Updates SFIT4 version 1.0.20

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many others of the NDACC-IRWG

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NDACC Spa, June 2023

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NOTE Spectroscopic parameters have to correspond to each other, the calculation of extra parameters will affect to 'Voigt' lineshape.

The lineshapes

When choosing fw.lineshape=4 several other parameters can be optionally added:

fw.lineshape.sdv switch on speed depency

fw.linemixing=T Linemixing (only 1st order, [Ros75])

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```
aux = gal sdv lm
aux.gal.nr = 2
aux.gal.files = 014_HF/14_hit16_Galatry.txt
                015_HCL/15_hit16_Galatry.txt
aux.sdv.nr = 1
aux.sdv.files = 005_CO/05_hit16_SDV.txt
aux.lm.nr = 1
aux.lm.files = 002_CO2/002_CO2.hit16_LM1ST.par
```

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Note:the test_case directories are still work in progress.

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Be aware when copying of hbin.ctl, hbin.input, isotope.ctl or reference.prf files.

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Preferably use provided tools and templates.

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create_testcase creates a testcases from a running directory. Reads all the files needed for running hbin and sfit4 and packs them into in tarball release.tgz. This can be sent to the maintainers along with description of the problem.

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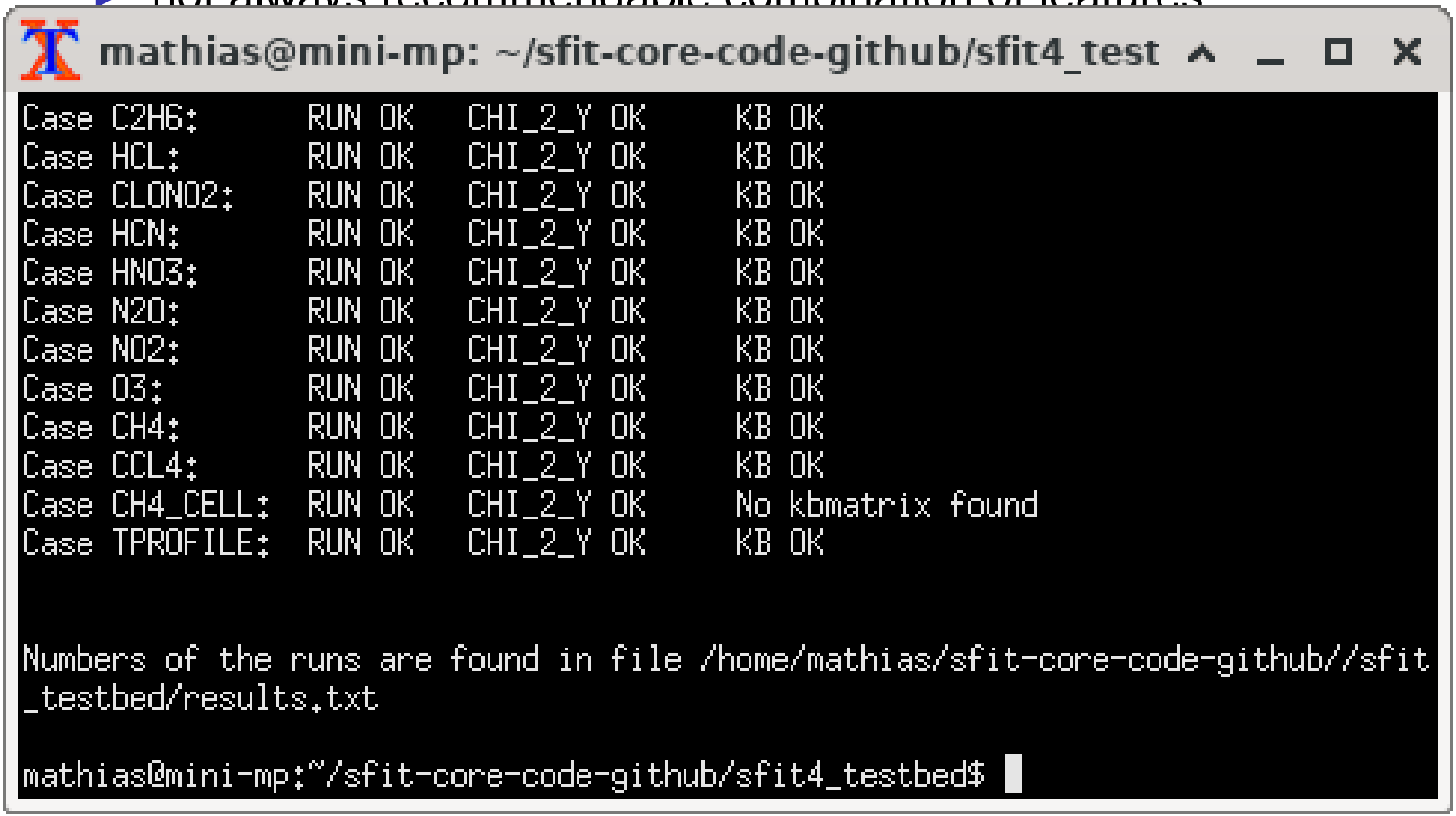

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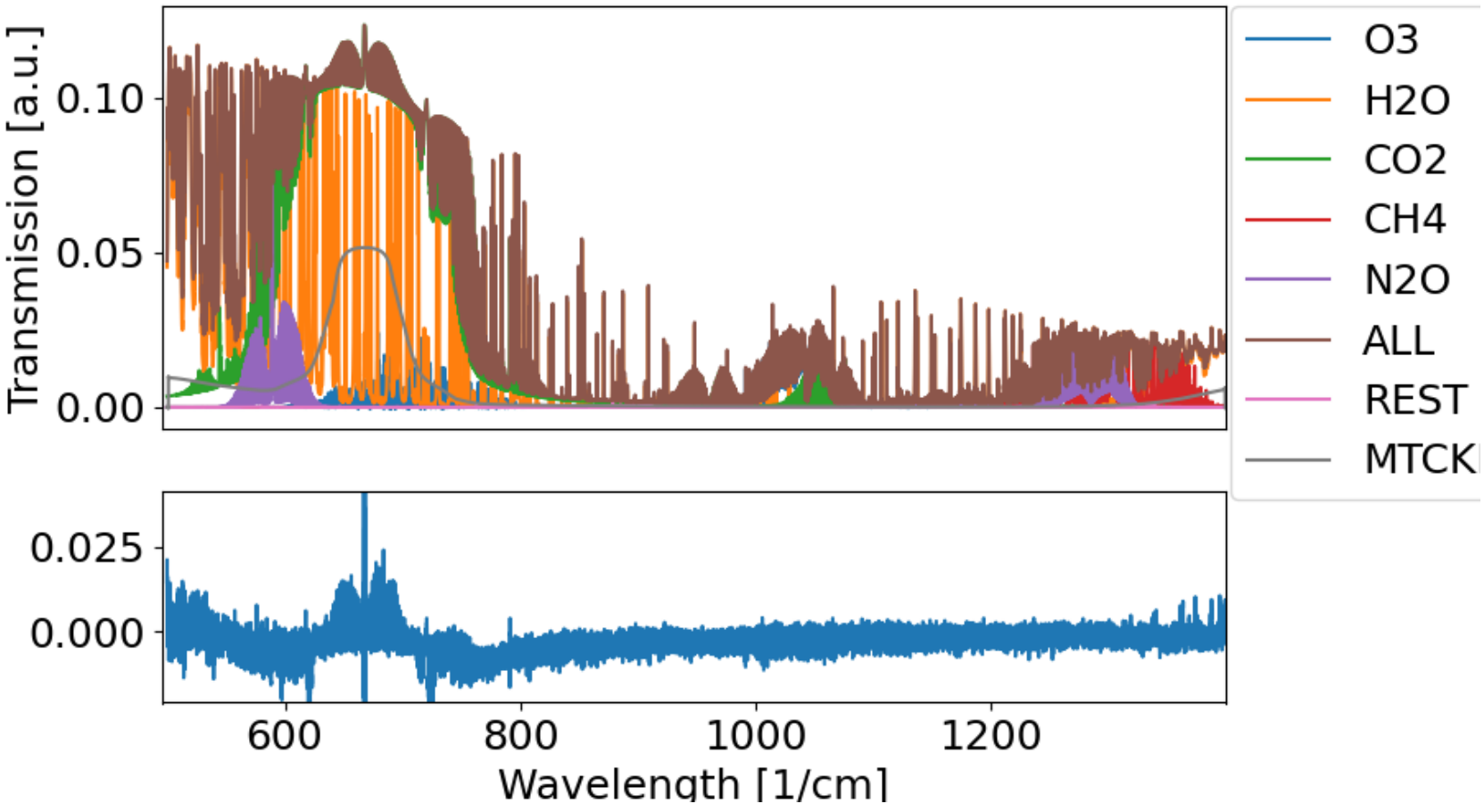
- all output should be ok.
- More detailed output can be found in results.txt

Implementation of continuum absorption

- planned for the next major upgrade (SFIT4 v1.1 or v2.0)
- implemented the AER radiation code (www.aer.com) in the version 3.0
- MT-CKD code is available from https://github.com/AER-RC/MT_CKD
- described in [MPM+12]
- SFIT4 v1.1 is already used by the Toronto group and recent results are at the poster of Lukas Heizmann
- Tests and finalization are ongoing. Code available on request for testing and validating.

Implementation of continuum absorption



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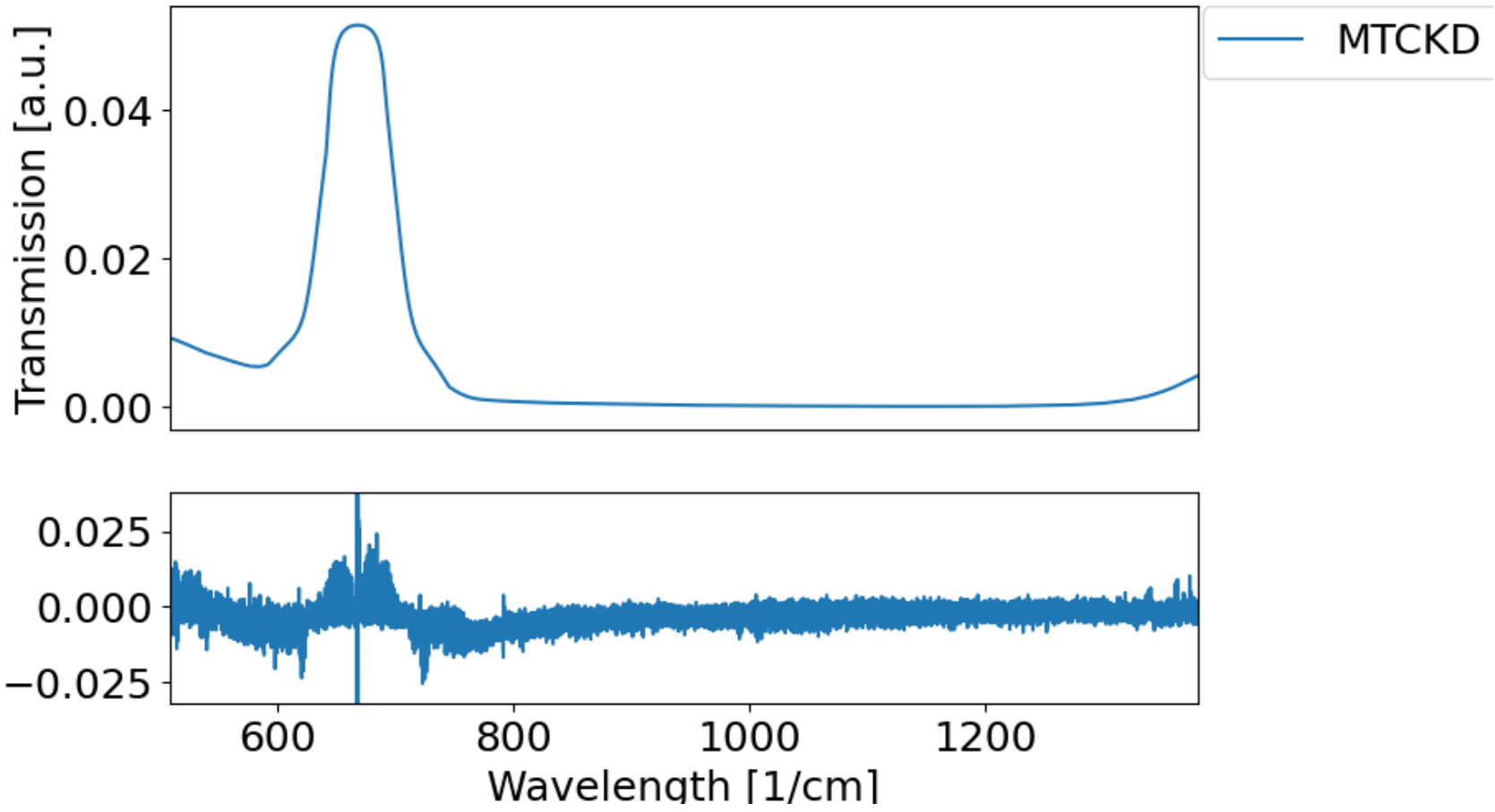

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Thanks for your attention

[BWB11] Chris D. Boone, Kaley A. Walker, and Peter F. Bernath. An efficient analytical approach for calculating line mixing in atmospheric remote sensing applications. *J. Quant. Spectrosc. Radiat. Transfer*, 112:980 – 989, 2011.

[Gal61] Louis Galatry. Simulateanous Effect of Doppler and Foreign Gas Broadening on Spectral Lines. *Phys. Rev.*, 122(4), 1961.

[MPM+12] Eli J. Mlawer, Vivienne H. Payne, Jean-Luc Moncet, Jennifer S. Delamere, Matthew J. Alvarado, and David C. Tobin. Development and recent evaluation of the MT_CKD model of continuum absorption. *PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A-MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES*, 370(1968):2520–2556, JUN 13 2012.

[Ros75] PW Rosenkranz. Shape of 5 mm Oxygen Band In Atmosphere. *IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION*, AP23(4):498–506, 1975.