Spectroscopy and gas absorption at mm/submm wavelengths: Recent progress from ground-based observatories

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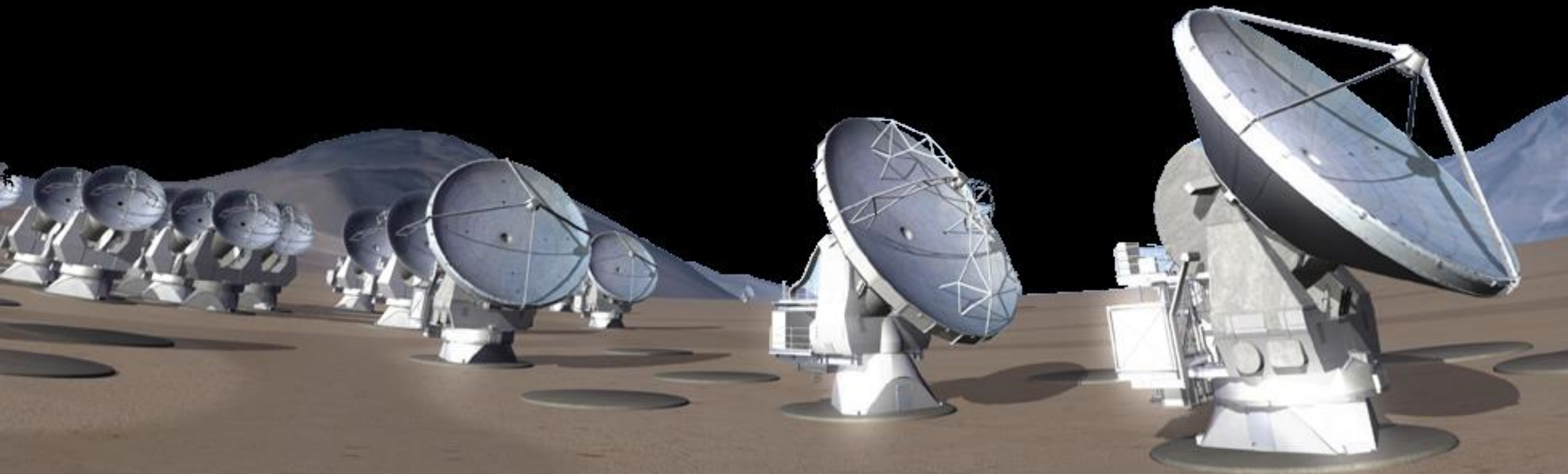


ASPECTS IN ATMOSPHERIC RT MODELS:

- Background
    - CBR
    - Astronomical source
    - Sea,
    - Land(s),…
- Scattering
    - Single
    - Multiple
    - Shapes of scatterers
    - Refraction indexes
- Polarization
    - Stokes parameters
    - E, B fields
- Spectroscopy
    - Main gases
    - Minor gases
    - Isotopologues
    - Vibrationally excited states
- Vertical profiles
    - Latitude, longitude
    - Day / Night
    - Season
- (Pseudo)continua
    - Collision induced
    - Syncrotron
    - Other
- Special effects
    - Zeeman
    - Stark
    - Other
- Geometry
    - 1D
    - 2D
    - 3D

- Operational constraints:
    - Spectral resolution
    - Fast codes for real time processing
    - Accuracy

3D atmospheric radiative transfer equation (coordintates: z, μ=cos(θ), φ)

$$\mu \frac{dI(z,\mu,\varphi)}{dz} = K(z,\mu,\varphi)I(z,\mu,\varphi) -$$

$$- \int_{-1}^{1} d\mu' \int_{0}^{2\pi} d\varphi' Z(z,\mu,\varphi,\mu',\varphi')I(z,\mu',\varphi') - \sigma(z,\mu,\varphi)B[T(z)]$$

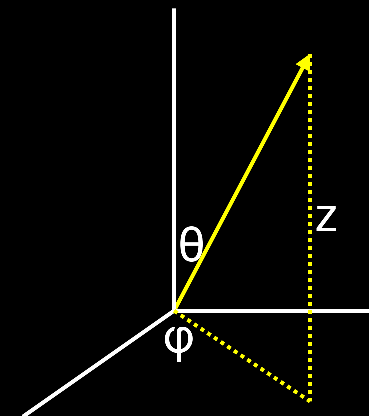
$I=(I,Q,U,V)^T$ Radiation field (Stokes column vector)

K 4x4 extinction matrix

Z 4x4 phase matrix (describing scattering)

σ 4x1 emission column vector

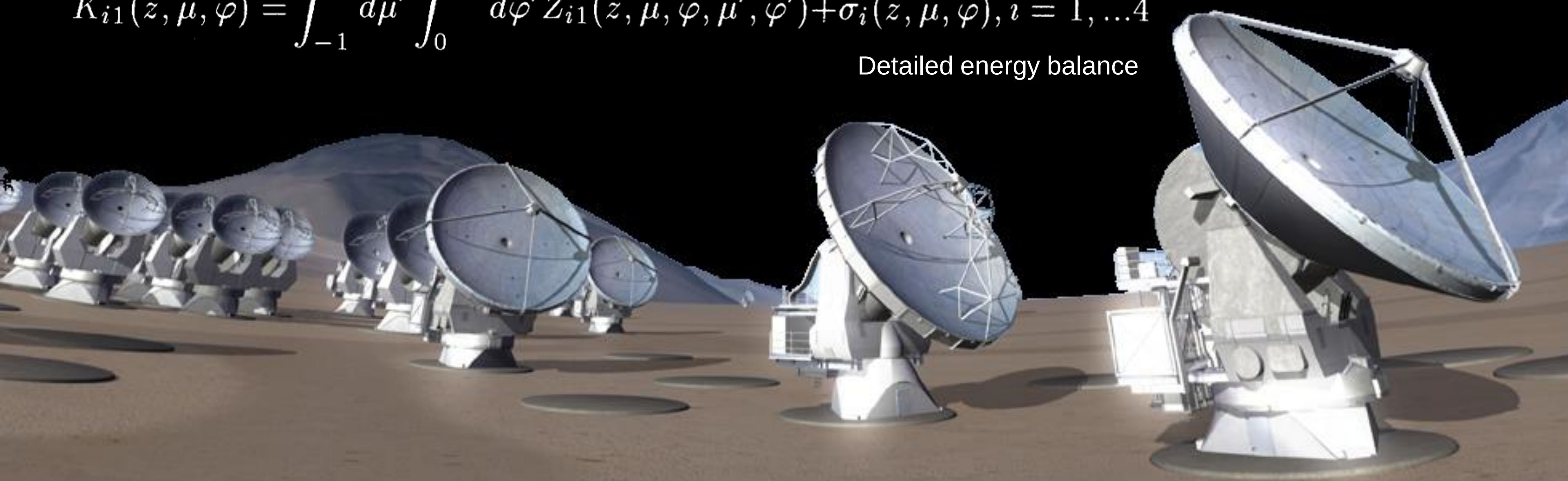
B Blackbody radiance at temperature T (due to LTE)



Frequency dependence is implicit

$$K_{i1}(z,\mu,\varphi) = \int_{-1}^{1} d\mu' \int_{0}^{2\pi} d\varphi' Z_{i1}(z,\mu,\varphi,\mu',\varphi') + \sigma_i(z,\mu,\varphi), i = 1,...4$$

Detailed energy balance



Another way of performing the radiative transfer: Propagate fields and take the average of the Poynting’s vector

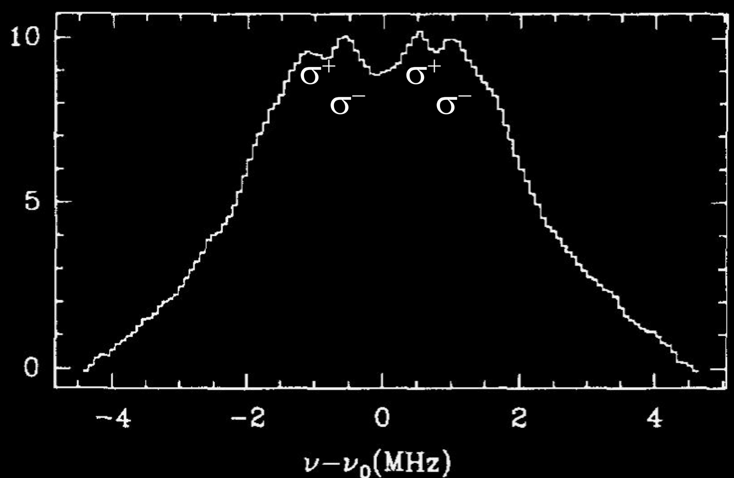
$$E_z = \exp[ikz(I + N_z 10^{-6})]E_0$$

We use this approach to study polarization introduced in the gas phase by Zeeman splitting on O_2 lines

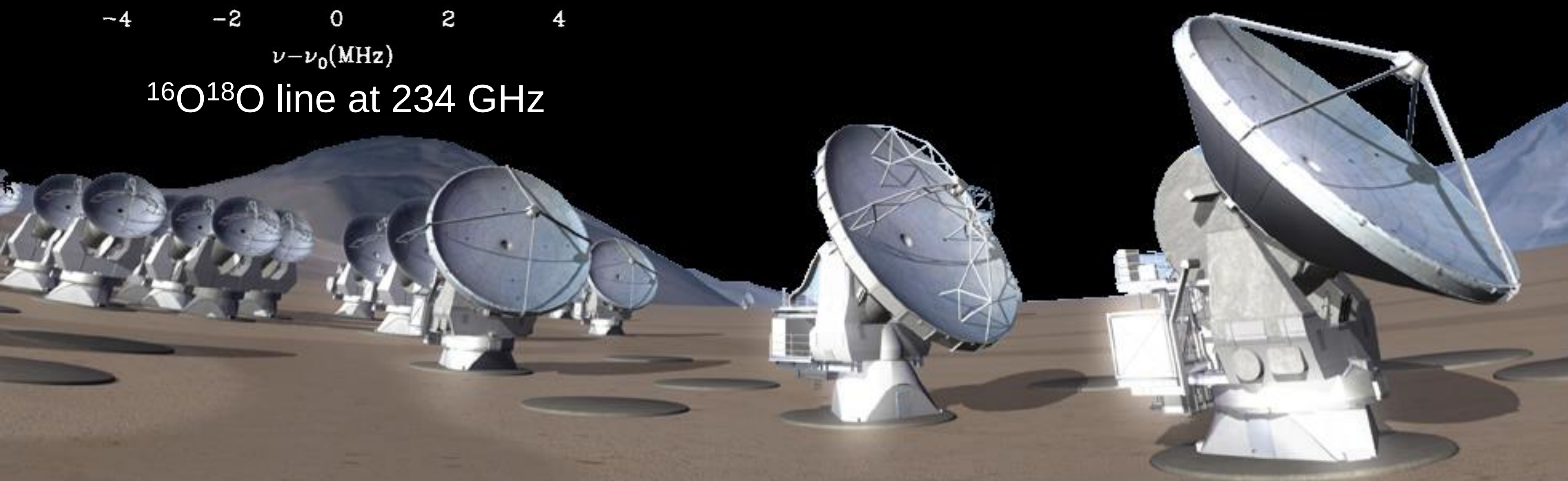
Refractivity is a complex matrix

$$\begin{bmatrix} N_0 \sin^2\phi + (N_+ + N_-)\cos^2\phi & -i(N_+ - N_-)\cos\phi \\ i(N_+ - N_-)\cos\phi & N_+ + N_- \end{bmatrix}$$

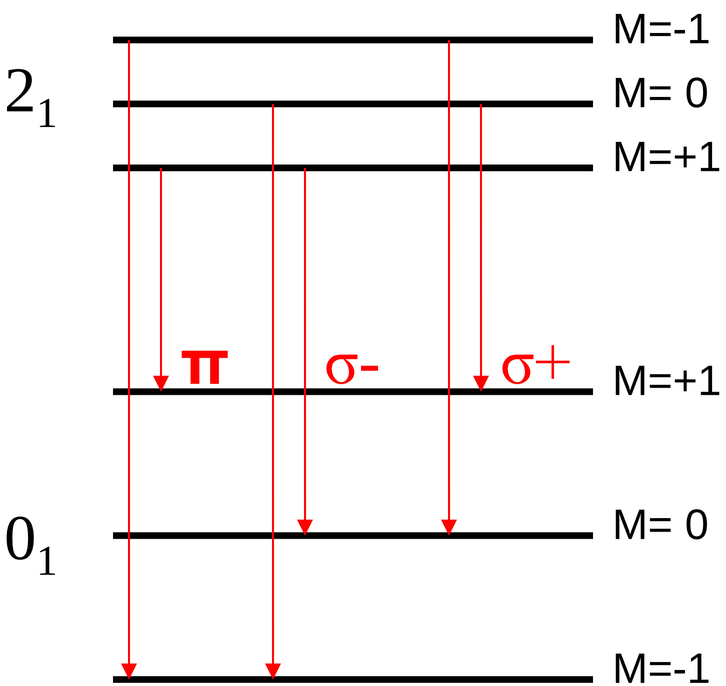
Angle between direction of propagation and geomagnetic field



$^{16}O^{18}O$ line at 234 GHz



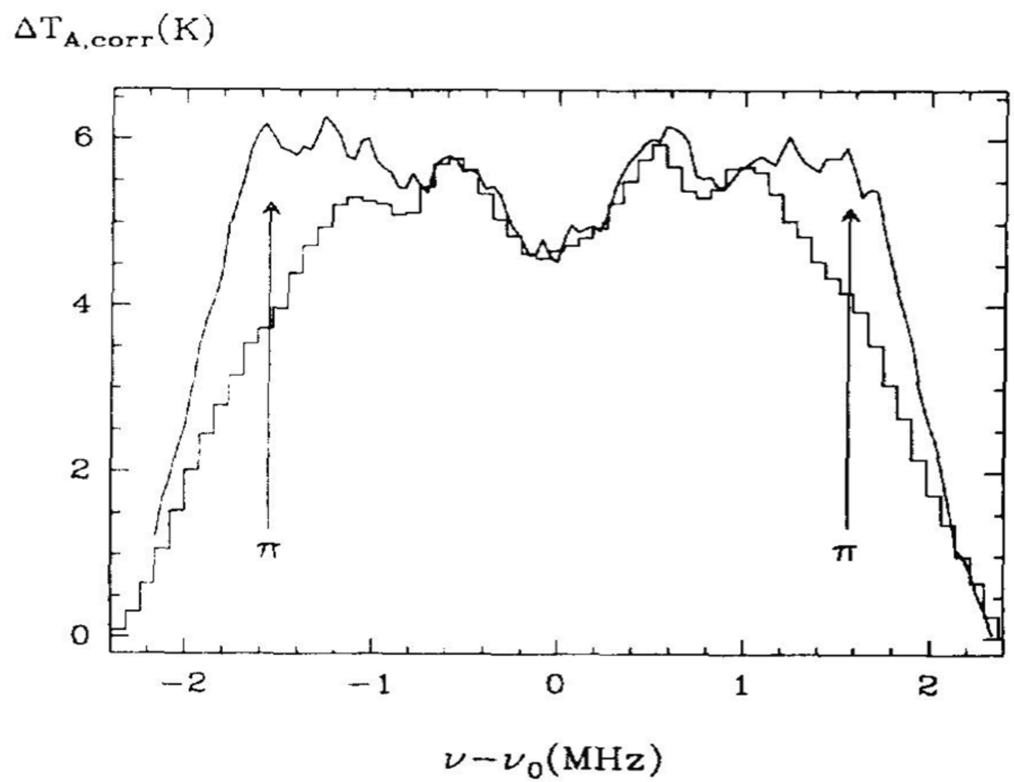
N_J $^{16}O^{18}O$ $v=0$



$$\Delta\nu(GHz) = 14.015 \cdot 10^{-6} H_{\mu T}(M_u + 2M_l)$$

Transitions π (ΔM=0): Radiation linearly polarized in the direction of the geomagnetic field.

Transitions σ (ΔM=±1): Radiation circularly polarized (right-hand or left-hand in the plane perpendicular to the direction of the geomagnetic field.



We should expect differencies in the line profile depending on the line of sight, the type of polarization detected, and the orientation of our detector with the geomagnetic field.

Under clear atmosphere →

$$\frac{dI_\nu(s')}{d\tau_\nu} = -I_\nu(s') + B_\nu(T[s'])$$

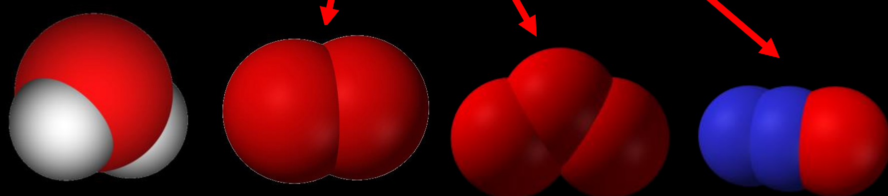
s'	coordinate along the path;
$S_\nu = \epsilon_\nu / \kappa_\nu$	source function;
$d\tau_\nu = \kappa_\nu ds$	differential opacity.

$$(\kappa_\nu)_{lu} = \frac{8\pi^3 N\nu}{3hcQ}\left(e^{-E_l/kT} - e^{-E_u/kT}\right) \cdot |< u \mid \mu \mid l >|^2 \, f(\nu, \nu_{l\to u})$$

gas-phase absorption

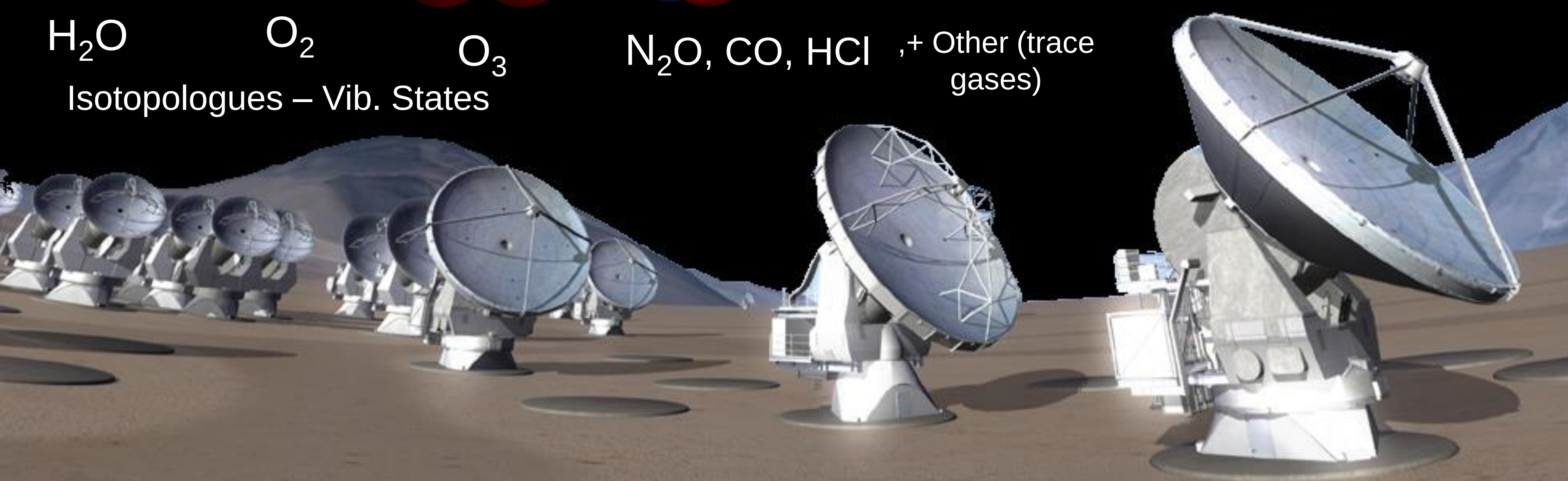
Line-by-line absorption

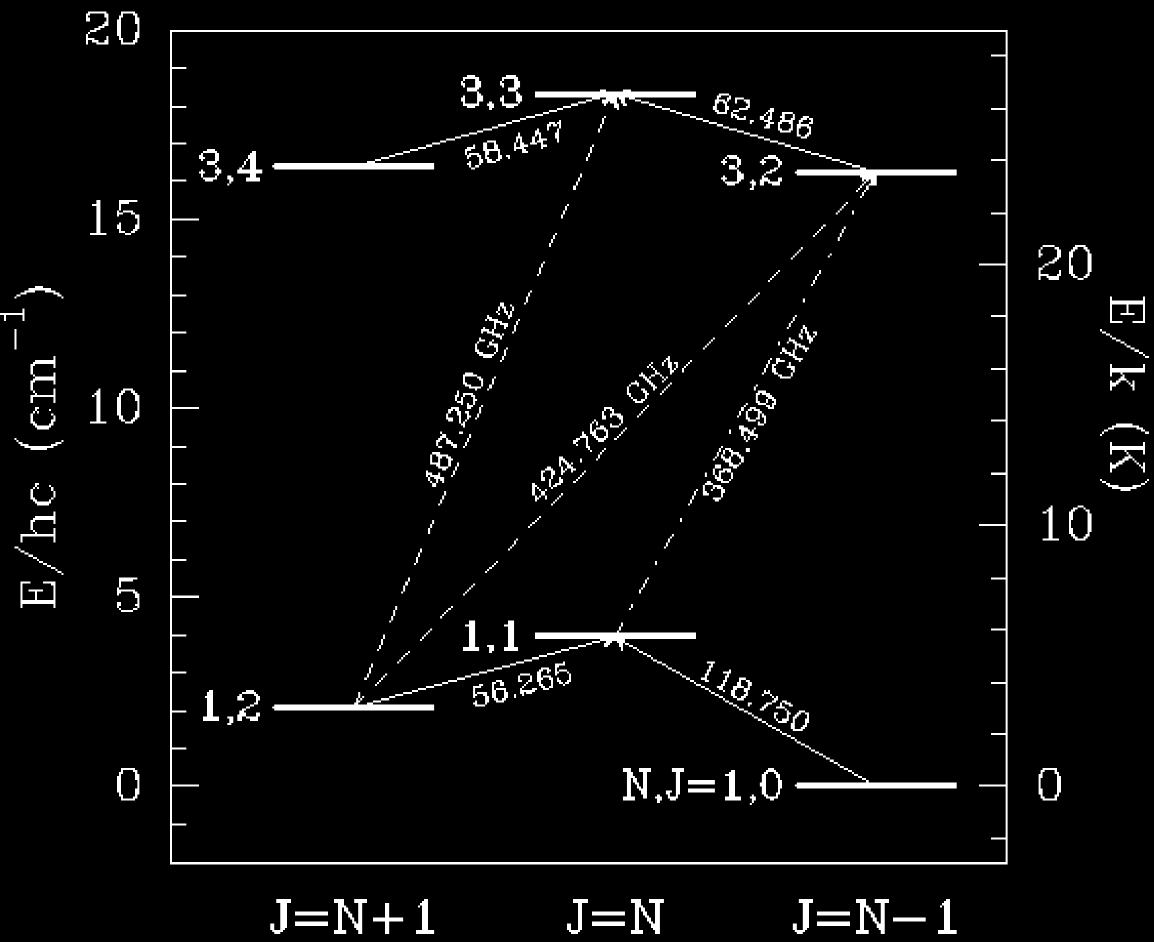
Collison-induced absorption (CIA)



H_2O O_2 O_3 N_2O, CO, HCl ,+ Other (trace gases)

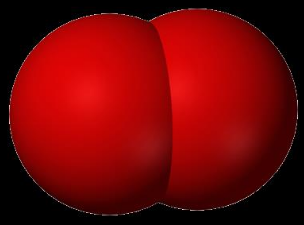
Isotopologues – Vib. States





Lowest rotational transitions

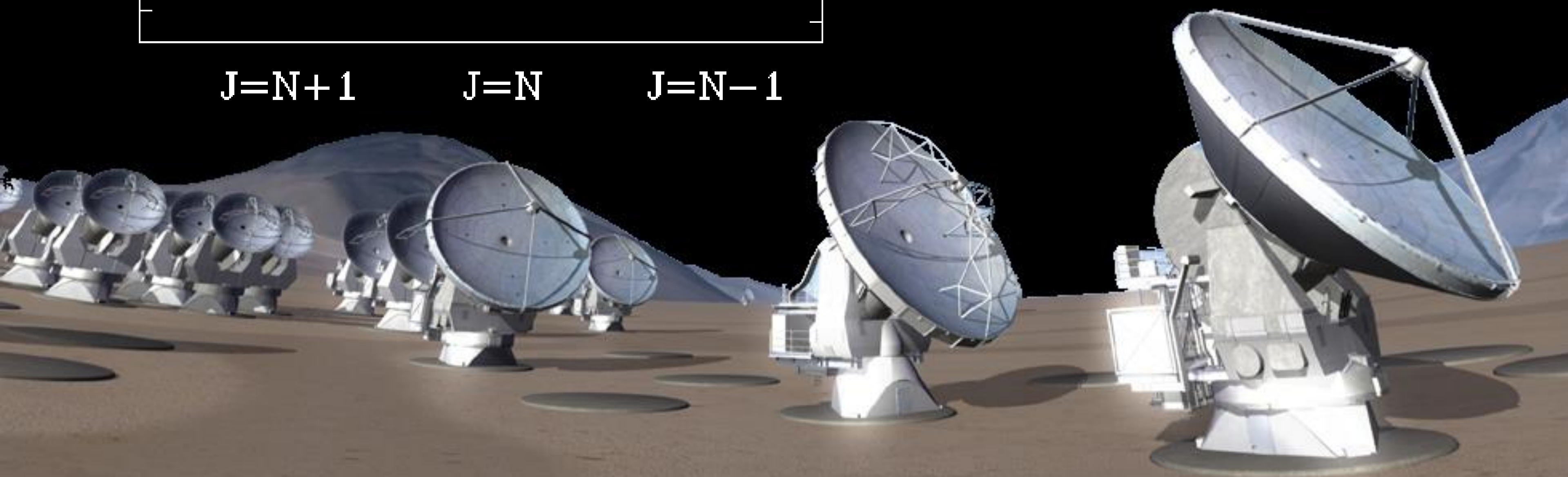
(M1)

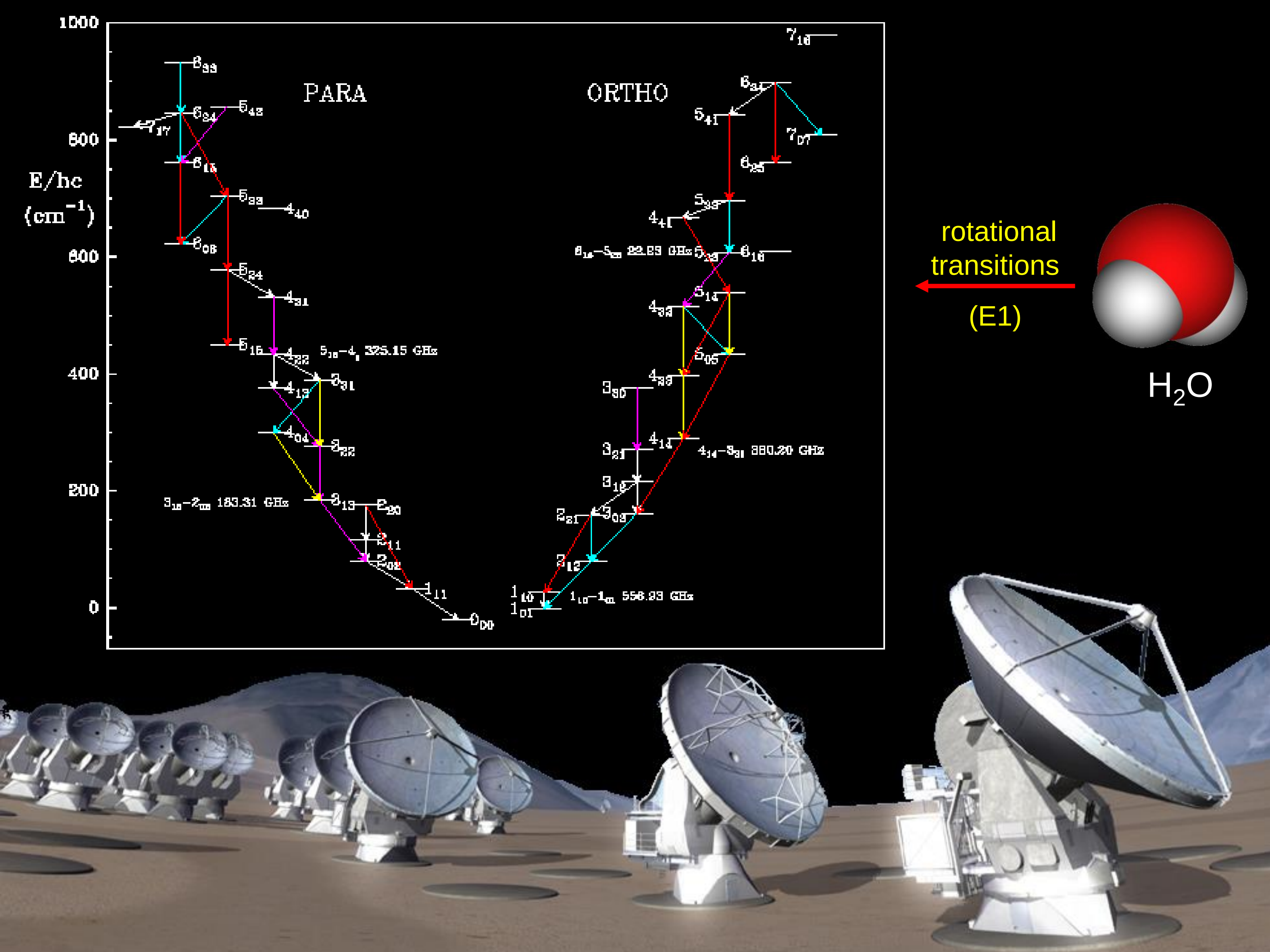


O_2

Paramagnetic molecule: Coupling of its permanent dipole moment with and external magnetic field causes ZEEMAN SPLITTING.

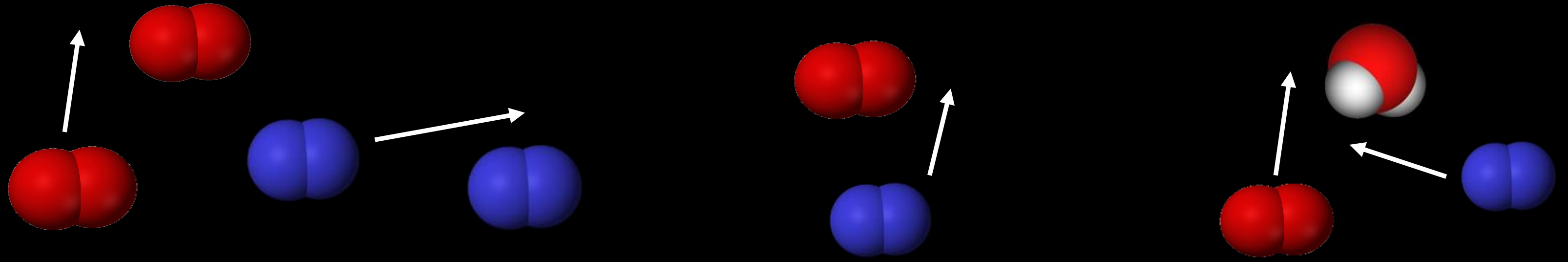
Modeling this effect is rather complex because of anisotropy, polarization, etc…

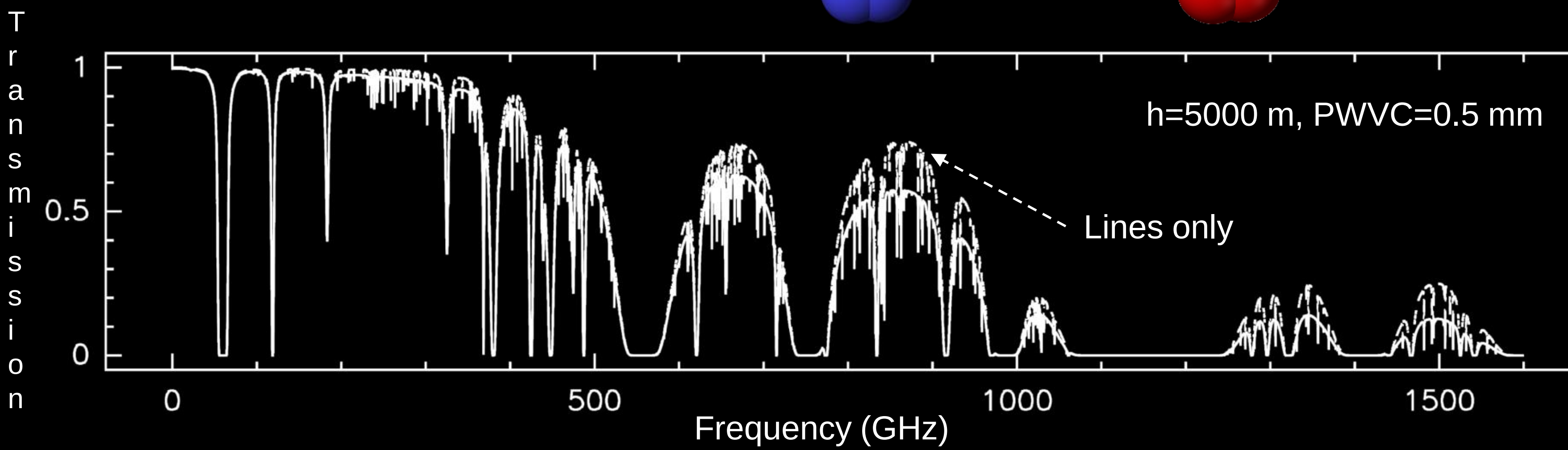


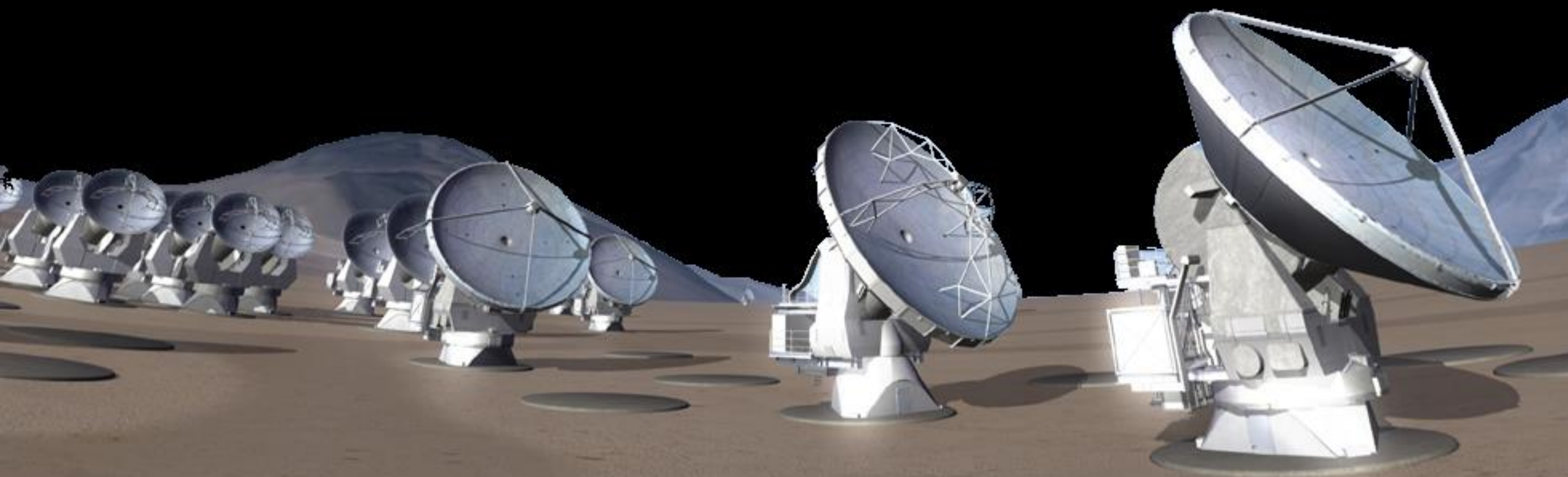


PARA
ORTHO
E/hc
(cm^{-1})
1000
800
600
400
200
0
$6_{16}-5_{23}$ 22.23 GHz
$5_{15}-4_{22}$ 325.15 GHz
$3_{13}-2_{20}$ 183.31 GHz
$4_{14}-3_{21}$ 380.20 GHz
$1_{10}-1_{01}$ 556.93 GHz
rotational
transitions
(E1)
H_2O

Collision-Induced absorption produces excess of sky opacity in the submm







SINCE ATMOSPHERIC RT MODELS ARE DESIGNED FOR SPECIFIC APPLICATIONS, EACH ONE OVERLOOKS DIFFERENT ASPECTS

- Background
  - CBR
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  - Single
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- Phase effects
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  - 1D
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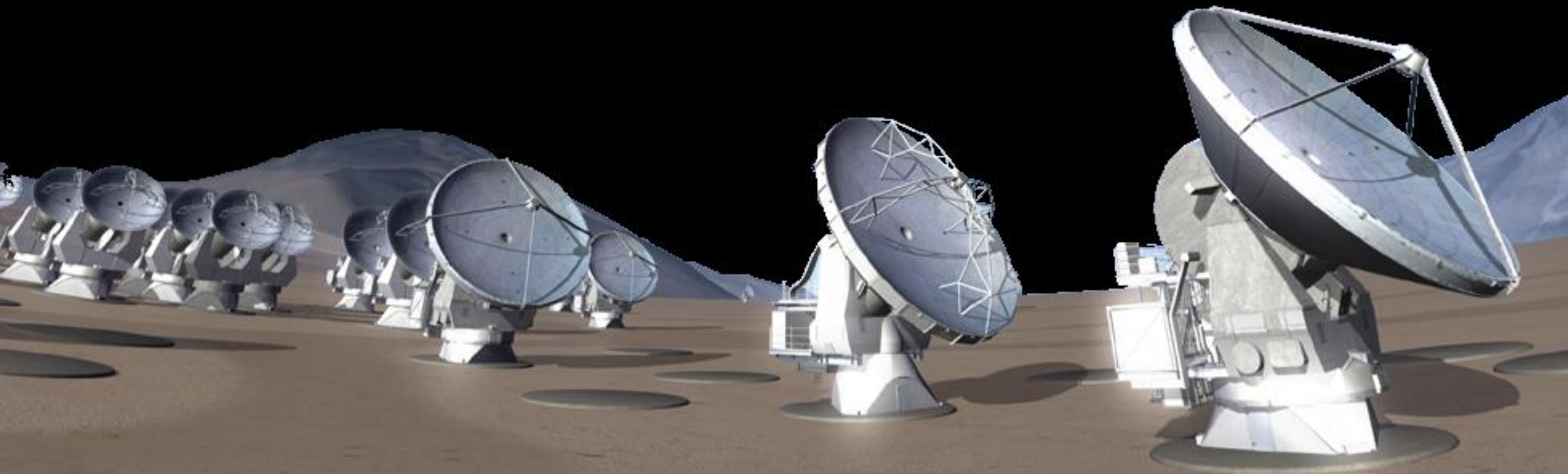
GROUND-BASED OBSERVATORIES FOR ATMOSPHERE RT STUDIES:

- It is not their primary goal.
- However the have to deal with the artmosphere and need a good model.
- Up to date instrumentation is available.
- The instrumentation can be replaced.
- Weight and size is not a big problem
- Wide Frequency coverage.
- Extremely fine frequency resolution
- Good stability is now possible as well as clean spectra.
- Specific calibrations for atmospheric measurements now available.
- Interest in the phase (real part of refraction index).



Atmospheric Phase fluctuations

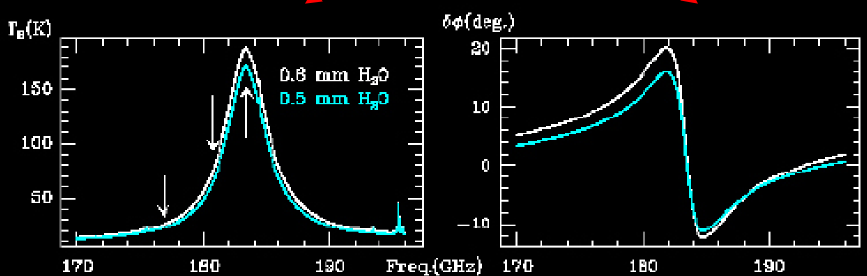
$$(\kappa_\nu)_{lu} = \frac{8\pi^3 N\nu}{3hcQ}\left(e^{-E_l/kT} - e^{-E_u/kT}\right) \cdot |< u \mid \mu \mid l >|^2 f(\nu, \nu_{l\rightarrow u})$$

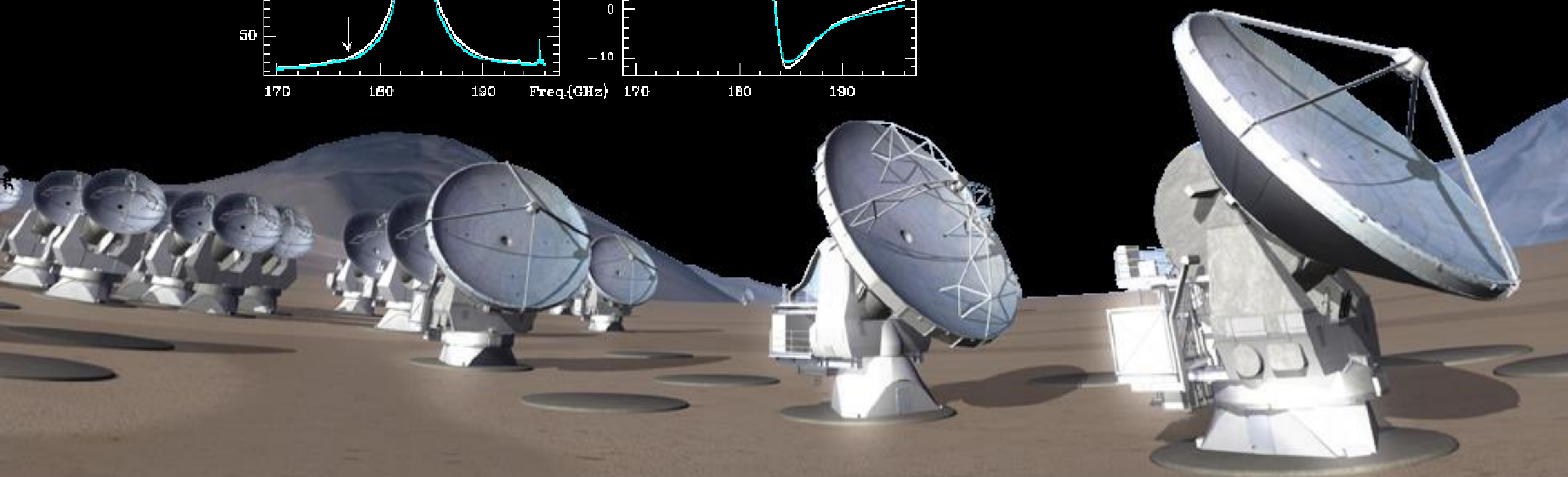
κ_ν Is a complex number

$$\mathcal{F}(\nu, \nu_{u\leftrightarrow l}) = \frac{\nu}{\pi\nu_{u\leftrightarrow l}}\left[\frac{1 - i\delta}{\nu_{u\leftrightarrow l} - \nu - i\Delta\nu} + \frac{1 + i\delta}{\nu_{u\leftrightarrow l} + \nu + \Delta\nu}\right] \quad (1)$$

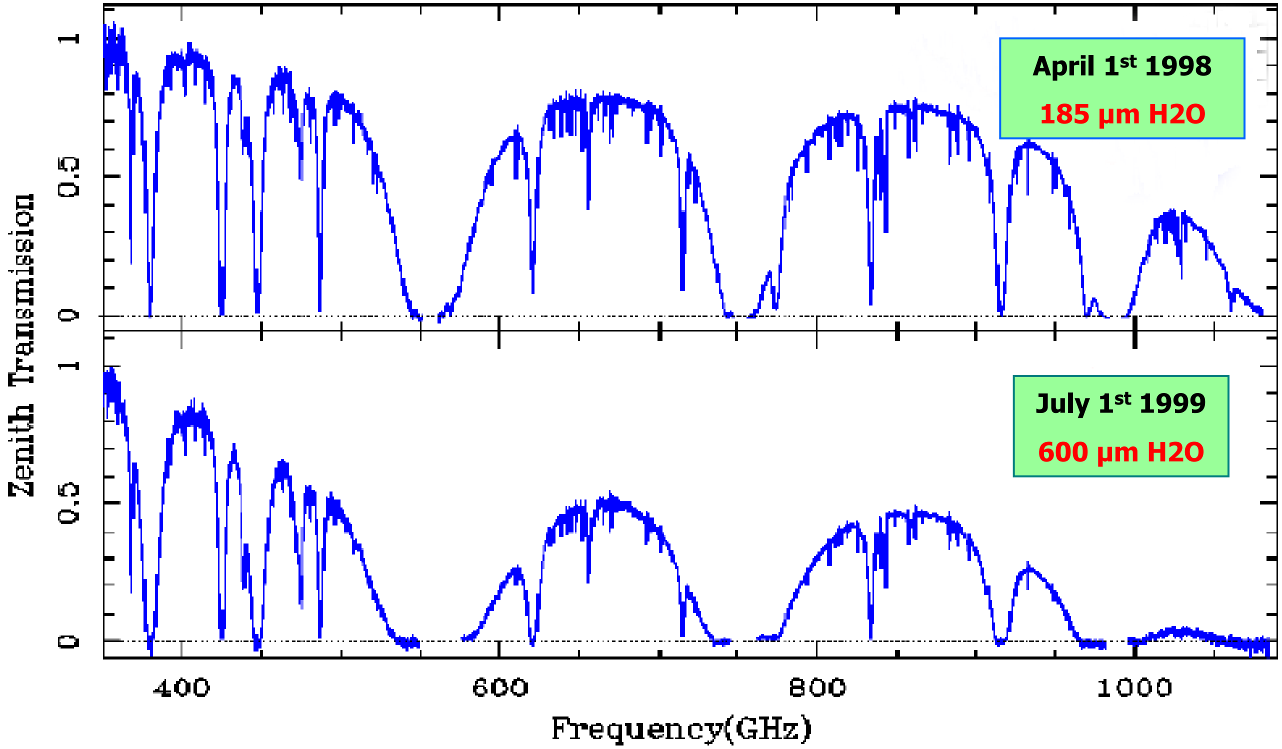
Imaginary part (absorption)

Real part (phase delay or pathlength variation)





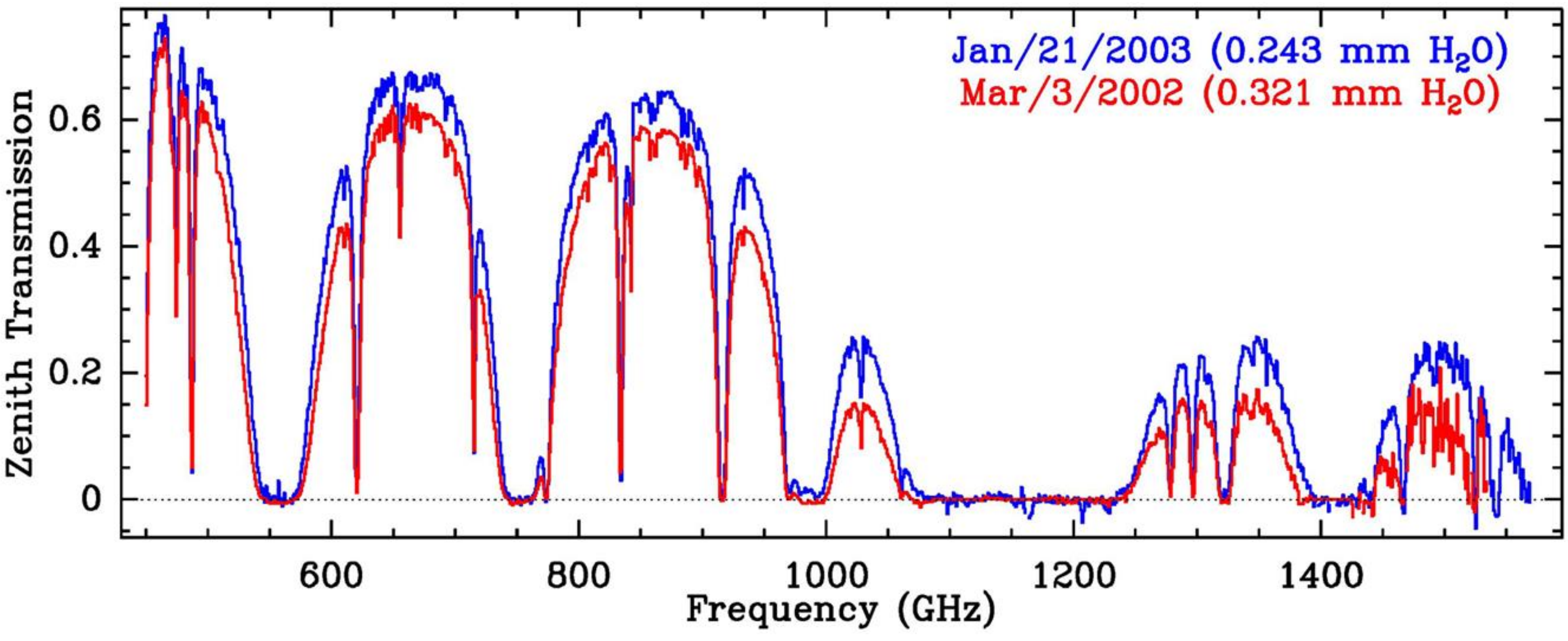

Mauna Kea (4200 m, -5 ºC), Hawai'i
Hapuna Beach (0 m, 25 ºC, Hawai'i)



Aproach to study the Collision Induced Absorption

- Use well calibrated scans under dry and stable conditions.
- Ground temperature at CSO altitude ~ 270 +/- 3 K
- Ground pressure at CSO altitude ~ 620 +/- 1.5 hPa

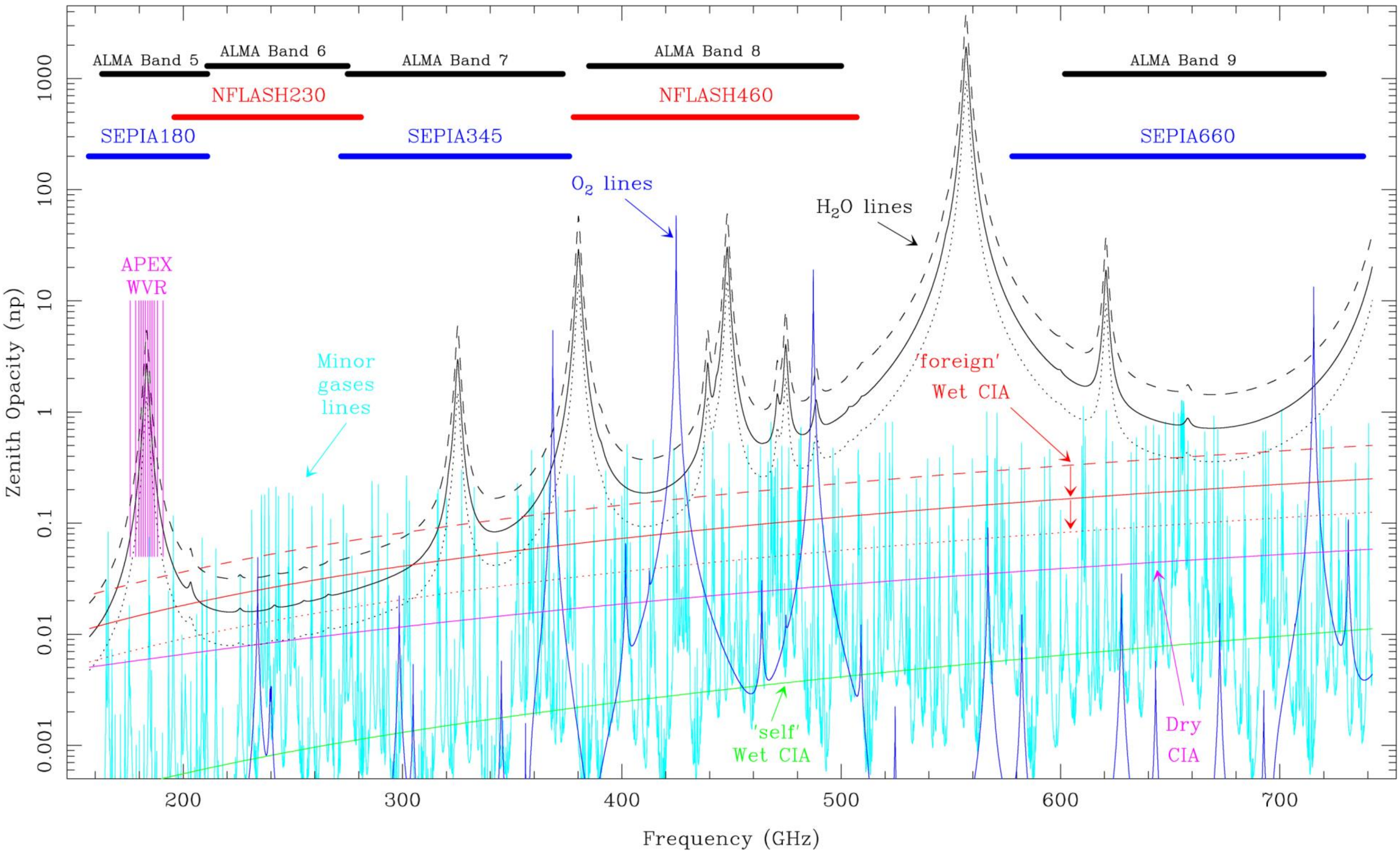
The“dry” absortion is basically the same (within 1-3 %). The remaining opacity is proportional to the PWV. The PWV can be determined from strong water lines.



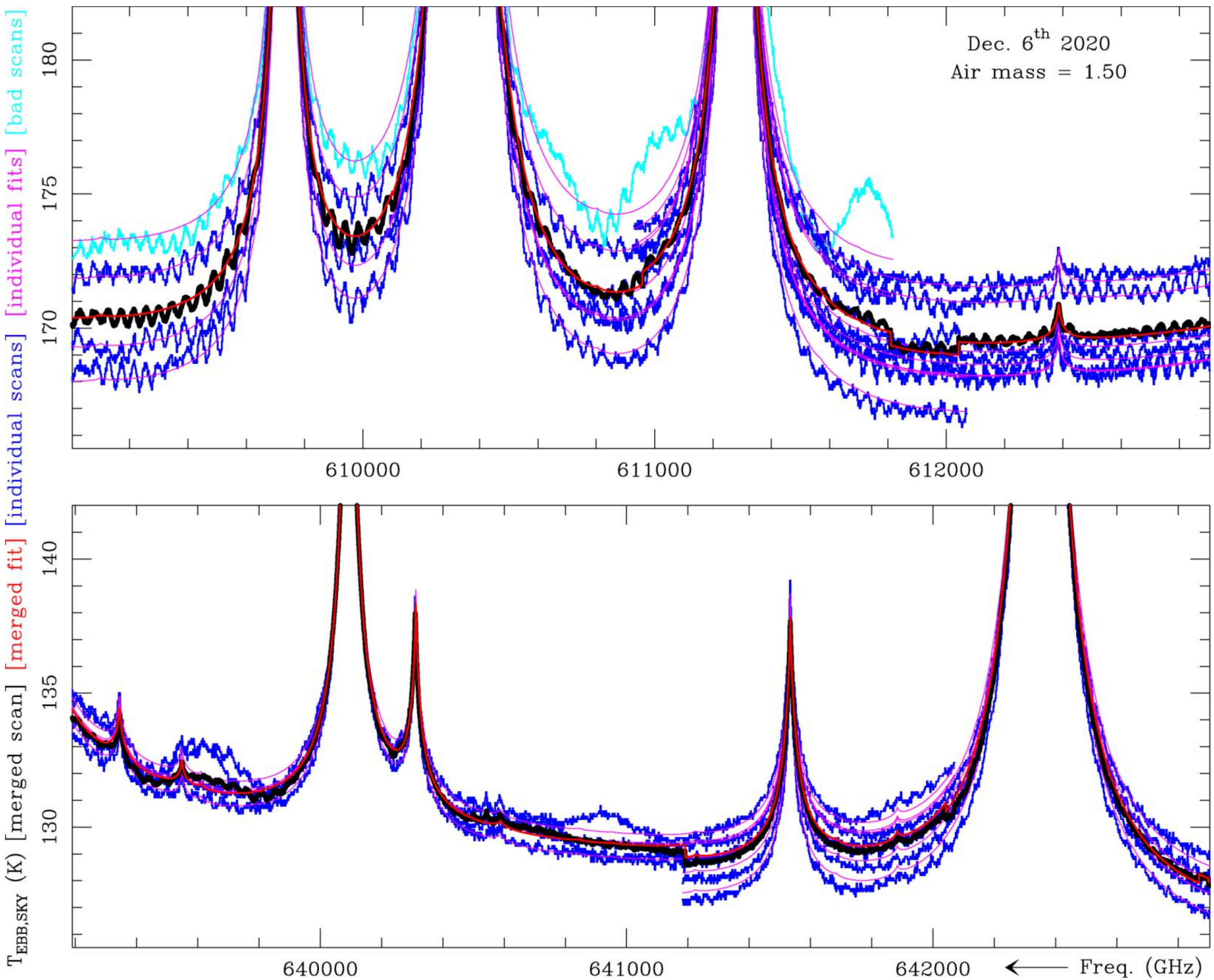

PETZL

Since our ATM model is used in ALMA, APEX was the perfect choice for a study to validate and refine it.

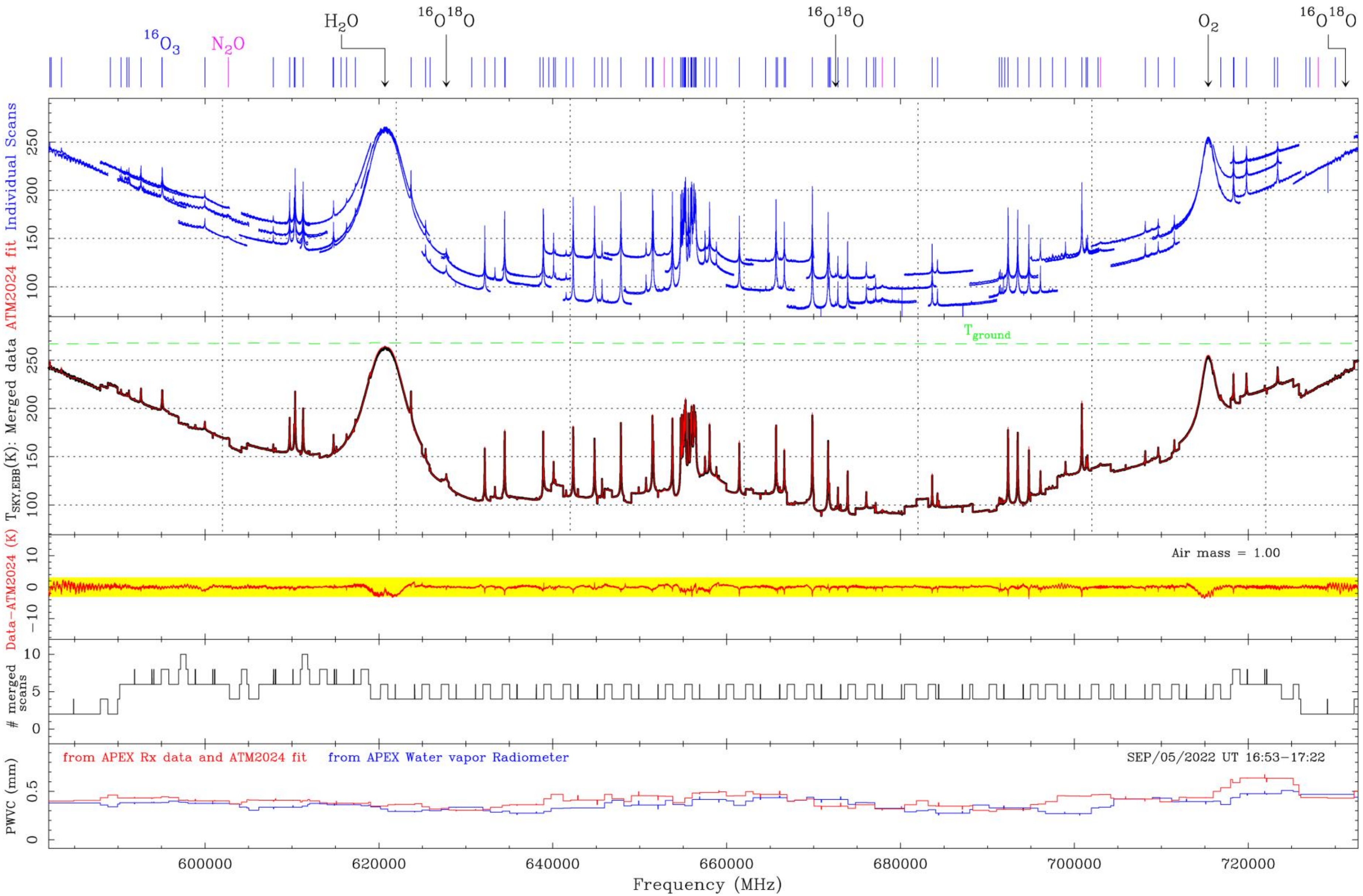
Atmospheric model (150-750 GHz) and available APEX instrumentation



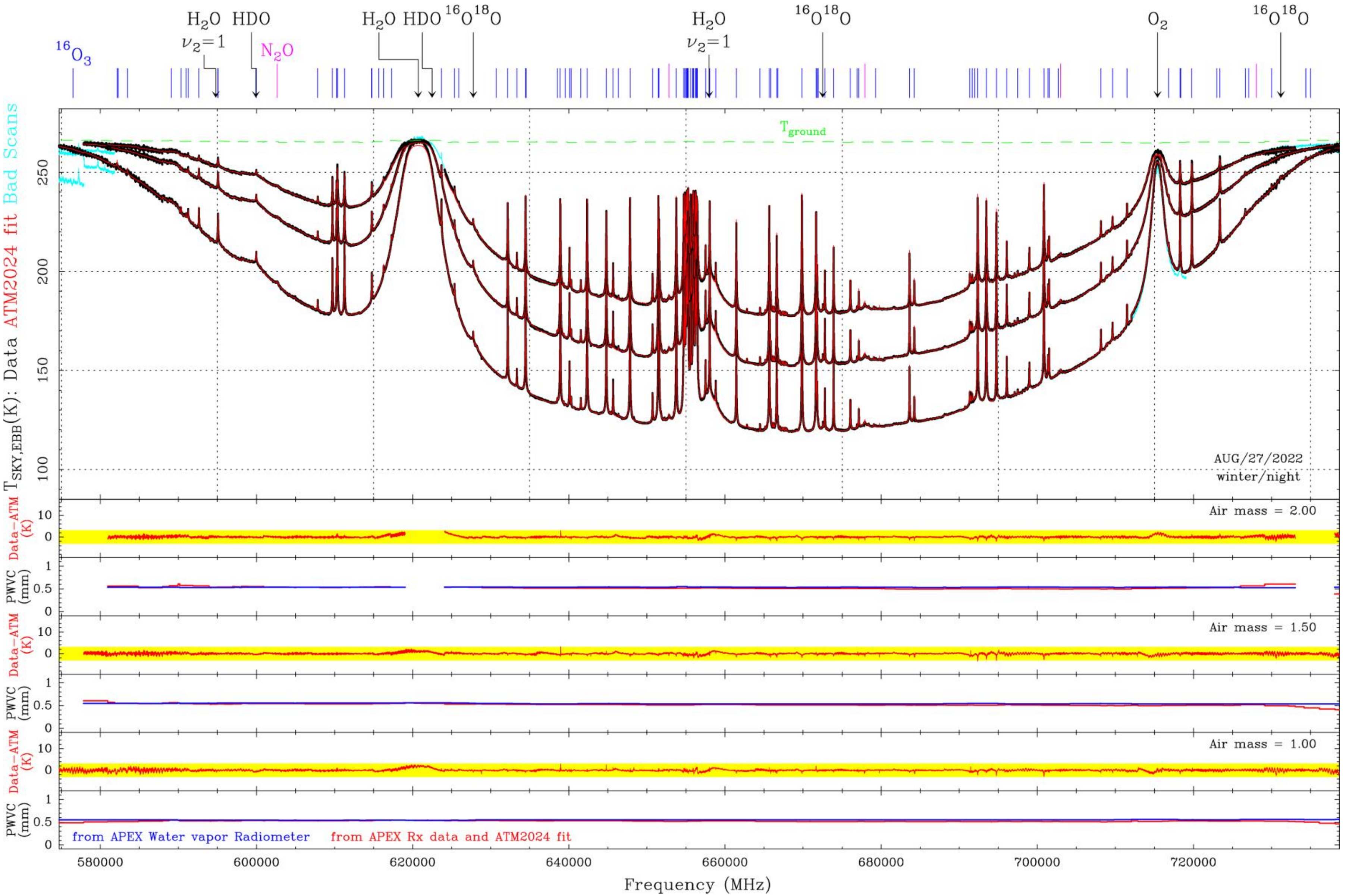
Good Scans are **fitted individually** and then **added.** **Bad scans are discarded.**



In some observing sessions the atmosphere was not very stable (here Sep. 5th 2022)



…but in other sessions the atmosphere was very stable



O_3

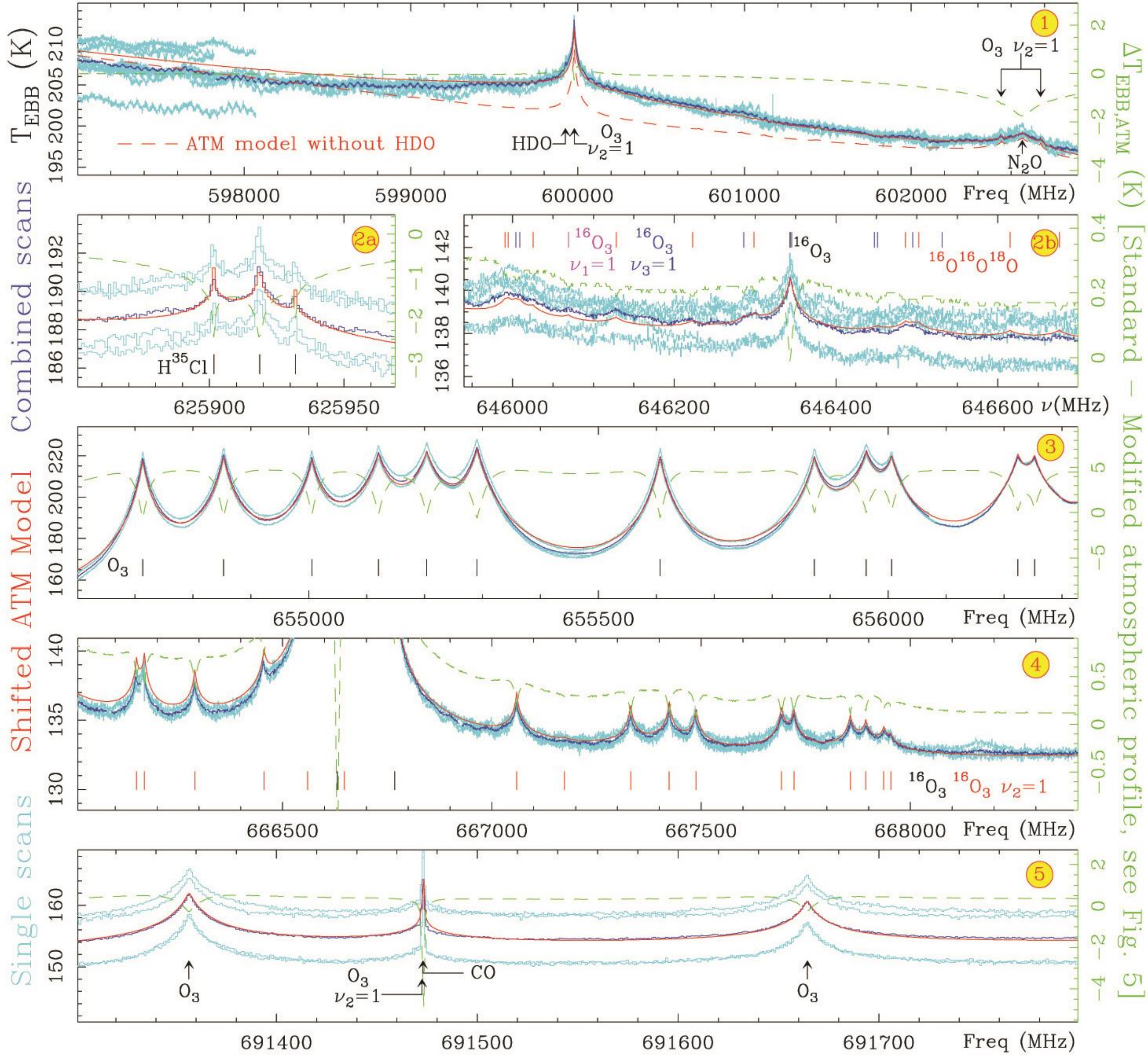
O_3 isot.

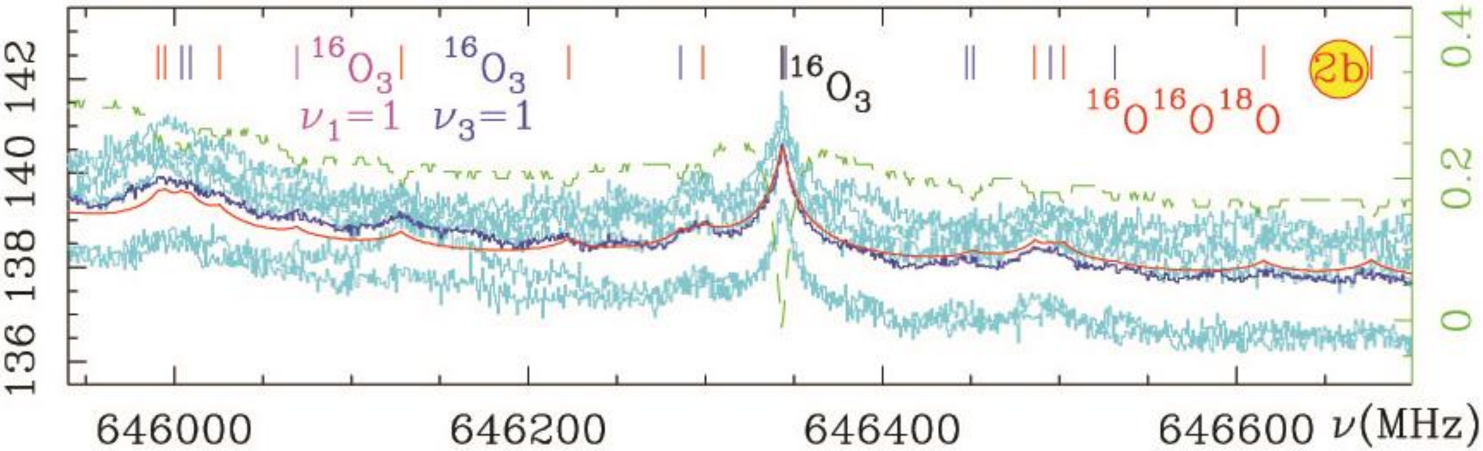
O_3 vib

N_2O

HCl

CO





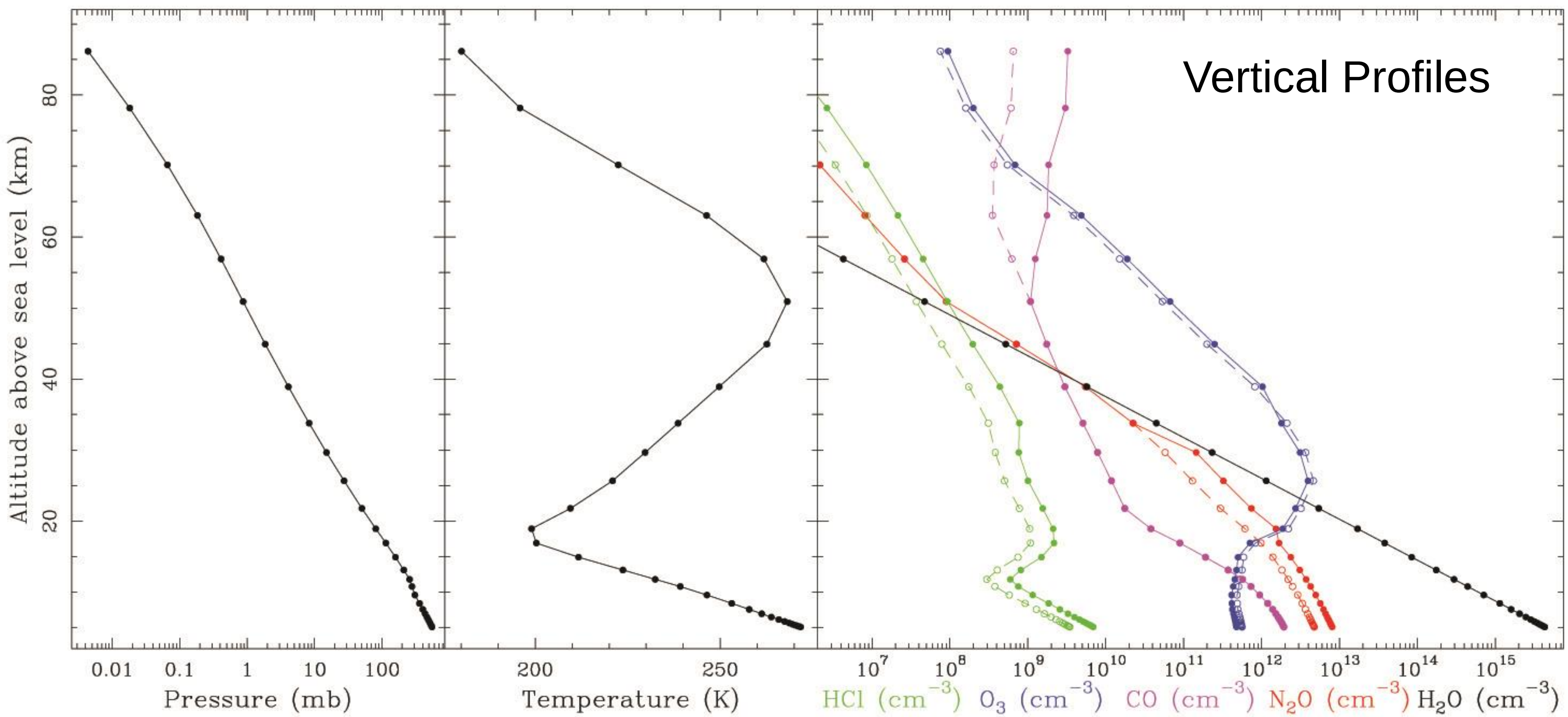
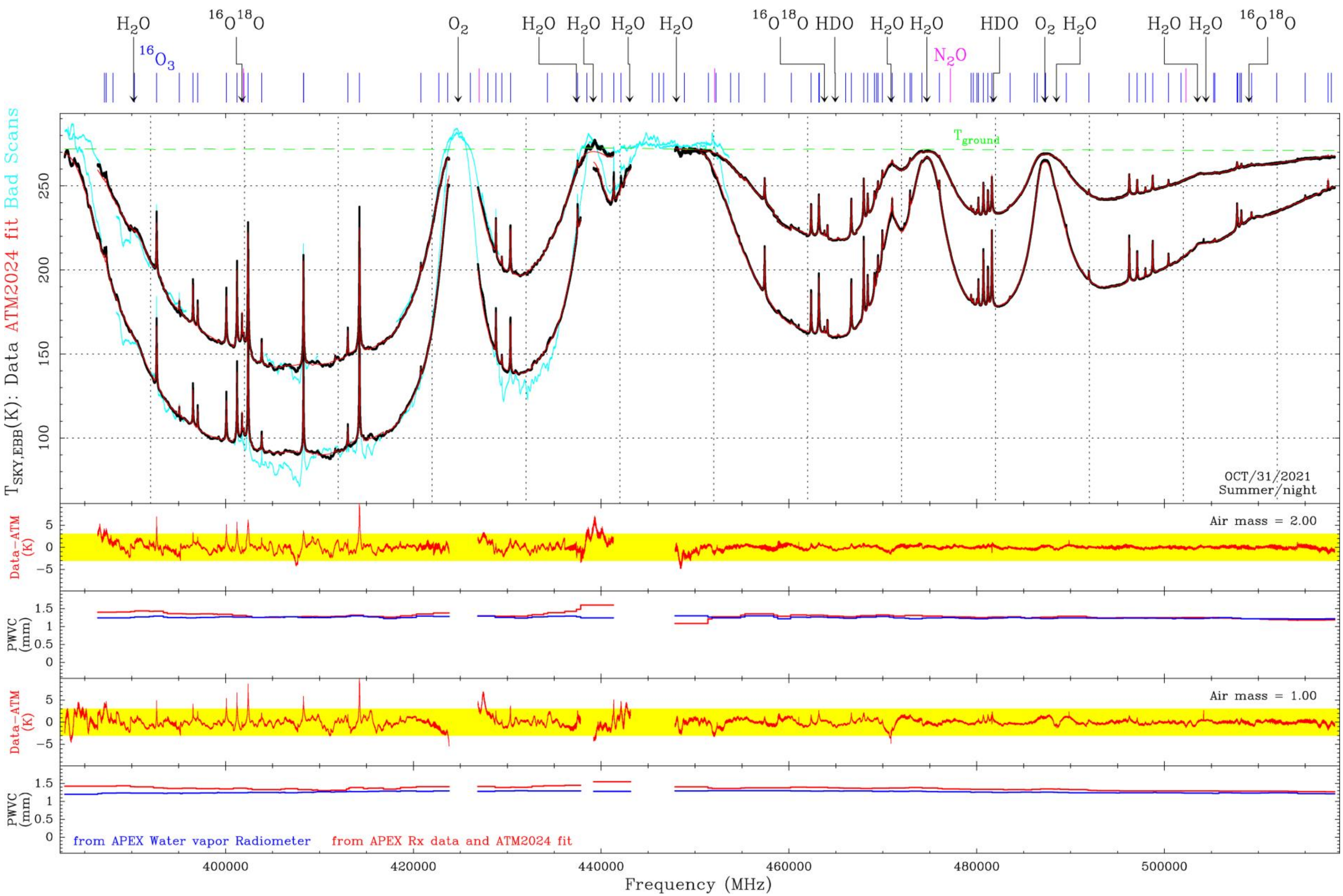
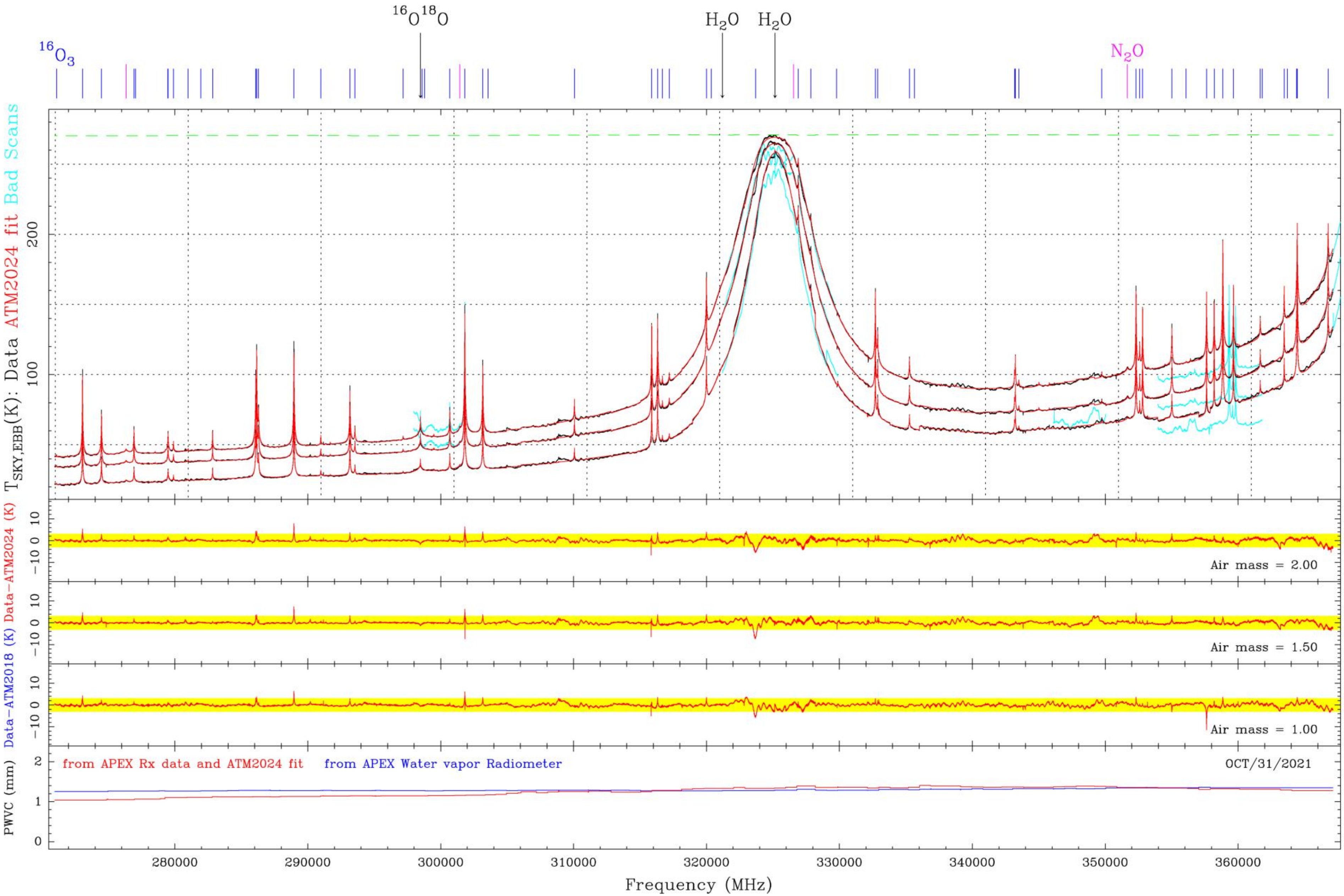


Fig. 5. Vertical profiles (solid lines) used as inputs to the ATM model for the model spectra shown in this work. The dots indicate the average values for the different layers (of increasing thickness) in which the atmosphere has been divided for the calculations. The dashed lines and open circles indicate profiles from U.S. Standard Atmosphere (1976) before being modified in order to better fit the observed lines of O_3, N_2O and CO.

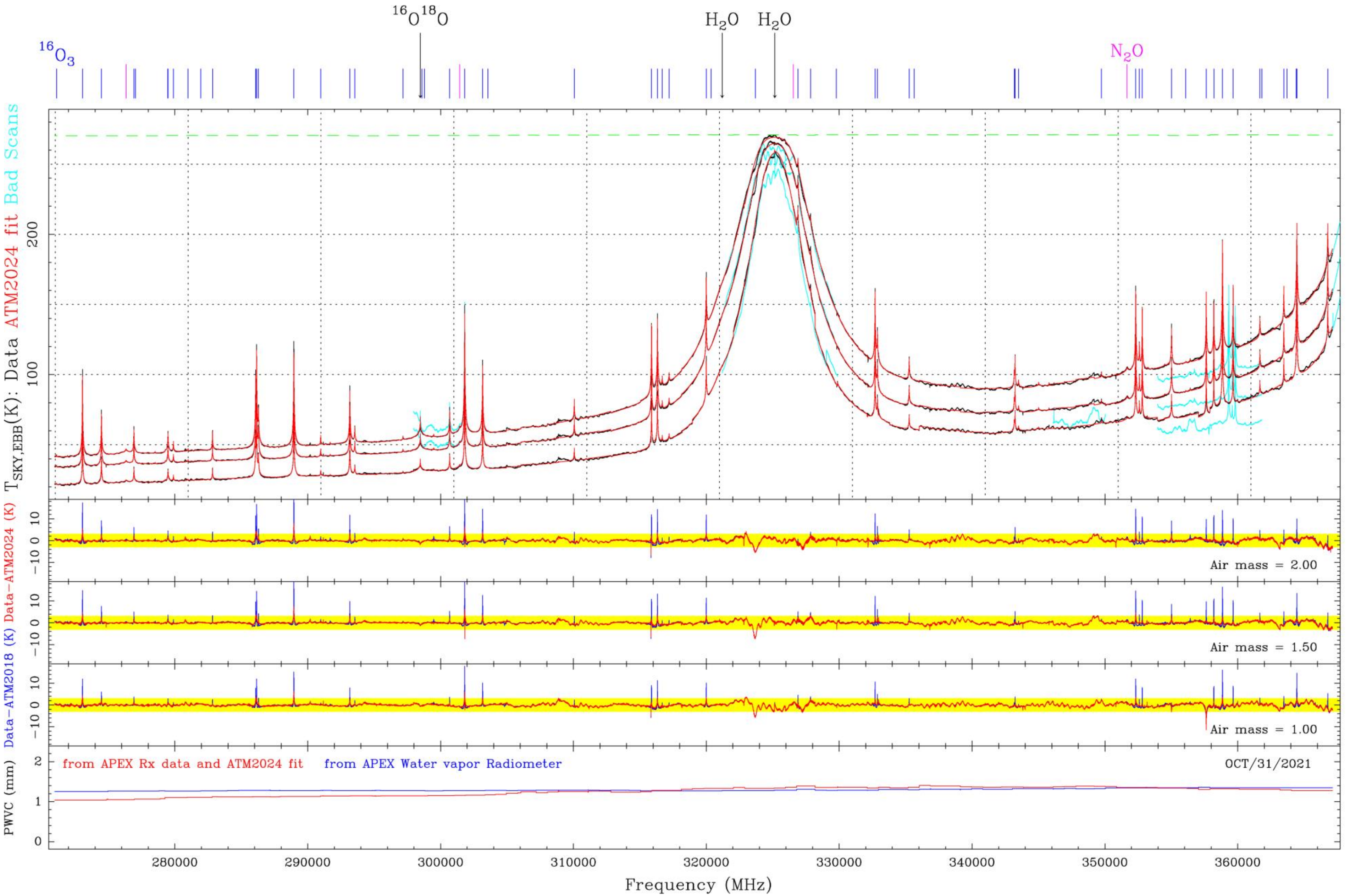
Other atmospheric "windows" (and receivers): 380 to 520 GHz, Oct 31st 2021

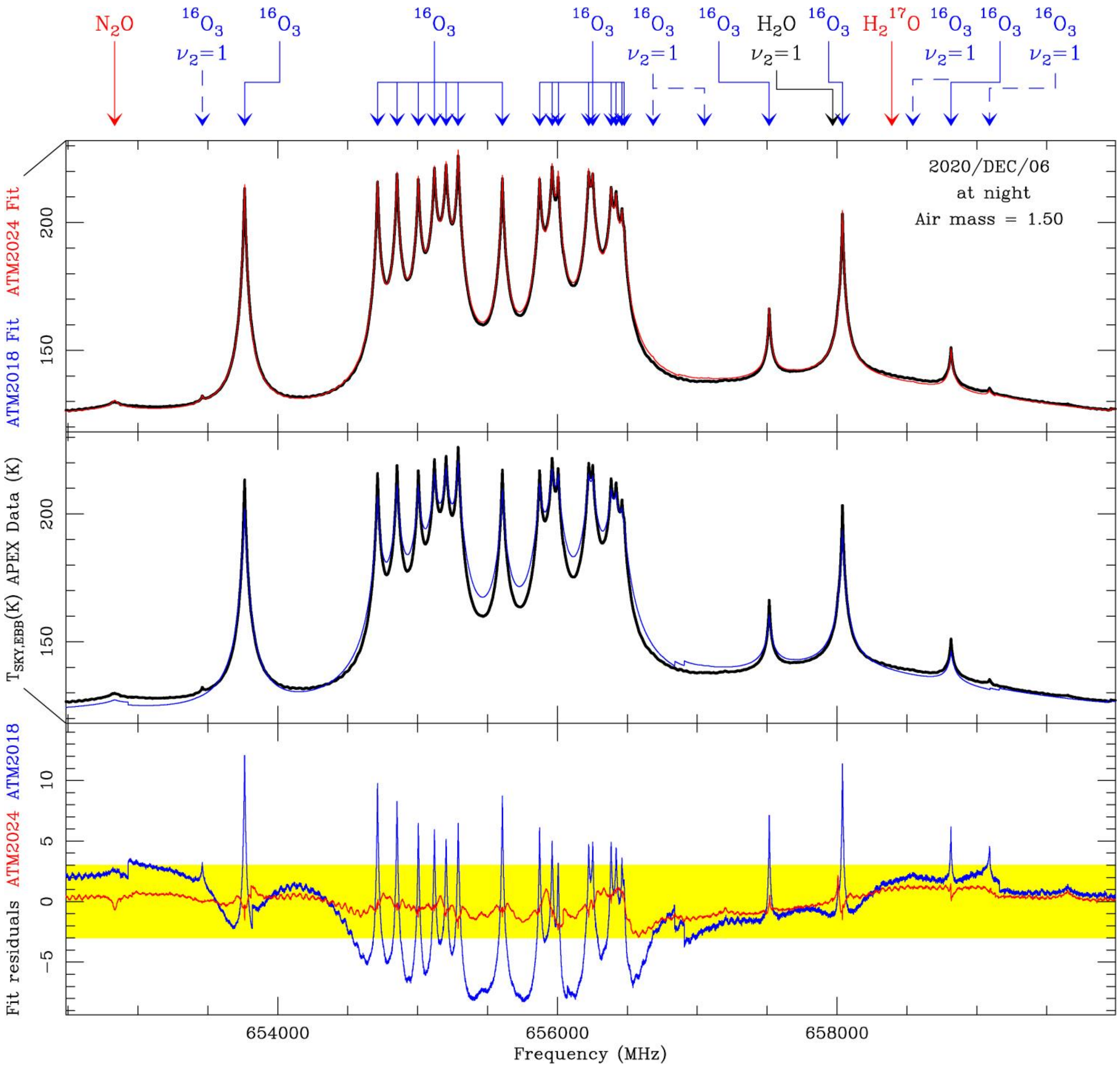


Around the 325 GHz water line, with best O_3 profile



With standard (default) O_3 vertical profile

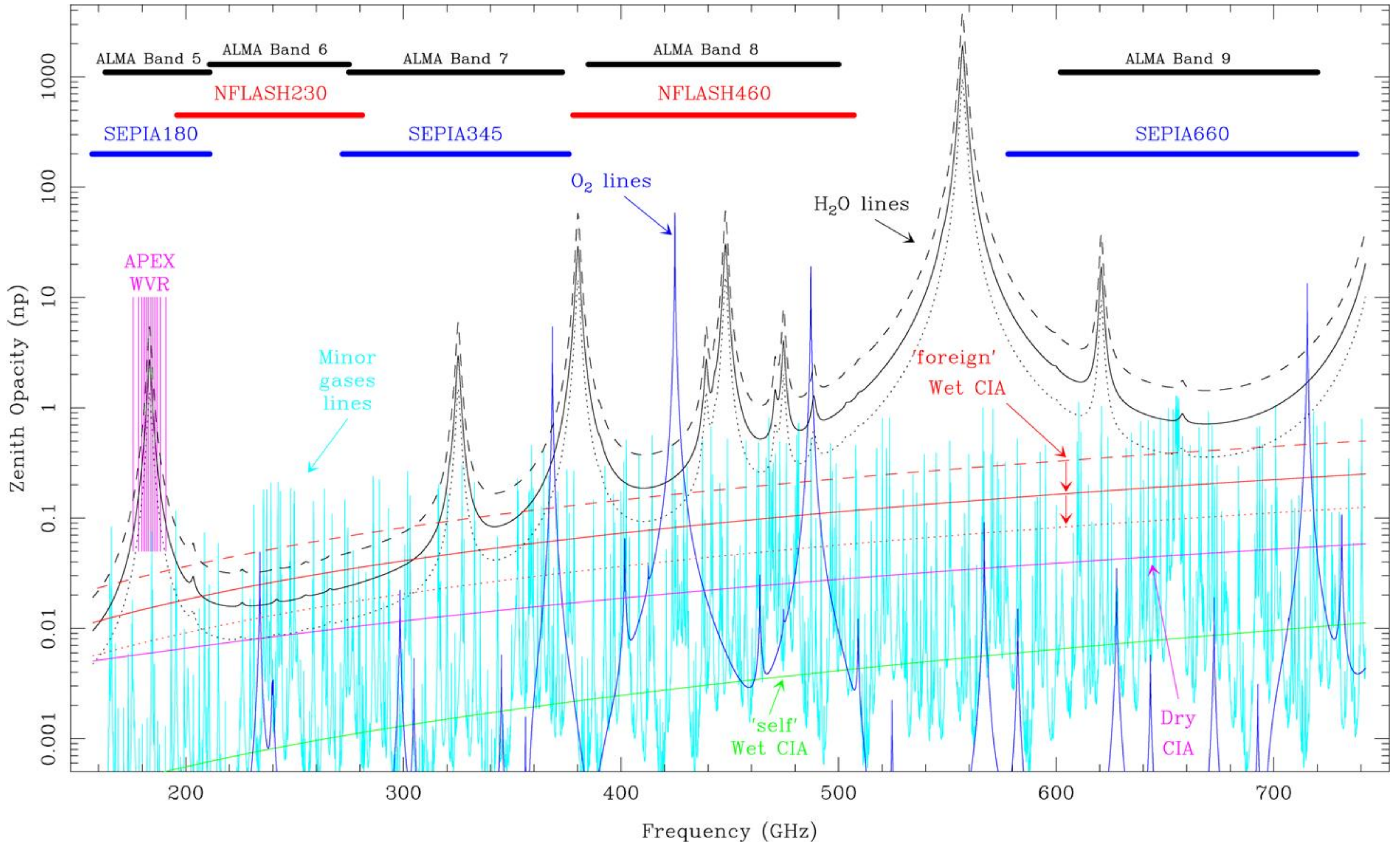




Fitting “minor” gases vertical profiles

Validating "excess" of line-by-line absorption in the submillimeter

- Dry CIA (N_2-N_2, O_2-O_2, O_2-N_2 mechanisms.
- Foreign wet CIA (O_2-H_2O, N_2-H_2O).
- Far wings of H_2O lines centered beyond 1 THz.



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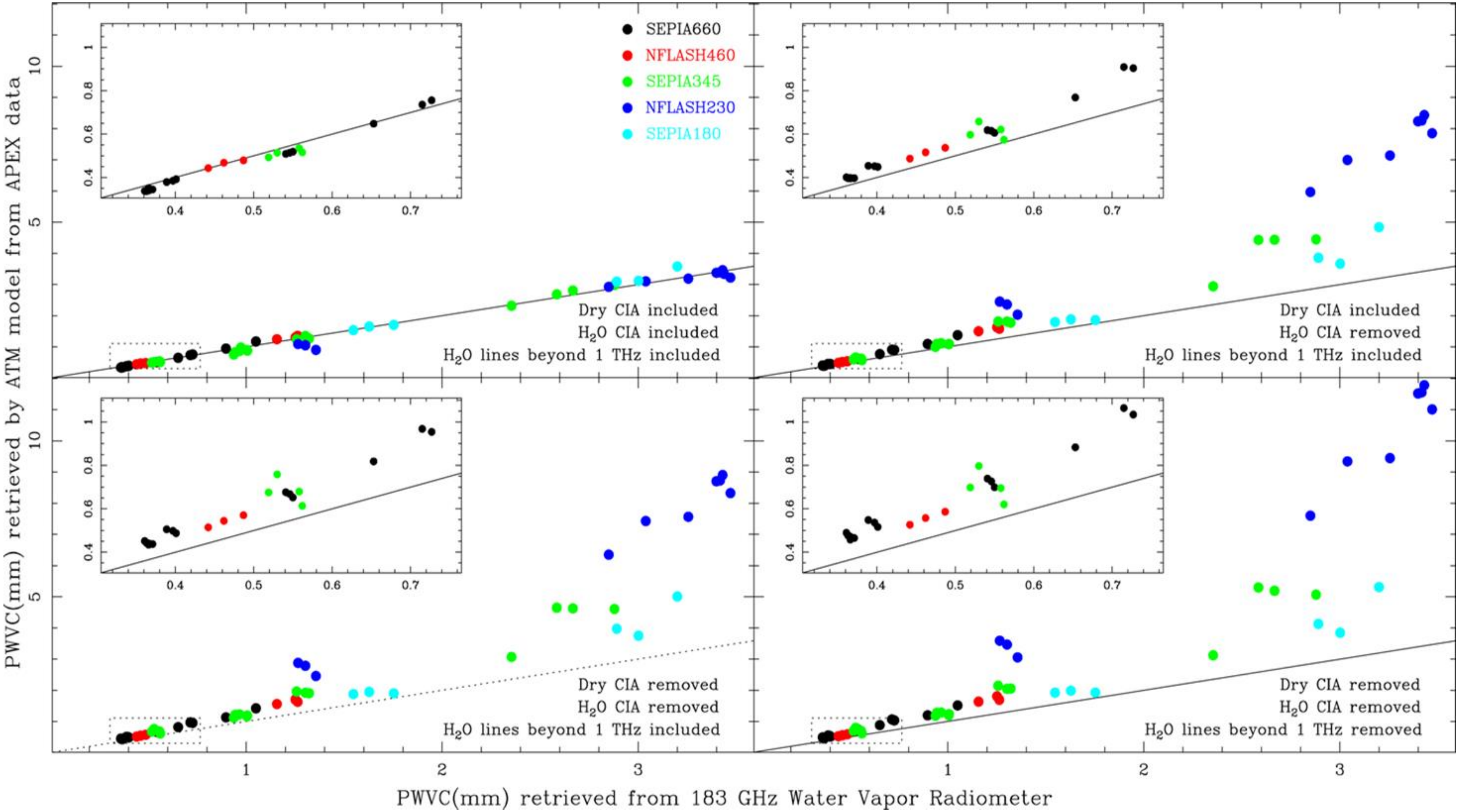

SUMMARY AND CONCLUSIONS

- Ground-based astronomical observatories have now very stable receivers + FFTS backends that allow to get absolutely calibrated atmospheric spectra covering hundreds of GHz at kHz resolution.
- Many fine aspects of the molecular spectroscopy parameters used for atmospheric models currently have been validated and/or improved.
- In particular the Dry and “foreign” wet CIA have been revisited
- Seasonal and day-night reference profiles can be updated.
- For satellite applications the ground-based observations form astronomical observatories provide very good validation databases.
- The effort will continue form other sites poviding access to complementary geographical and altitude conditions.