaling factor of 1.34 is:
# J. Boissoles et al.
# Theoretical calculation of the translation-rotation collision-induced
# absorption in N2-N2, O2-O2, and N2-O2 pairs
# JQSRT, vol. 82 (2003) 505-516.
# For the Odin frequencies it is sufficient to use this constant
# scaling factor and not the frequency dependent factors given in the paper.
# The scaling incluses CIA contributions from O2-O2 and N2-O2 besides
# the original N2-N2 CIA.
# One has to note that Boissoles et al. used their own N2-N2- CIa model
# and not the B&F model to deduce this scaling factors. However, for the
# Odin frequencies the difference between these two models should be
# very small, implying that the 1.34 scaling factor is also appropriate
# in connection with the B&F model within the uncertainty range.

# MPM93 N2 continuum model:
```

```
abs_cont_descriptionAppend( abs_cont_names, abs_cont_models, abs_cont_parameters,
  "N2-SelfContMPM93",
  "MPM93Scale",
  [ 1.34 ]
)

# ----- End of absorption models used for Odin-SMR ------------------------

}
```

2.2.2 Odin/SMR linedata

```
A summary around the 556 GHz line:
---
Articles:
* Seta et al., JQSRT, 2008
* Hoshina et al., JQSRT, 2008
* Golubiatnikov et al., JQSRT, 2008
* Dick et al, JQSRT, 2009

ga = P_dry*ga_air*(300/T)^x_air + P_H2O*ga_self*(300/T)^x_self

Source  ga_air[MHz/hPa] x_air[-] ga_self[MHz/hPa] x_self[-]

MPM87           3.00 0.60 14.40 1.10
MPM89           3.21 0.69 13.20 1.00
MPM93           3.21 0.69 13.20 1.00
PWR98           3.21 0.69 13.20 1.00
HITRAN00        3.06 0.64     0    -
HITRAN04        3.11 0.78 13.83    -
HITRAN12        3.14 0.75 14.40 0.75
Seta            2.98    -     -    -
Hoshina         2.98    -     -    -
Golubiatnikov   3.10    - 14.06    -
Dick            3.55 0.27     -    -   Table 1, measurements at 200K
Dick            3.13    -     -    -   Table 3, measurements at 296K

The MPM89/93 and PWR98 values are not independent and should be taken as a
single "vote". Seta+Hoshina give the lowest ga_dry (most important variable).
Golubiatnikov is in the middle. Note that all data are not at the same
reference temperature, that can explain differences up to 1%.

For 547, 552 and 557 GHz lines, pressure broadening parameters are taken from
Golubiatnikov et al., JQSRT, 2008. Note that article data are for 299 K. These
data were scaled to 296K by multiplication with (299/296)^0.75. All this
resulted in these values:

For the 488.5 GHz line, the pressure broadening parameter is taken from
Tretyakov et al, JQSRT, 2013, Table 1, column Air (measured)

Line    HITRAN2012   Used
---
488GHz     26007     26100
547GHz     31362     31096
552GHz     31362     31768
556GHz     31362     31260
```

```
Pressure shift parameter is taken from same articles (no temperature scaling
applied)

Line    HITRAN2012   Used
---
488GHz     533       1800
489GHz    -917          0    (no source for this change)
490GHz       0          0
547GHz    2012       1838
552GHz    2012       1822
556GHz    2012       1867


Note that no data have been found for the isotopologue lines at 489.05 and 490.60 GHz


H2O continuum absorption is taken from Podobedov et al., JQSRT, 2008 (Table 3,
experiment b). More recent measurements include Koshelev et al, JQSRT, (2011)
and Yang et al, JQSRT, (2014).


O3:
-----
Line centre and strength replaced with JPL:
501.22 GHz, df +0.66 MHz (JPL higher), dI +12.9% (JPL higher, but no T-correction)
501.48 GHz, df -1.50 MHz, dI +2.4%
544.49 GHz, df +0.15 MHz, dI +6.0%
544.86 GHz, df -0.32 MHz, dI -0.4%
550.99 GHz, df +0.91 MHz, dI +0.0%
551.44 GHz, df +0.49 MHz, dI +2.8%
556.71 GHz, df -1.22 MHz, dI +2.4%
576.52 GHz, df -1.01 MHz, dI +0.5%

Change of air broadening:
544.86 GHz: 24942 -> 30500 (based on tests made by Ashley)


H2O:
-----
Line centre and strength replaced with JPL:
488.49 GHz, df +0.21 MHz, dI -0.6%
489.05 GHz  df + 5kHz,    dI -2.9%
490.60 GHz, df +0.01 MHz, dI -3.1%
547.68 GHz, df +0.11 MHz, dI -2.6%
552.02 GHz, df -0.05 MHz, dI -2.6%
556.94 GHz, df -3 kHz,    dI -3.1%

For pressure broadening, see h2o_notes.txt


N2O:
-----
Line centre and strength replaced with JPL:
502.30 GHz, df +2.25 MHz, dI -8.0%
```

```
CO:
-----
Line centre and strength replaced with JPL:
576.3 GHz, df -2 kHz, dI -2.6%


NO:
-----
Line centre and strength replaced with JPL:
551.19 GHz, df -0.26 MHz, dI -3.6% (just main three lines modified)
551.53 GHz, same as 551.19


ClO:
-----
501.27 GHz: Line positions and strengths look to agree well between JPL and HITRAN
```

Bibliography

P. Eriksson. Odin/SMR algorithms theoretical basis document - Level2 processing. Technical report, Department of Earth and Space Sciences, Chalmers University of Technology, 2020.

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