GEOPHYSICAL RESEARCH LETTERS, VOL. 34, L01802, doi:10.1029/2006GL026684, 2007

Fast forward radiative transfer modeling of 4.3 μm nonlocal thermodynamic equilibrium effects for infrared temperature sounders

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Received 24 April 2006; revised 30 August 2006; accepted 24 November 2006; published 3 January 2007.

[1] Retrieval algorithms for downlooking infrared sounders typically avoid using channels from the 4.3 μm CO_2 region that probe the mid- and upper-atmosphere due to very high altitude Non Local Thermodynamic Equilibrium (NLTE) emission, which can add as much as 10 K to the measured daytime brightness temperatures (BT). In this paper we report a fast radiative transfer model for a nadir sounding instrument (AIRS) that includes the effects of NLTE, allowing the retrieval algorithm to use many short wave CO_2 channels for upper-air soundings. Model biases and standard deviations are very similar for both day and night. This work allows an infrared sounder to probe the upper atmosphere much more completely using only short wave 4.3–4.5 μm channels. **Citation:** DeSouza-Machado, S. G., L. L. Strow, S. E. Hannon, H. E. Motteler, M. Lopez-Puertas, B. Funke, and D. P. Edwards (2007), Fast forward radiative transfer modeling of 4.3 μm nonlocal thermodynamic equilibrium effects for infrared temperature sounders, *Geophys. Res. Lett.*, *34*, L01802, doi:10.1029/2006GL026684.

1. Introduction

[2] Weather satellite sounding of the atmosphere in the infrared has traditionally avoided spectral regions where Non Local Thermodynamic Equilibrium (NLTE) occurs. NLTE emission occurs high in the atmosphere, generally above the stratopause, where solar pumping populates the vibration-rotation energy levels more quickly than collisions can thermally redistribute the energy. NLTE emission is most noticeable in nadir-sounding high-altitude channels where the CO_2 bands are strong enough for NLTE emission to significantly alter LTE emission seen from lower altitudes. Our experience with the Atmospheric Infra-Red Sounder (AIRS) on the EOS-AQUA platform, the first of an upcoming generation of high-spectral resolution satellite atmospheric sounders, has shown that NLTE emission is unimportant at 15 μm, but impacts all stratospheric as well as a number of upper atmosphere sounding channels in the 4.3 μm spectral region. In this paper, we introduce a NLTE radiative transfer algorithm that models NLTE emission in the 4.3 μm spectral region accurately enough to allow many more 4.3 μm channels to be used for upper-tropospheric and stratospheric sounding.

[3] Previous atmospheric studies by limb viewing satellite instruments have shown that solar pumping strongly affects the vibrational temperatures of CO_2 bands in the 4 μm region. NLTE effects can be seen above tangent heights as low as 45 km. Spaceborne instruments measuring the radiance at the top of the atmosphere (TOA) are able to see the enhancement in observed brightness temperature (BT) [*Drossart et al.*, 1993; *Picard et al.*, 1998]. NLTE effects have been studied in detail with limb viewing instruments, from which kinetic temperatures have been retrieved [*Edwards et al.*, 1993; *Miller et al.*, 2000; *Lopez-Puertas and Taylor*, 2001] but few observations have been made with polar-orbiting nadir viewing instruments, and none that we know of with a continuous spectrum in the 4.3 μm region such as that of NASA's AIRS instrument.

[4] AIRS [*Aumann et al.*, 2003] was launched into polar orbit on board the AQUA platform on May 4, 2002. AIRS covers the spectral range between 650 cm^{-1} (15 μm) to 2700 cm^{-1} (3.7 μm) using 2378 channels. Assuming a constant CO_2 mixing ratio, the current AIRS retrieval algorithm uses 15 μm CO_2 channels and 4.3 μm channels beyond 2386 cm^{-1} to sound the atmospheric temperature profile. NLTE emission adds a maximum of $\sim$10K to the observed radiances at 2310 cm^{-1}, dropping to a 0.2K addition at 2385 cm^{-1} and 2386 cm^{-1}. The channels between 2350 and 2386 cm^{-1} are very clean sounding channels that only depend upon CO_2 emission. Presently NLTE limits the use of channels with weighting functions peaking above 350 mbar. The addition of NLTE to the forward model now allows use of sounding channels at 4.3 μm with weighting functions that peak as high as 10 mbar.

[5] The effects of NLTE has previously been modeled in monochromatic line-by-line (MNLBL) codes such as GENLN2 [*Edwards*, 1992]. The NLTE model includes identifying the vibrational bands that deviate from equilibrium and computing their excitation (vibrational) temperature profiles as a function of altitude. For these, using the local kinetic and band vibrational temperatures, the optical depths and source (Planck) function modifications needed for radiative transfer calculations have to be computed, from which a final TOA monochromatic radiance can be calculated. This is then convolved over the instrument Spectral Response Functions (SRF).

[6] For any given solar angle and kinetic temperature profile, line-by-line codes are too slow to be of any practical use for routine operational atmospheric retrievals. In this paper we discuss the development of a much faster NLTE model for use in the AIRS operational retrieval algorithm.

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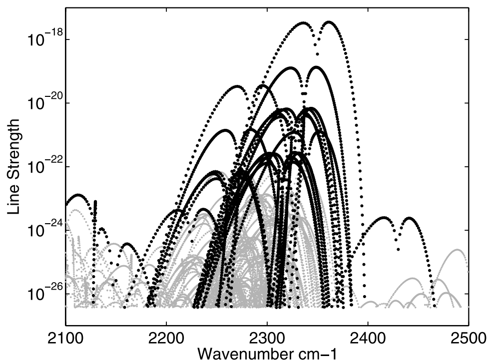

Figure 1. CO_2 bands used by kCARTA for calculations in the 2100–2500 cm^{-1} region. The gray lines are assumed to be in LTE, and their optical depths come from a compressed database. The black lines are assumed to be in NLTE, with the strongest band being the main isotope of the 00011 band.

Although specific to AIRS, the modeling technique should be applicable to other high resolution sounders.

[7] Extensive testing of this fast model shows that the (BT(observed) − BT(calculated)) biases and standard deviations are similar for both day and night cases. The AIRS Science Team is currently modifying the temperature retrieval algorithm to include many of the 4.3 μm channels and showing increased retrieval skill [*Susskind*, 2006]. The addition of channels sensitive to NLTE allows retrievals covering both the troposphere and stratosphere using just 4.3 μm channels, of course with a vertical resolution that depends on the instrument spectral resolution.

[8] We begin by summarizing the important physics adjustments to the MNLBL code kCARTA, so that it could be used for NLTE calculations. We then describe the fast forward model developed from kCARTA, followed by results comparing the fast code to AIRS observations.

2. NLTE Radiative Transfer Algorithm

2.1. Modifications to the kCARTA Line-by-Line Model

[9] kCARTA is the reference monochromatic radiative transfer code for the AIRS instrument (S. De Souza-Machado et al., kCARTA: An atmospheric radiative transfer algorithm using compressed lookup tables, http://asl.umbc.edu/pub/packages/kcarta.html), and is the basis of the current (version 4) AIRS Radiative Transfer Algorithm (AIRS-RTA) [*Strow et al.*, 2003], that only includes LTE effects. kCARTA assumes all gases are in LTE, and differs from MNLBL codes in that instead of spectroscopic calculations for each absorption line of each gas, it computes transmittances from compressed look-up tables of atmospheric optical depths at 0.0025 cm^{-1} resolution, resulting in very fast computation times. The lookup tables were generated with a slow but accurate MNLBL that includes CO_2 P/R-branch line-mixing at 4.3 and 15 microns [*Tobin*, 1996], especially important in the temperature sounding regions. The accuracy of kCARTA is only limited by that of the line parameters and lineshapes used to generate the lookup tables.

[10] The original kCARTA code uses a standard atmosphere that extends only to 80 km, since the weak bands close to LTE (during night time) have very little upper atmospheric emission compared to the upwelling radiance from lower altitudes. However, daytime solar pumping of the strongest band produces significant emission in the lower thermosphere, so NLTE model atmospheres that extend to 120 km were used. At these heights the lineshape is predominantly Doppler and very narrow, for which a higher resolution (0.0005 cm^{-1}) was needed, which is $\times 5$ more than that used in other wavenumber regions.

[11] kCARTA has a variable user-set height (nominally 30 km) below which it uses LTE optical depths computed using the compressed database. While most gases are still treated as before (LTE), the NLTE correction factors and source function modifiers [*Edwards et al.*, 1993; *Lopez-Puertas and Taylor*, 2001] were added for relevant 4 μm region CO_2 bands. The criteria for NLTE selection is based on the population of the upper vibrational states and the relative (NLTE/LTE) contribution to the TOA radiances as some hot bands, with excited lower vibrational states, have weak strengths but still contribute significantly. The lineshapes for these NLTE bands are computed within kCARTA using a traditional MNLBL approach. This is computationally expensive and significantly slows the code. The remaining lines are assumed to be in LTE, with their optical depths coming from the kCARTA compressed database. Figure 1 shows the CO_2 bands between 2100 – 2500 cm^{-1}; those in gray are the weak lines assumed to be in LTE while the rest are assumed to be in NLTE (e.g. the 00011 isotope bands, and the 01111, 02211 bands). Testing was done against GENLN2 [*Edwards*, 1992], which was part of an inter-comparison of NLTE codes for limb sounders [*Clarmann et al.*, 2002].

2.2. NLTE Effects in AIRS Fast Model

[12] kCARTA was used to compute daytime radiances for 48 diverse profiles, as a function of 6 solar angles and 6 view angles to generate regression data for the parameterized AIRS fast NLTE RTA. The NLTE vibrational band temperatures for the bands shown in Figure 1 were computed using the Generic RAdiative traNsfer AnD non-LTE population Algorithm (GRANADA) model [*Funke et al.*, 2002], which uses the radiative and collisional schemes of [*Lopez-Puertas and Taylor*, 2001]. For the ith channel the difference between AIRS radiances computed including NLTE effects and those computed using only LTE was estimated using

$$\Delta r_i^{NLTE} = r_i^{NLTE} - r_i^{LTE} = \mathcal{A}X \quad (1)$$

where r_i^{LTE} and r_i^{NLTE} are the convolved radiances for AIRS channel i, computed using kCARTA. $\mathcal{A}$ is a matrix of profile based predictors, and X is a set of coefficients determined by regression. The predictors are shown in Table 1, and are ordered in order of importance. The solar

Table 1. Predictors for NLTE Fast Model

Number	Predictors
1	constant
2	$\cos(\theta_{sun}^{TOA})$
3	$\cos^2(\theta_{sun}^{TOA})$
4	$\cos(\theta_{sun}^{TOA}) \times \sec(\theta_{view})$
5	$\cos(\theta_{sun}^{TOA}) \times T^{avg}(5)$
6	$\cos(\theta_{sun}^{surf})$

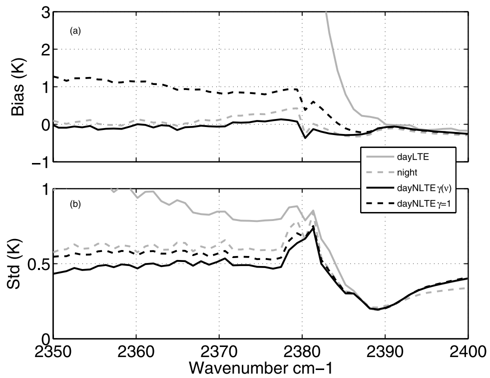

Figure 2. (a) Biases and (b) standard deviations for various tests of the RTA. Grey curves show the results when the LTE RTA is used, with solids showing daytime results, and dashed showing night time results. Black curves show daytime results when the NLTE RTA is used, with solids showing results with channel dependent γ_i, and dashed showing results with constant γ_i = 1.

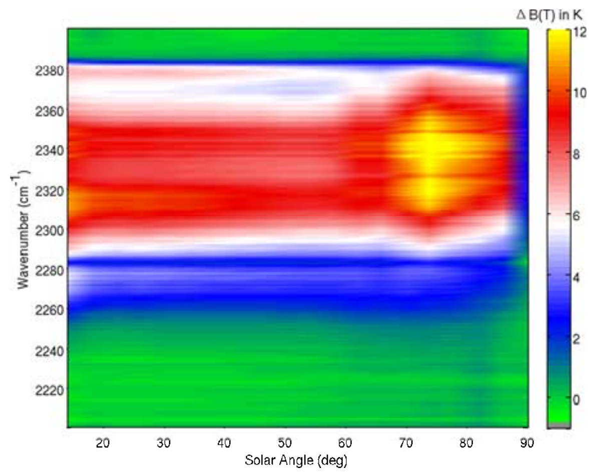

Figure 3. Daytime biases in the 4.3 μm CO_2 bands, between tens of thousands of AIRS observations and calculated TOA radiances, converted to BT (Kelvin). The horizontal axis is solar angle (degrees), the vertical axis are the AIRS channels in cm^{-1}, and the color scale is in degrees Kelvin. This plot was made using a Fast Model which does not have NLTE effects.

zenith angle is the main driver for the NLTE effects and is one of the main predictors, which are based on combinations of the solar angles at TOA and at the surface (θ_{sun}^{TOA}, θ_{sun}^{surf}), view angle (θ_{view}), and the average kinetic temperature of the uppermost five standard AIRS layers ($T^{avg}(5)$). These five layers (altitude $\geq$ 55 km) are typically above the stratopause, and have non negligible amounts of CO_2 present. The strong 4.3 μm bands have daytime vibrational temperatures in these layers that are as much as 50–100 K larger than the kinetic temperature.

[13] The NLTE radiance computed by the new AIRS-RTA is therefore

$$r_i^{NLTE} = \Delta r_i^{NLTE} + r_i^{LTE} \quad (2)$$

The simplicity of this NLTE model means it can easily be included in the AIRS-RTA with only a negligible impact on processing speed. The fitting errors for the fast model Δr_i^{NLTE} were on the order of 7% *rms* for most channels. Improvements were made by by comparing against a set of clear sky AIRS observations made over the Tropical Western Pacific Atmospheric Radiation Measurements site (ARM: A Science Research Program for Global Climate Change, http://www.arm.gov/) where coincident radiosondes were launched as part of an AIRS validation campaign [*Tobin et al.*, 2005], with 15 μm AIRS retrievals used for temperatures above 0.1 mbar. The comparisons showed that equation (2) slightly under-estimates the observed radiances $r_i^{NLTE} \simeq 0.96\ r_i^{obs}$ (or a BT bias of about +1 K). A channel varying adjustment factor γ_i so that $r_i^{NLTE} = \gamma_i \Delta r_i^{NLTE} + r_i^{LTE} \simeq r_i^{obs}$ was introduced to empirically correct for these observed biases. The biases for the 4.3 μm channels were then reduced to a level comparable with those from the 15 μm region. Note that the 15 μm AIRS temperature retrievals were used as the "truth" for NLTE predictor #5 in Table 1, and errors in these retrievals could be the source of the need for the empirical γ adjustments. γ has a mean value of 1.25 ± 0.08.

3. Results Using the AIRS NLTE Fast Forward Model

[14] The NLTE Fast Forward Model was tested on four days of AIRS observations over open water, whose radiances passed a strict spatial uniformity test, reducing the effects of possible contamination by clouds or spatially varying humidity. These data consisted of AIRS radiances from 24 hours worth of observations (typically 10000 night time and 30000 day time), with no latitudinal restrictions (with corresponding seasonal effects on the local sun angles) other than avoidance of ice covered regions near the poles. A random day in each of February,

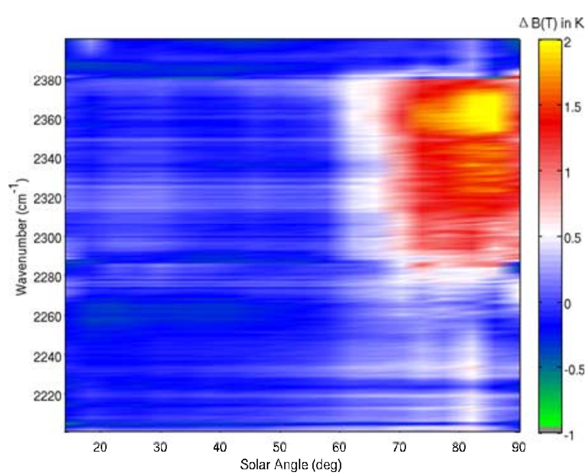

Figure 4. Same as Figure 3, except using the NLTE RTA described in this paper. Vertical units are in cm^{-1}, horizontal units are in degrees, and the color scale is in degrees Kelvin.

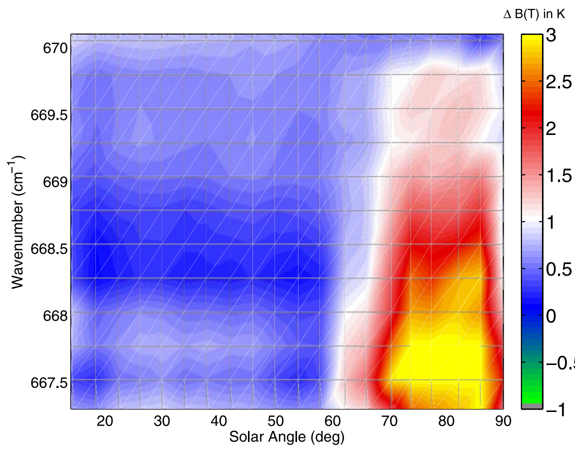

Figure 5. Same as Figure 4 except for high altitude channels in the 15 μm sounding region. Vertical units are in cm^{-1}, horizontal units are in degrees, and the color scale is in degrees Kelvin.

May, July and October 2005 were used for the figures in this paper. For all sets, we used a constant CO_2 mixing ratio of 370 ppm in the lower atmosphere. The water vapor, ozone and temperature profiles used in the results shown below are from the ECMWF model fields. As the DECEM profiles ended at 0.1 mbar, we again used a simple climatology based on latitude and month to add on one of six profiles [*Anderson et al.*, 1986] above this pressure level (tropical, mid-latitude summer and winter, sub-arctic summer and winter, or standard).

[15] Figure 2 summarizes the biases and standard deviations between AIRS and ECMWF for the four days tested. The biases using the NLTE model with variable γ during the day are almost zero and very similar to the nighttime LTE biases. If the empirical γ factor is set to unity (no effect), the daytime NLTE biases rise to slightly above 1K, compared to a daytime LTE model that would have biases larger than 10K (see Figure 3). The γ factor does appear to slightly lower the standard deviations, which are more dominated by ECMWF than AIRS noise below 2380 cm^{-1}. AIRS channels at 15 μm that peak at similarly high altitudes also have increased standard deviations.

[16] Figure 3 shows another view of the biases in the 4 μm region between AIRS observations and calculated TOA radiances, converted to BT, when only a LTE model is used. The horizontal axis is solar angle while the vertical axis is the AIRS channel center wavenumbers. The biases in the CO_2 channels between 2260–2380 cm^{-1}, which sound radiances high in the atmosphere can be as large as 10 K, but drop to about 0.25 K for the rest of the channels that sound lower in the atmosphere. A similar plot for solar angles larger than 90 degrees (nighttime) shows biases for all channels are about 0.2–0.3 K.

[17] Figure 4 shows the biases in the 4 μm region between the same AIRS observations and calculated TOA radiances using the NLTE model, again converted to BT. Note the colorscale range has changed. It is clearly evident that the NLTE model has largely reduced the biases for the 2300–2378 cm^{-1} channels to about 0.2K, independent of solar angle below $\sim$70 degrees. Beyond this angle, the biases then increase for larger solar angles. For the AQUA/AIRS polar orbit, observations for the larger solar angles are for sub-polar and polar winter regions where ECMWF upper atmosphere fields have known biases. Consequently, we believe the larger biases in Figure 4 are more likely due to errors in the ECMWF fields rather then the NLTE RTA.

[18] We tested this by finding 15 μm AIRS channels that have weighting functions that peak at the same nominal altitudes as the channels in the 2280–2380 cm^{-1} region that exhibit the high biases at high solar angles. Figure 5 plots biases for the same observations as shown in Figure 4 but for the 15 μm channels with similar weighting functions. These channels, which are not sensitive to NLTE behavior, also show increasing biases at high solar angles, and confirm that the high biases in Figure 4 are most likely due to the ECMWF fields rather than poor behavior in the NLTE RTA. Note that the AIRS channels near 667.5 cm^{-1} peak higher in the atmosphere than any of the 4 μm channels, and consequently show even higher BT biases, while the higher wavenumber channels (669.5 cm^{-1}) contain slightly lower altitude information than those in the 2300–2378 cm^{-1} region and consequently have slightly lower biases at the higher solar angles.

4. Conclusions

[19] We have demonstrated fast forward modeling of NLTE effects in the temperature sounding 4.3 μm CO_2 band for a high resolution nadir viewing instrument. The accuracy of this model is sufficient to make the daytime computed radiances as accurate as the nighttime computed radiances. Future work on this physics-based algorithm may include resolving the γ_i factors used across this spectral region and assessing the impact of using some of these NLTE channels on the quality of retrievals. Preliminary studies [*Susskind*, 2006] have shown improved upper-atmospheric soundings using this new NLTE radiative transfer algorithm. Moreover, an accurate NLTE RTA allows retrievals covering both the troposphere and stratosphere using only 4 μm channels.

[20] **Acknowledgments.** The authors thank ECMWF for use of forecast and analysis model fields. This work was supported by NASA contract NNG04GG03G-2. The IAA team has been partially supported by Spanish projects REN2001-3249/CLI and ESP2004–01556 and by EC FEDER funds. The National Center for Atmospheric Research is sponsored by the National Science Foundation.

References

Anderson, G., S. Clough, F. Kneizys, J. Chetwynd, and E. Shettle (1986), AFGL atmospheric constituent profiles (0–120 km), *Tech. Rep. AFGL-TR-86-0110*, Air Force Geophys. Lab., Hanscom Air Force Base, Mass.

Aumann, H., et al. (2003), AIRS/AMSU/HSB on the Aqua mission: Design, science objectives, data products and processing systems, *IEEE Trans. Geosci. Remote Sens.*, *41*(2), 253–264.

Clarmann, T., et al. (2002), Intercomparison of radiative transfer codes under non-local thermodynamic equilibrium conditions, *J. Geophys. Res.*, *107*(D22), 4631, doi:10.1029/2001JD001551.

Drossart, P., et al. (1993), Earth global mosaic observations with NIMS-Galileo, *Planet. Space Sci.*, *41*, 551.

Edwards, D. (1992), GENLN2: A general line-by-line atmospheric transmittance and radiance model, *NCAR Tech. Note 367+STR*, Natl. Cent. for Atmos. Res., Boulder, Colo.

Edwards, D. P., M. Lopez-Puertas, and M. López-Valverde (1993), Non-local thermodynamic equilibrium studies studies of 15 um bands of

CO2 for atmospheric remote sensing, *J. Geophys. Res.*, *98*, 14,955–14,977.

Funke, B., M. Martín-Torres, F. J. López-Puertas, M. Höpfner, F. Hase, M. A. López-Valverde, and M. García-Comas (2002), A generic non-LTE population model for MIPAS–ENVISAT data analysis, *Geophys. Res. Abstr.*, *4*, Abstract XXXXXX.

Lopez-Puertas, M., and F. Taylor (2001), *NONLTE Radiative Transfer in the Atmosphere*, World Sci., Hackensack, N. J.

Miller, S., J. Winick, and H. Snell (2000), Non-LTE effects om retrieval of temperature from the CO_2 laser bands using CIRRIS 1A data, *J. Geophys. Res.*, *105*, 10,193–10,202.

Picard, R., et al. (1998), Remote sensing of discrete stratospheric gravity-wave structure at 4.3-μm from the MSX satellite, *Geophys. Res. Lett.*, *25*, 2809.

Strow, L., S. Hannon, S. DeSouza-Machado, D. Tobin, and H. Motteler (2003), An overview of the AIRS radiative transfer model, *IEEE Trans. Geosci. Remote Sens.*, *41*, 303–313.

Susskind, J. (2006), Contribution of the AIRS shortwave sounding channels to retrieval accuracy, in *Algorithms and Technologies for Multispectral, Hyperspectral, and Ultraspectral Imagery XII*, *Proc. SPIE Int. Soc. Opt. Eng.*, *6233*.

Tobin, D. C. (1996), Infrared spectral lineshapes of water vapor and carbon dioxide, Ph.D. thesis, Univ. of Md. Baltimore County, Baltimore.

Tobin, D. C., et al. (2005), Arm site atmospheric state best estimates for airs temperature and water vapor retrieval validation, *J. Geophys. Res.*, *111*, D09S14, doi:10.1029/2005JD006103.

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