KOPRA installation

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1 Modules

For the basic version of KOPRA the following modules are necessary (in required order of compilation):

precis_m.f90
param_m.f90
co2coe_m.f90
ckdcoe_m.f90
types_m.f90
inpdat_m.f90
outdat_m.f90
modat_m.f90
varsub_m.f90
recipe_m.f90
give_m.f90
parchk_m.f90
inismw_m.f90
inider_m.f90
inipar_m.f90
inspec_m.f90
xinput_m.f90
input_m.f90
ray_m.f90
rayctl_m.f90
modgeo_m.f90
modlev_m.f90
linpac_m.f90
linmix_m.f90
addlin_m.f90
gascon_m.f90
transf_m.f90
xintpl_m.f90
ilsfov_m.f90
abco_m.f90
radtra_m.f90
offsca_m.f90
iniout_m.f90
wriout_m.f90
deallo_m.f90
kopfwd_m.f90
kopra.f90 (main program)

2 Run KOPRA

KOPRA reads its main input from standard input. The command line to start the program is:

```
kopra < filename_main_input_file
```

The file names of further input and the output are given in the main input file which is described in the following.

3 Required files

Basic principle:
For most of the input files: input will be read beginning directly in the line following a $ in the first column and ending when all the relevant input for this topic is read. No fixed format is required for this input. Until the next $ there can be any number of comment lines.

3.1 Main input file

This is the basic input file for kopra. All other file names and directories are read from this file. All the topics $ are indicated also by a number which is, however, not used by kopra and only meant to facilitate referencing. In the following a commented main input file is given:

```
============================================================
============================================================
KOPRA main input file
version 9-3-99



============================================================
0. version of input file
------------------------


This is the version number of the kopra input-file and identical to the second
number in the kopra version number. Kopra is downward compatible and supports
all lower input file versions.

$0.1
  0.8

============================================================
1. input files and directories for fixed data
---------------------------------------------


1.1 and 1.2 are fixed data used for the calculation of absorption coefficients
in module addlin_m.

File with Doppler cut-offs for calculation of the absorption coefficient
$1.1
input/data/cutdop.dat

File with Lorentz cut-offs for calculation of the absorption coefficient
$1.2
input/data/cutlor.dat

Data file with information on each hitran molecule and isotope
  (number of isotopes, molecular weights, hitran isotope abundancies,
  Gamache coefficient for partition sum calculation, state energies)
$1.3
input/data/hitmol.dat

File with line-mixing data. This file is only necessary if $12.1 is set
```

```
to 'T', i.e. line mixing is switched on.
  (y-coefficients, ...)
$1.4
input/data/linemix.dat

Directory with spectroscopic data
  (The files have to be in the form: fXXXXX, where XXXXX is the wavenumber;
  they are produced with the program 'hitsort.f90')
$1.5
/home/amelib/data/kopra/hitran96/

Directory with cross-section data for the heavy molecules.
This file is only necessary if cross-section species are calculated.
$1.6
/home/amelib/data/cross/


============================================================
2. input files and directories for atmospheric/instrumental data
---------------------------------------------------------------

File with p,T profiles.
$2.1
input/profiles/pt.prf

File with p,T - gradient profiles.
  (will only be used if p or T gradients are switched on in $5.9)
$2.2
input/profiles/ptgra.prf

File with vmr profiles
$2.3
input/profiles/vmr.prf

File with vmr - gradient profiles
  (will only be used if vmr gradients are switched on in $5.9)
$2.4
input/profiles/vmrgra.prf

File with continuum profiles
  (for each microwindow one profile)
$2.5
input/profiles/cont.prf

File with vibrational temperature profiles
  (will only be used if nlte is switched on in $13.1)
$2.6
input/profiles/Tvib.gabi

File with Tvib gradient profiles
  (will only be used if Tvib gradients are switched on in $5.9)
$2.7
input/profiles/Tvibgra.prf
```

```
File with isotope abundance profiles
$2.8
input/profiles/isoabu.prf

File with (apodized) instrumental line shape per microwindow
  (will only be used if $9.7==3)
$2.9
input/instrument/ails.dat

File with broadband-aerosol profiles:
  number densities, mode-radii, mode-widths
  (will only be read if $14.1==T)
$2.10
input/profiles/brdaero.prf

File with broadband-aerosol altitude and wavenumber dependent refraction indices
  (will only be read if $14.1==T and $14.2==T)
$2.11
input/profiles/brdaero.refra

File with broadband-aerosol altitude and wavenumber dependent cross-sections
  (will only be read if $14.1==T and $14.2==F)
$2.12
input/profiles/brdaero.cross11


============================================================
3. output files and directories
-------------------------------

Spectra on fine grid
  (directory and first letters of output file;
  numbers for microwindows and geometries will be added;
  type  F  for no output; if end letter is  e  the spectral will
  be on the equidistant fine grid, else on the non-equidistant)
$3.1
output/x

Spectra on coarse grid
  (directory and first letters of output file;
  numbers for microwindows and geometries will be added;
  type  F  for no output)
$3.2
output/y

Test-output grade for logfile
  0 = no log-output
  1 = total log-output
$3.3
  1

Filename for logfile
  screen = output to screen
$3.4
```

```
screen

Filename for error-file
  screen = output to screen
$3.5
output/errors


============================================================
4. header for output files [a80]
--------------------------------

 (the version number will be added to this header)
$4.1
   test run 25-04-2000


============================================================
5. mode of observation and definition of geometry
-------------------------------------------------

1= satellite / limb / tangent altitude
2= satellite / limb / nadir angle and observer altitude
3= balloon / limb / tangent altitude and observer altitude
4= balloon / limb / nadir angle and observer altitude
5= upward / nadir angle and observer altitude
6= upward+limb / nadir angle and observer altitude
7= homogeneous path (cuvette)
$5.1
   1

Background temperature [K]
  (for negative values only the transmission is calculated)
  {default: 2.7 K for emission, 6000 K for solar absorption}
$5.2
   2.7

Number of observational geometries ('sweep')
  *** implies changes in $5.3-$5.7, $8.3, $8.4, $9.11, $9.12 ***
  (for observation mode 1-6)
$5.3
   2

Tangent altitudes [km]        (observation mode 1,3)
Viewing nadir angles [rad]    (observation mode 2,4,5,6)
Homogeneous path length [km]  (observation mode 7)
  (# observation geometries)
  -->   (ordering: low -> high observation geometry)
$5.4
  10.0 13.0

Observer altitude [km]
  (# observation geometries)
  -->   (ordering: low -> high observation geometry)
```

```
$5.5
  800.0 800.0

Latitude of the tangent points [rad]   (observation mode 1,3)
Latitude of the observer [rad]         (observation mode 2,4,5,6)
  (# observation geometries)
  -->   (ordering: low -> high observation geometry)
$5.6
   0.78539 0.78539

Longitude of the tangent points [rad]  (observation mode 1,3)
Longitude of the observer [rad]        (observation mode 2,4,5,6)
  (# observation geometries)
  -->   (ordering: low -> high observation geometry)
$5.7
     0.0 0.0

Azimuth of the observation [rad]
  (i.e. the direction in which the instrument is looking)
  (south=0,direction S->O->N->W)
  (# observation geometries)
  -->   (ordering: low -> high observation geometry)
$5.8
  0.0 0.0

Which horizontal inhomogeneity should be considered?
  (be careful that the related input file is defined in $2.2,$2.4,$2.7)
 p      vmr
 |   T   |  Tvib
 |   |   |   |
$5.9
 F   F   F   F


============================================================
6. wavenumber discretization
----------------------------

Smallest wavenumber interval for calculation of absorption coefficients [cm-1]
  (will internally be adjusted so that $6.2 is an integer multiple of $6.1)
$6.1
   0.0005

Output grid interval [cm-1]
$6.2
   0.025


============================================================
7. parameters for the adjustment of computational accuracy
----------------------------------------------------------

Wavenumber range outside the microwindow where lines are taken into account [cm-1]
  {default 25.0}
```

```
$7.1
    25.00

Accuracy for absorption coefficient calculation
  absolute accuracy for optical              =0 lines my be rejected and truncated
  depth calculation of each line             =1 all lines retained, no truncation
  (negative for slow reference calculation)
              |                               |  {default 0}
$7.2          |                               |
           1.0e-6                             0


Constant base-levels for the forward-model layering:
  the input-profile levels are used exclusively               : 0
  the input-profile levels are used and additional
    levels with respect to criteria $7.3-7.6 are added        : 1
  the levels under $7.32 are used exclusively                 : 2
  the levels under $7.32 are used and additional
    levels with respect to criteria 7.3-7.6 are added         : 3
  the levels are set up automatically with respect            : 4
    to criteria $7.3-7.6
$7.31
   0

Number of base-levels and
Base level altitudes [km]
  (only used if $7.31 = 2,3)
$7.32
  3
  0.0 30.0  120.0


Maximum allowed temperature variations between two forward model levels [K] for
      lower and higher altitude regions and altitude [km] which divides this regions
        |        |                             |
  (only used if $7.31 = 1,3,4)
$7.3
      10.0      3.0                         40.0

Maximum variation of the Lorentz line width between two model levels
  (values > 1.0)
  (only used if $7.31 = 1,3,4)
$7.4
  1.4

Maximum forward model layer thickness above the tangent altitude [km] and altitude
  above the tangent altitude up to which this maximum thickness is valid [km]
  (only used if $7.31 = 1,3,4)
  {default 100 , 2 to use only input levels}
$7.5
   100.0             2.0

Minimal layer thickness [km]
  (only used if $7.31 = 1,3,4)
```

```
$7.6
   0.4

Definition for the recalculation of the absorption coefficients (extra paths)
  -1 = all absorption coefficients recalculated
   0 = all absorption coefficients above the lowest geometry
       are taken from lowest geometry
   1 = new calculation only of tangent-layer, all others
       are taken from lowest geometry
   2 = new calculation for tangent-layer and the one above, all others
       are taken from lowest geometry
   {default 2}
$7.7
    2

Accuracy of apodization (defines the microwindow extension)
    1 = apodization function decreases to  1%    of center value
    2 = apodization function decreases to  0.1%  of center value
    3 = apodization function decreases to  0.01% of center value
    {default 1}
$7.8
    1

Number of the geometry ('sweep') up to which the $7.10 criterion no. 1 is used
  for addition of simulated geometries for field of view calculation;
  for the geometries above $7.10 criterion no. 2 is used
$7.9
    3

2 Criteria for the addition of simulated geometries for field of view calculation:
    0 = no addition of extra geometries, only one below the lowest observation
        and/or one above the highest
   negative values:
   -1 = between all observed geometries one extra will be added
   -2 = between all observed geometries two extra will be added
   -3 = ...
   positive values (only odd values >= 3 allowed !)
    3 = for fov calculation of each observed geometry 3 geometries at least will be
        used
    5 = for fov calculation of each observed geometry 5 geometries at least will be
        used
    7 = ...

   crit. 1 for low geometries      crit. 2 for high geometries
   {default  0  0   for no extra geometries}
$7.10
          3                                3

Integration step length for ray-tracing and Curtis-Godson/mass calculation [km]
  {default 1.0}
$7.11
         1.000

Gas/isotope number of the main gas
```

```
  (it must appear in all microwindows under $8.6)
 >0 = gas/isotope number of the main gas: it's Curtis-Godson T will be used for
      Planck function
  0 = for no main gas (mix Curtis-Godson T's of all species for Planck function)
      (this is necessary for nlte calculations and is the slowest choice)
 -1 = use Curtis-Godson T of air for Planck function
$7.12
         -1


============================================================
8. microwindow definition
-------------------------

Number of microwindows
  *** implies changes in $8.2-$8.6,$9.10-9.12 ***
$8.1
   1

Wavenumber ranges [cm-1] (ordering low -> high first wavenumbers)
  *** implies changes in $8.3 ***
  --> mw
$8.2
  (940.,941.)

Number of sub-microwindows for each microwindow and
  each observational geometry
  (if = -1: the mircowindows from 8.2 will be used for all altitudes and
   input $8.4 is not valid)
  --> mw
 g
 e
 o
$8.3
  1
  2

Wavenumber range [cm-1] for each sub-microwindow and
  each observational geometry  (must be inside ranges of $8.2)
  --> sub-mw
 g
 e
 o
$8.4
  (940.,941.)
  (940.,940.5) (940.6,940.8)

Number of gases/isotopes to be considered in each microwindow
  *** implies changes in $8.6 ***
  --> mw
$8.5
   2

Gases/isotopes (i4: xxxy, xxx=molecule number, y=hitran isotope number,
```

```
                y=0: use all isotopes)
  (e.g. for separate calculation of HDO and all other isotopes give: 011 010 )

 (line-data gases:)
 1=H2O    2=CO2    3=O3     4=N2O    5=CO     6=CH4    7=O2     8=NO     9=SO2
10=NO2   11=NH3   12=HNO3  13=OH    14=HF    15=HCL   16=HBr   17=HI    18=CLO
19=OCS   20=H2CO  21=HOCL  22=N2    23=HCN   24=CH3CL 25=H2O2  26=C2H2  27=C2H6
28=PH3   29=COF2  30=SF6   31=H2S   32=HCOOH 33=HO2   34=O     35=ClNO3 36=NO+
37=HOBr  38=C2H4

 (additional non-hitran line-data gases:)
101=HNO4

 (pseudo-line data gases:)


 (x-section gases:)
351=CFC-11(CCL3F)            352=CFC-12(CCl2F2)            353=CFC-22(CHClF2)
354=SF6                      355=CFC-14(CF4)               356=CCl4
357=CFC-113(CCl2FCClF2)      358=CFC-114(CClF2CClF2)       359=N2O5
360=ClONO2

  --> gas
 m
 w
$8.6
   10 20

Spectral shift of lines for each gas/isotope
  --> gas
 m
 w
$8.7
 0.0 0.0

continuum is considered for (but only if the related gas number is chosen in $8.6)
artificial continuum (as defined for each mw in file $2.5)
(default=T)

                  N2        O2       H2O       CO2    artificial
$8.8              |         |         |         |         |
                  F         F         T         T         T

============================================================
9. instrumental parameters
--------------------------

Kind of apodization
  1= boxcar in ifg == sinc in spectrum
  2= triangle in ifg == sinc^2 in spectrum
  3= Hamming (Happ-Genzel)
  4= 3 term Blackmann-Harris
  5= 4 term Blackmann-Harris
  6= Norton-Beer weak
```

```
  7= Norton-Beer medium
  8= Norton-Beer strong
    (for MIPAS ENVISAT (i.e. $9.7 =2) only Norton-Beer strong allowed)
$9.1
   8

Maximum optical path difference of the interferometer [cm]
$9.2
   20.0

Should field-of-view be taken into account?
  *** implies changes in $7.9, $7.10 ***
$9.3
   T

Should field-of-view effect on the instrumental profile be taken into account (F/T)?
$9.4
   F

Number of channels (the microwindows must lie in these channels)
$9.43
  1

Wavenumber range [cm-1] for each channel of $9.43
$9.46
  (100.,6000.)

Half vertical field-of-view extension [rad]
  (one number for each channel of $9.43)
$9.5
   6.1e-4

Relative weighting function for vertical field-of-view
  (20 values along vertical fov extension, ordered by elevation,
  the vertical fov is subdivided in 20 bands of equal thickness
  and the values give the relative weighting (integral!) of each band)
  (one function for each channel of $9.43)
$9.6
  1.,3.,5.,6.,6.,6.,6.,6.,6.,6.,6.,6.,6.,6.,6.,6.,6.,5.,3.,1.

Ils is calculated for circular aperture with phase and lin. apo. error:  1
Ils is calculated using ESA parametrization:                             2
Ils is read in for each microwindow from file($2.9):                     3
  (in case 3 the area under the ils must be normalized to 1!)
$9.7
  1

In case of $9.7 = 1:
====================
->maximum inclination of the ray in the interferometer [rad]
   [max. value = 1/sqrt({$9.2} * max_wavenumber_of_interferometer) ]
->part of linear Apodization in interferogram
   (1.0 = perfect instrument, 0.0 = triangle) {default 1.0}
->phase error [rad] {default 0.0}
```

```
In case of $9.7 = 2:
====================
 ESA parameters:
->infrared misalignment y-direction [rad]
->infrared misalignment z-direction [rad]
->retroreflector linear shear along y [cm]
->retroreflector linear shear along z [cm]
->linear shear variation along y [-]
->linear shear variation along z [-]
->full interferometer divergence along y [rad]
->full interferometer divergence along z [rad]
->blur angular width along y [rad]
->blur angular width along z [rad]
->laser misalignment along y [rad]
->laser misalignment along z [rad]
->optical speed of interferometer [cm/s]
->initial sampling perturbation [dxnull]
->time constant of exponential attenuation of initial sampling perturbation [s]
->time constant of exponential attenuation of initial speed fluctuation [s]
->initial relative speed fluctuation at beginning of scan [cm/s]
->gain slope of IR electrical response [-]
->mismatched delay between electronic response and ADC trigger [s]
->laser wvnr [cm-1]
->relative drift rate of laser wvnr [-]
->bandwidth laser white noise [Hz]
->bandwidth laser 1/f noise [Hz]

$9.8
   4.6e-5  1.0  0.0

   0.0, 0.2e-3, 0.004, 0.004, 0.0, 0.0, 5.4e-3, 9.0e-3
   5.2e-4, 3.3e-4, 0.15e-3, 0.15e-3, 10.0, 4.0e-8, 0.16, 0.016, 0.03
   -0.22, 1.4e-6, 7692.0, 1.0e-8, 20.0e6, 0.0

Wavenumber shift [cm-1]
   --> m i c r o w i n d o w
$9.9
   0.0 0.0

Offset per mw and geometry [nW/cm2Srcm-1]  (Spectrum*scale + offset)
  *** implies changes in $8.1, $5.2 ***
   --> m i c r o w i n d o w
 g
 e
 o
$9.10
   0.0 0.0

Scale per mw and geometry [nW/cm2Srcm-1]   (Spectrum*scale + offset)
  *** implies changes in $8.1, $5.2 ***
   --> m i c r o w i n d o w
 g
 e
```

```
 o
$9.11
   1.0 1.0

Should noise be added to the spectra?
$9.12
  F

Rms value of the noise in the sinc-spectrum
 (independent grid-values of distance 1/2*opdmax) [nW/cm2Srcm-1]
 --> mw
$9.13
 30.0 30.0

Seed-value for noise
 ( >= 0: same noise in two runs, < 0: noise always changes)
$9.14
   -1

============================================================
10. derivative definition
-------------------------

Which derivatives shall be calculated?
  in case of esa-ils-parameters ($9.7==2):
    phase is parameter 1 and apolin is parameter 2

Temp  artific. shift  offset   phase   Tgrad   press    aerosol         weighting
 |    continuum  |       |       |       |       | nlte numden          fuction
 |  vmr  |  LOS  |  Tvib | scale | apolin|vmrgrad| model | Mie-para     |
 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |    |         |
$10.1
 T   T   F   F   F   F   F   F   F   F   F   F   F   F   F    F         F

How many gases/isotopes for VMR derivative?
  *** implies changes in $10.3 ***
$10.2
    1

Which gas/isotope for VMR derivative?
  --->
$10.3
   010

How many gases/isotopes for VMR-gradient derivative?
  *** implies changes in $10.5 ***
$10.4
    1

Which gas/isotope for VMR-gradient derivative?
  --->
$10.5
   020
```

```
Which gas/isotope (nlte-species) for Tvib derivative?
$10.6
   021

How many vibrational temperature profiles (states) for this gas/isotope?
  *** implies changes in $10.8 ***
$10.7
   2

Which Tvib-state(s) (HITRAN state number)?
  --->
$10.8
   1 2


============================================================
11. profile definition
----------------------

Should the profiles be recalculated for hydrostatic equilibrium
  (no:0) and should the level-pressures (1) or the level-altitudes (2) be adjusted?
  {default  0}
$11.1
   0

Number of base levels for p,T,vmr,Tvib,continuum and gradient profiles
$11.2
   50

Latitude of the profiles read from files $2.1-2.7 [rad]
$11.3
   0.78539

Longitude of the profiles read from files $2.1-2.7 [rad]
$11.4
   0.0

Level altitudes [km]
$11.5
       0.0,       1.0,       2.0,       3.0,       4.0,
       5.0,       6.0,       7.0,       8.0,       9.0,
      10.0,      11.0,      12.0,      13.0,      14.0,
      15.0,      16.0,      17.0,      18.0,      19.0,
      20.0,      21.0,      22.0,      23.0,      24.0,
      25.0,      27.5,      30.0,      32.5,      35.0,
      37.5,      40.0,      42.5,      45.0,      47.5,
      50.0,      55.0,      60.0,      65.0,      70.0,
      75.0,      80.0,      85.0,      90.0,      95.0,
      100.0,     105.0,     110.0,     115.0,     120.0


============================================================
12. line mixing
```

```
---------------

Should line mixing be considered (F/T)?
$12.1
  F

Direct diagonalization (1), Rosenkranz (2)
$12.2
  2

Only Q- (1), Q- and PR- coupling (2)
$12.3
  2

============================================================
13. NLTE
--------

Should NLTE be considered (F/T)?
$13.1
  F

Should fq be set to 1.0?
  {default  T}
$13.2
  T

Should rotational-spin nlte for NO be calculated (F/T)?
  {default  F}
$13.25
  F

NLTE for how many different species?
   *** implies changes in 13.6, 13.8 ***
$13.3
  1

Species identifier(s) [(hitran molecular code) *10 + (hitran isotope number)]
  -->
$13.4
   021

How many Tvib profiles (states) for each species?
   *** implies changes in 13.6 ***
  -->
$13.5
  2

Which Tvib-states for each species?
  states -->
 s
 p
 e
 c
```

```
 i
$13.6
  5 9

How many transitions should be calculated for each species?
   *** implies changes in 13.8 ***
  -->
$13.7
   1

Which transitions (ground state =1)?
 (higher,lower state)

  transitions -->
 s
 p
 e
 c
 i

$13.8
   (9,5)

Should the nlte-model be used (F/T)?
$13.9
   F

Nlte-model for which nlte-species?
   *** must be one of 13.4 ***
$13.10
   021


================================================================================
14. broadband-aerosol
---------------------

Should broadband-aerosol be considered?
   *** input files $2.10 and $2.11 or $2.12 must exist ***
$14.1
  F

Should the KOPRA internal Mie-model be used?
   (=T: wavenumber and altitude dependent refraction indices must be provided: $2.11)
   (=F: wavenumber and altitude dependent cross-sections must be provided: $2.12)
$14.2
  T

============================================================
end KOPRA main input file



============================================================
```

```
============================================================
```

3.2 Files with fixed data

The fixed data files are delivered together with the source-files of KOPRA. The directory tree is not fixed but given under \$1.* in the main input file.

3.2.1 Files with Doppler and Lorentz cut-offs

```
============================================================

   Files with Doppler ($1.1) and Lorentz ($1.2) cut-offs for calculation of the
   absorption coefficient. There are two versions of each file:
   For normal accuracy calculations:
     cutdop.dat  and cutlor.dat
   For very high accuracy:
     cutdop3.dat and cutlor3.dat
============================================================
```

3.2.2 Molecule information data file

```
============================================================

   Data file with information on each hitran molecule and isotope
   (number of isotopes, molecular weights, hitran isotope abundancies,
   Gamache coefficient for partition sum calculation, state energies)
   ($3.3)
============================================================


$ number of hitran molecules, additional molecules, pseudo-line molecules
  38, 3, 10

$  number of isotopes per HITRAN molecule
  4,8,5,5,6,3,3,3,2,1,2,1,3,1,2,2,1,2,5,3,2,1,3,2,1,2,1,1,1,1,3,1,1,1,2,1,2,2

$  number of isotopes per additional line gas molecule
   1,1,1

$  number of isotopes per pseudo line gas molecule
   1,1,1,1,1,1,1,1,1,2

$  molecular weights per HITRAN molecule
   18., 20., 19., 19.
   44., 45., 46., 45., 47., 46.,48.,47.
   48., 50., 50., 49., 49.
   44., 45., 45., 46., 45.
   28., 29., 30., 29., 31., 30.
   16., 17., 17.
   32., 34., 33.
   30., 31., 32.
   64., 66.
```

```
   46.
   17., 18.
   63.
   17., 19., 18.
   20.
...
...

$  molecular weights per additional gas molecule, to be VERIFIED
   79.
   44.
   30.

$  molecular weights per pseudo-line gas molecule
   1.
   1.
   1.
   1.
   8.
   1.
   0.0004
   0.
   0.001
   97. 99.

$  isotope abundancies of HITRAN
  0.997317,0.00199983,0.000372,0.00031069
  0.98420,0.01106,0.0039471,0.000734,0.00004434,0.00000825,0.0000039573,0.00000147
  0.992901,0.00398194,0.00199097,0.000740,0.000370
  0.990333,0.0036409,0.0036409,0.00198582,0.000369
  0.98654,0.01108,0.0019782,0.000368,0.00002222,0.00000413
  0.98827,0.01110,0.00061575
  0.995262,0.00399141,0.000742
  0.993974,0.0036543,0.00199312
  0.94568,0.04195
  0.991616
  0.9958715,0.0036613
  0.989110
  0.997473,0.00200014,0.00015537
  0.99984425
  0.757587,0.242257
  0.50678,0.49306
  0.99984425
  0.75591,0.24172
  0.93739,0.04158,0.01053,0.00739908,0.0018797
  0.98624,0.01108,0.0019776
  0.75579,0.24168
  0.9926874
  0.98511,0.01107,0.0036217
  0.74894,0.23949
...
...

$  isotope abundancies of additional line gases
```

```
  1.0
  1.0
  1.0

$  isotope abundancies of pseudo-line gases
  1.0
  1.0
  1.0
...
...

  Total internal partition sums for 70 - 500 K and
  500 - 1500 K coefficients for temperature interpolation
  for hitran molecules
$
 !...   H2O  --   161
  -.44405E+01, .27678E+00, .12536E-02,-.48938E-06
  -.94327E+02, .81903E+00, .74005E-04, .42437E-06
 !...   H2O  --   181
  -.43624E+01, .27647E+00, .12802E-02,-.52046E-06
  -.95686E+02, .82839E+00, .68311E-04, .42985E-06
 !...   H2O  --   171
  -.25767E+02, .16458E+01, .76905E-02,-.31668E-05
  -.57133E+03, .49480E+01, .41517E-03, .25599E-05
...
...

  Total internal partition sums for 70 - 500 K and
  500 - 1500 K coefficients for temperature interpolation
  for additional molecules
$
 !...HNO4  --  146                            ! derived from Toon
    -93323.15,1501.75154,-7.63597,0.01955      !160-350 K
    -1.36049E6, 12156.008, -37.79588,0.0483    !350-500 K
 !...C3H8  --  221
  .10000E+01, .0000E+00,.0000E+00, .0000E+00
  .10000E+01, .0000E+00,.0000E+00, .0000E+00
 !...  H2CO  --   126, taken from hitran-gas 20 (H2CO)
  -.11760E+03, .46885E+01,.15088E-01, .35367E-05
  -.11760E+03, .46885E+01,.15088E-01, .35367E-05


  Total internal partition sums for 70 - 500 K and
  500 - 1500 K coefficients for temperature interpolation
  for pseudo-line gas molecules
$
 !...ccl3f  f11                               ! from Toon
    -0.3529, 1.00617, -3.15636E-5, 4.90591E-8
    32.7266, 0.89325, 5.73225E-5, 6.49571E-8
 !...ccl2f2  f12                               ! from Toon
    2.70287 0.99566, -5.51294E-4, 3.26664E-6
   -1330.38301, 6.58174, -0.00826, 6.78855E-6
 !...chf2cl  f22                               ! from Toon
    -1.2063, 1.02228, -1.23158E-4, 2.11691E-7
```

```
    62.86447, 0.74045, 2.71348E-4, 4.48698E-8
...
...

   total internal partition sums at reference temperature 296 K
   for hitran molecules
$
  .174626E+03, .176141E+03, .105306E+04, .865122E+03
  .286219E+03, .576928E+03, .607978E+03, .354389E+04, .123528E+04, .714432E+04,
  .323407E+03, .376700E+04
  .348186E+04, .746207E+04, .364563E+04, .430647E+05, .212791E+05
  .499183E+04, .334938E+04, .344940E+04, .526595E+04, .307008E+05
  .107428E+03, .224704E+03, .112781E+03, .661209E+03, .236447E+03, .138071E+04
  .589908E+03, .117974E+04, .477061E+04
  .215726E+03, .452188E+03, .263998E+04
  .339730E+04, .157040E+04, .358252E+04
...
...

   total internal partition sums at reference temperature 296 K
   for additional molecules
$
    189178.416             ! HNO4 derived from Toon
   .100000E+01             ! C3H8
   .268388E+04             ! taken from hitran-gas 20 (H2CO)

   total internal partition sums at reference temperature 296 K
   for pseudo-line gas molecules
$
   2.959803E+02
   3.338342E+02
   2.960880E+02
   2.959858E+02
...
...

   State Energies  for hitran gases
     number of states
     state energies
     number of ground states
     hitran ground state number
$
 !...   H2O  --   161
   4
   0.0,1594.750,3151.630,3657.053
   1
   1
 !...   H2O  --   181
   2
   0.0,1588.279
   1
   1
 !...   H2O  --   171
...
```

```
...

   State Energies  for additional line-gases
     number of states
     state energies
     number of ground states
      ground state number
$
!...HNO4  --  146
   1
   0.
   1
   1
!...C3H8   --  221
...
...

   State Energies  for pseudo line-gases
     number of states
     state energies
     number of ground states
      ground state number
$
   !...ccl3f
   1
   0.
   1
   1
   !...ccl2f2
...
...
============================================================
```

3.2.3 Line-mixing data file

For a detailed description of this file see Part VI: 'Line mixing'.

```
============================================================
============================================================

   File with line-mixing data. This file is only necessary if $12.1 is set
   to 'T', i.e. line mixing is switched on.
   (y-coefficients, ...) ($3.4)

============================================================
```

3.2.4 Spectroscopic data files

Files with spectroscopic data of HITRAN molecules, additional molecules, and pseudo-lines. (The file-names have to be in the form: fXXXXX, where XXXXX is the wavenumber; the files are produced with the auxiliary program 'hitsort.f90') ($3.5)

3.2.5 Cross-section data files for heavy molecules

Files with cross-section data for the heavy molecules. (Only necessary if cross-section species are calculated.) For each molecule one binary direct-access data file is necessary and is produced with the auxiliary program 'hitX2bin.f90' from standard hitran cross-section files. The cross-section file-names are given in the file xfiles.dat which is in the same directory as the cross-section files (name given under $3.6).

3.3 Input files for atmospheric profiles

The altitudes of the profiles and the number of levels can be different from file to file. All profiles will be interpolated to the grid under $11.5 in the main input file. Be careful: if the altitude range of $11.5 extends the altitude ranges in the profile-files the values will also be extrapolated to the levels of $11.5! This can sometimes lead to implausible values. So care should be taken that the altitude range of $11.5 includes all ranges given in the profiles.
All input-profiles are assumed to be at the same geolocation which is given under $11.3-11.4 in the main input file.

3.3.1 p,T profiles

```
============================================================

   File with p,T profiles. The filename is given under $2.1
   in the main input file.
============================================================

Number of levels
$
  50


Altitude [km]
$
    0.0,       1.0,       2.0,       3.0,       4.0,
    ...

Pressure [hPa]
$
  1.013E+03, 8.988E+02, 7.950E+02, 7.012E+02, 6.166E+02,
  ...

Temperature [K]
$
    288.20,    281.70,    275.20,    268.70,    262.20,
    ...
============================================================
```

3.3.2 p,T gradient profiles

```
============================================================

   File with p,T gradient profiles. The filename is given
   under $2.2 in the main input file.
```

```
============================================================
Number of levels
$
 50

Level altitudes [km]
$
       0.0,       1.0,       2.0,       3.0,       4.0,
     ...

Pressure lat. gradient [hPa/km], i.e. the gradient is parallel to
  (along) the latitude circles.
  Positive to the east and negative to the west.
$
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
  ...

Pressure lon. gradient [hPa/km], i.e. the gradient is parallel to
  (along) the longitude circles (meridians).
  Positive to the south and negative to the north.
$
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
  ...


Temperature lat. gradient [K/km], i.e. the gradient is parallel to
  (along) the latitude circles.
  Positive to the east and negative to the west.
$
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
  ...

Temperature lon. gradient [K/km], i.e. the gradient is parallel to
  (along) the longitude circles (meridians).
  Positive to the south and negative to the north.
$
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
  ...
============================================================
```

3.3.3 vmr profiles

```
============================================================

   File with vmr profiles. The filename is given under $2.3
   in the main input file.
   There must exist a profile for each molecule which
   should be calculated under $8.6 of the main input file.
============================================================
Number of levels
$
  50

Level altitudes [km]
```

```
$
       0.0,       1.0,       2.0,       3.0,       4.0,
       ...

Number of gas profiles given below (at least for the gases which have to be
considered in all microwindows)
$
  2

Hitran gas number
Profile [ppmv]

H2O
$
   1
 7.745E+03 6.071E+03 4.631E+03 3.182E+03 2.158E+03 1.397E+03 9.254E+02 5.720E+02
 ...
CO2
$
   2
 3.300E+02 3.300E+02 3.300E+02 3.300E+02 3.300E+02 3.300E+02 3.300E+02 3.300E+02
 ...


============================================================
```

3.3.4 vmr gradient profiles

```
============================================================

   File with vmr - gradient profiles. The filename is given under $2.4 in
   main input file.
   There must exist a profile for each molecule which
   should be calculated under $8.6 of the main input file
   (even if its gradients are zero).
============================================================
Number of levels
$
10

Level altitudes [km]
$
0.0,   9.0,      16.0,      24.0,      31.0,      39.0,
      48.0,      57.0,      66.0,     120.0


Number of gas gradient profile pairs given below
 (at least for the gases which have to be
  considered in all microwindows)
$
 2

Hitran gas number
```

```
Profile [ppmv/km]

H2O   lat. gradient [ppmv/km], i.e. the gradient is parallel to
  (along) the latitude circles.
  Positive to the east and negative to the west.
$
   1
 3.375E-01 3.375E-01 4.050E-03 2.400E-03 2.000E-03 1.500E-03
 1.800E-03 2.200E-03 2.200E-03 2.200E-03

H2O   lon. gradient [ppmv/km], i.e. the gradient is parallel to
  (along) the longitude circles (meridians).
  Positive to the south and negative to the north.
$
   1
 3.375E-01 3.375E-01 4.050E-03 2.400E-03 2.000E-03 1.500E-03
 1.800E-03 2.200E-03 2.200E-03 2.200E-03

CO2   lat. gradient [ppmv/km], i.e. the gradient is parallel to
  (along) the latitude circles.
  Positive to the east and negative to the west.
$
   2
 0.000E-02 0.000E-02 0.000E-02 0.000E-02 0.000E-02
 0.000E-02 0.000E-02 0.000E-02 0.000E-02 0.000E-02

CO2   lon. gradient [ppmv/km], i.e. the gradient is parallel to
  (along) the longitude circles (meridians).
  Positive to the south and negative to the north.
$
   2
 0.000E-02 0.000E-02 0.000E-02 0.000E-02 0.000E-02
 0.000E-02 0.000E-02 0.000E-02 0.000E-02 0.000E-02
============================================================
```

3.3.5 continuum profiles

```
============================================================

   File with continuum profiles. The filename is given under $2.5 in
   main input file. (For each microwindow one profile has to be given.)
============================================================
aerosol absorption and scattering
coefficient profiles (for each microwindow) [km-1]


Number of levels
$
  50

Level altitudes [km]
$
```

```
       0.0,       1.0,       2.0,       3.0,       4.0,
     ...

Number of microwindows for which profiles are given below
$
 2

Continuum absorption coefficient profiles (for each microwindow) [km-1]

Microwindow number
Profile

$
 1
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 ...

$
 2
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 ...


Continuum scattering coefficient profiles (for each microwindow) [km-1]

Microwindow number
Profile

$
 1
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 ...

$
 2
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 ...
============================================================
```

3.3.6 Vibrational temperature or non-LTE/LTE population ratio profiles

```
============================================================

   File with vibrational temperature or population ratio profiles.
   The filename is given under $2.6 in
   main input file.
============================================================

Number of levels
$
```

```
  50

Level altitudes [km]
$
       0.0,       1.0,       2.0,       3.0,       4.0,
     ...

Vibrational temperatures (F),  population ratios (T)
$
  F

Total number of following profiles
$
  1

Species
Vibrational state
Vibrational temperatures or population ratios

co2  2 (vib state 01101)
$
 021
 2
 2.8820E+02 2.8170E+02 2.7520E+02 2.6870E+02 2.6220E+02 2.5570E+02 2.4920E+02
 ...

============================================================
```

3.3.7 Vibrational temperature or non-LTE/LTE population ratio gradient profiles

```
============================================================

   File with vibrational temperature or population ratio gradient profiles.
   The filename is given under $2.7 in
   main input file.
============================================================
Number of levels
$
  50

Level altitudes [km]
$
       0.0,       1.0,       2.0,       3.0,       4.0,
     ...

Vibrational temperatures (F),  population ratios (T)
$
  F

Total number of following latitude/longitude profile-pairs
$
```

```
  1

Species
Vibrational state
Vibrational temperature gradients

co2  2 (vib state 01101) lat. gradient [K(or 1)/km], i.e. the gradient is parallel to
  (along) the latitude circles.
  Positive to the east and negative to the west.
$
 021
 2
 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2
  ...
co2  2 (vib state 01101)  lon. gradient [K(or 1)/km], i.e. the gradient is parallel to
  (along) the longitude circles (meridians).
  Positive to the south and negative to the north.
$
 021
 2
 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2 1.000E-2
 ...
============================================================
```

3.3.8 Isotope abundance profiles

```
============================================================

   File with isotope abundance profiles.
   The filename is given under $2.8 in
   main input file.
============================================================


The isotope (relative) abundance profiles for all isotopes of all hitran gases:

Number of levels for gas: 1
$
 1

Altitude levels for this gas [km]
$
 1.0

Isotope abundances on the levels
$ iso 1
   0.997317
$ iso 2
   0.00199983
$ iso 3
   0.000372
$ iso 4
```

```
   0.00031069

Number of levels for gas: 2
$
 1

 ...
 ...
============================================================
```

3.3.9 Broadband aerosol number density, mode-radius and -width profiles

```
============================================================

  File with broadband-aerosol profiles:
  number densities, mode-radii, mode-widths.
  The filename is given under $2.10
  in the main input file.
============================================================

Number of altitude levels
$
  4

Altitude [km]
$
  0.0  22.0  25.0  120.0

Broadband-aerosol number density [particles/cm-3]
$
  0.0  10.0  0.0 0.0


The following input data is only necessary if the KOPRA internal Mie-model is used:

Number of modes for distribution function (1 or 2)
$
  1

Mode-radius for mode 1 [micrometer]
$
  0.2   0.2  0.2  0.2

Mode-width for mode 1
$
  0.4   0.4  0.4  0.4



The following input data is only necessary if 2 modes are considered:

Mode-radius for mode 2 [micrometer]
$
```

```
   0.9   0.9  0.9  0.9

Mode-width for mode 2
$
  0.4 0.4 0.4 0.4

Weight for mode 1
 (range: 0.0 - 1.0)
$
  1.0
============================================================
```

3.3.10 Broadband aerosol altitude and wavenumber dependent refraction indices

```
============================================================

  File with broadband-aerosol altitude and wavenumber
  dependent refraction indices.
  The filename is given under $2.11
  in the main input file.
============================================================

Number of altitude levels
$
  2

Altitude [km]
$
  0.0  120.0



The following section is repeated (number of levels) times:

Number of wavenumber grid points for refraction indices:
$
  1691

Wavenumber, real-part, imaginary part of refraction index
$
   482.12 2.172E+00 3.333E-01
   485.97 2.121E+00 4.082E-01
   489.83 2.077E+00 4.928E-01
   493.69 2.010E+00 5.676E-01
   497.54 1.917E+00 6.039E-01
    ...

Number of wavenumber grid points for refraction indices:
$
  1691

Wavenumber, real-part, imaginary part of refraction index
$
```

```
   482.12 2.172E+00 3.333E-01
   485.97 2.121E+00 4.082E-01
   489.83 2.077E+00 4.928E-01
   493.69 2.010E+00 5.676E-01
   497.54 1.917E+00 6.039E-01
    ...


============================================================
```

3.3.11 Broadband aerosol altitude and wavenumber dependent cross-sections

```
============================================================

  File with broadband-aerosol altitude and wavenumber
  dependent cross-sections.
  The filename is given under $2.12
  in the main input file.
============================================================
Number of altitude levels
$
  2

Altitude [km]
$
  0.0  120.0


The following section is repeated (number of levels) times:


Number of wavenumber grid points for broadband-aerosol
  cross-sections:
$
  5

Wavenumber [cm-1], absorption cross-section [cm2/particle],
  extinction cross-section [cm2/particle]
$
 500.0  1.0e-17 1.2e-17
 955.0  1.0e-16 1.1e-16
 960.0  1.0e-18 1.2e-18
 1500.0 1.0e-18 1.3e-18
 2000.0 1.0e-18 1.4e-18

Number of wavenumber grid points for broadband-aerosol
  cross-sections:
$
  5

Wavenumber [cm-1], absorption cross-section [cm2/particle],
  extinction cross-section [cm2/particle]
$
```

```
 500.0  1.0e-17 1.2e-17
 955.0  1.0e-16 1.1e-16
 960.0  1.0e-18 1.2e-18
 1500.0 1.0e-18 1.3e-18
 2000.0 1.0e-18 1.4e-18



============================================================
```

3.4 Input file for AILS-function

```
============================================================

   File with (apodized) instrumental line shape (AILS) function per microwindow
   The filename is given under $2.9 in the main input file.
============================================================

 The apodized instrumental line shape (ails) function for
 each microwindow on the wavenumber fine grid.

Wavenumber distance between the ails points  [cm-1]
$
  0.0005

Number of grid points (must be odd!)
$
  303

Ails functions per microwindow
$  mw 1
    -0.01928
    -0.01878
    -0.01849
   ...

============================================================
```

3.5 Output files for spectra and derivative spectra

The file name convention for spectra and derivative spectra is:
For spectra:
directory/abcd...xxyyzz
For derivative-spectra of offset, scale, wavenumber-shift, ils-phase, ils-apolin, and line-of-sight:
directory/abcd...offxxyyzz
directory/abcd...scaxxyyzz
directory/abcd...shixxyyzz
directory/abcd...phaxxyyzz
directory/abcd...apoxxyyzz
directory/abcd...losxxyyzz
For derivative-spectra of temperature, temperature-gradient, pressure, and continuum:

directory/abcd...Txxyyzzvvv
directory/abcd...Tgraxxyyzzvvv
directory/abcd...pxxyyzzvvv
directory/abcd...aerxxyyzzvvv
For derivative-spectra of vmr, vmr-gradient, and vibrational temperature:
directory/abcd...vmrxxyyzzuuvvv
directory/abcd...vmrgraxxyyzzuuvvv
directory/abcd...Tvibxxyyzzuuvvv
Where:
directory/abcd... = directory and file-initials as given under $3.1 and 3.2$ xx = microwindow number yy = observation geometry number zz = sub-microwindow number uu = species number (in case of vmr and vmr-gradient) uu = vibrational state number (in case of Tvib) vvv = (altitude) retrieval-parameter number (e.g. altitude level)

```
============================================================

   Spectra and derivative spectra on the fine wavenumber (monochromatic) grid.
   The file name directory and initials are given under $3.1 and under $3.2
============================================================
#
#     number of wavenumber grid-points
  wavenumber          spectral value [nW/cm2srcm-1]
  wavenumber          spectral value [nW/cm2srcm-1]
  wavenumber          spectral value [nW/cm2srcm-1]
  wavenumber          spectral value [nW/cm2srcm-1]
     ...                     ...
============================================================
```

3.6 log- and error-files

If $3.3==1 the log-file is written to screen or file as selected under $3.4. The warnings and errors are written into the log-file and into an extra error-file with the filename of $3.5.