# Test of Jonas Zmuidzinas' ALI code

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## Test of the Zmuidzinas ALI code

With the goal of testing Jonas Zmuidzinas' ALI code, I have obtained results for the simple case of a two-level water molecule in an isothermal, constant density sphere.

### Cloud model

Outer radius = 0.1 pc
Inner radius = 0.001 pc
$H_2$ density = $10^4$ $cm^{-3}$
Temperature = 40 K
Gaussian line profile with FWHM = 1 km $s^{-1}$
No dust or velocity gradient

### Excitation model

Two level ortho-water molecule ($1_{01}$ and $1_{10}$ states)

Collisional excitation of 557 GHz transition by ortho and para-$H_2$ in 3:1 ratio*

➔ de-excitation rate coefficient, $q_{21}$ = $2.18 \times 10^{-10}$ $cm^3$ $s^{-1}$
excitation rate coefficient, $q_{12}$ = $1.12 \times 10^{-10}$ $cm^3$ $s^{-1}$
critical density, $n_{cr}$ = $1.59 \times 10^7$ $cm^{-3}$

*Realistically, the ratio is almost certainly smaller than 3

### Numerical details

The standard model* has:

200 radial shells, with the column density across the outermost shell 50,000 times that across the innermost shell. (The grid points were heavily concentrated near outer edge because that is where the level populations change rapidly.)
Grid input file = **grid.dat**

10 frequency points across the line

Convergence criterion: fractional change in population < $10^{-4}$

*To test the accuracy, models were also run (a) with only 100 radial shells; (b) with only 5 frequency points; and (c) with a convergence criterion of $10^{-3}$. The maximum change in any of the quantities plotted below for any of these cases was 10%.

### Parameters

Abundance $x(o\text{-}H_2O) = n(o\text{-}H_2O)/n(H_2) = 10^{-10}, 10^{-9}, 10^{-8}, 10^{-7}, 10^{-6}$ and $10^{-5}$

**<u>Results: level populations</u>**

Level populations for ortho-water abundance of $10^{-XX}$ are given in the files **popnXX.dat.**

**<u>Figure 1</u>** shows the population in $1_{10}$ as a function of radius for each ortho-water abundance considered.

**<u>Figure 2</u>** shows the fractional abundance $f(1_{10})$ at the center of the sphere as a function of the ortho-water abundance.

The results conform to expections:

(1) For low water abundances, radiative trapping is negligible and the equilibrium abundance is

$$f(1_{10})/f(1_{01}) = \exp(-\Delta E/kT)\,[1 + n_{cr} / n(H_2)]^{-1} = 0.512\,(1 + 1588)^{-1}$$

$\Rightarrow$ $f(1_{10}) = 3.23 \times 10^{-4}$ (dashed line in Figures 1 and 2)

If $f(1_{01}) >> f(1_{10})$, the optical depth at line center from the cloud surface to the center is $\tau_0 = 0.063\ x(o\text{-}H_2O)/10^{-10}$ $\Rightarrow$ radiative trapping of minor importance for $x(o\text{-}H_2O) < 10^{-9}$

(2) For high water abundances, radiative trapping drives the populations in the interior towards LTE. In the optically-thick case, radiative trapping reduces the *effective* critical density by a factor of a few x $\tau_0$ (i.e. escape probability ~ 1/[few x $\tau_0$] ). Thus the level populations at the center come close to LTE (within a factor ~ 2) for

$$\text{few} \times \tau_0 = n_{cr} / n(H_2) = 1588 \Rightarrow \tau_0 = \text{few} \times 10^2 \Rightarrow x(o\text{-}H_2O) \sim 10^{-6}$$

In the limit of high water abundance, we expect LTE populations at the center with

$f(1_{10})/f(1_{01}) = \exp(-\Delta E/kT) = 0.512$ $\Rightarrow$ $f(1_{10}) = 0.339$ (dotted line in Figs 1 and 2)

## Results: emergent spectrum

**Figure 3** shows the emergent spectrum ($T_A$ versus v), computed for a Gaussian beam of projected size 10 pc FWHM. (This value was chosen to be large enough that the cloud core can be considered a point source, but obviously leads to fluxes too small to be observed by SWAS.) Results are tabulated in the files **spectrumXX.dat**

## Results: total line luminosity

The total line luminosity is

$$L = 4\pi^2 R^2_{cloud}\, I = 4\pi^2 R^2_{cloud}\, (2\, k/\lambda^3) \int T_B\, dv$$

$$= 4\pi^2 R^2_{beam}\, (2\, k/\lambda^3) \int T_A\, dv$$

where $T_B$ is the brightness temperature averaged over the disk of the cloud,

$T_A = (R^2_{cloud} / R^2_{beam})\, T_B$ is the antenna temperature, and

$R_{beam}$ = (Projected FWHM beam size) / [2 (ln 2)$^{1/2}$ ] = 6.01 pc is the radius of the projected beam at the 1/e power point.

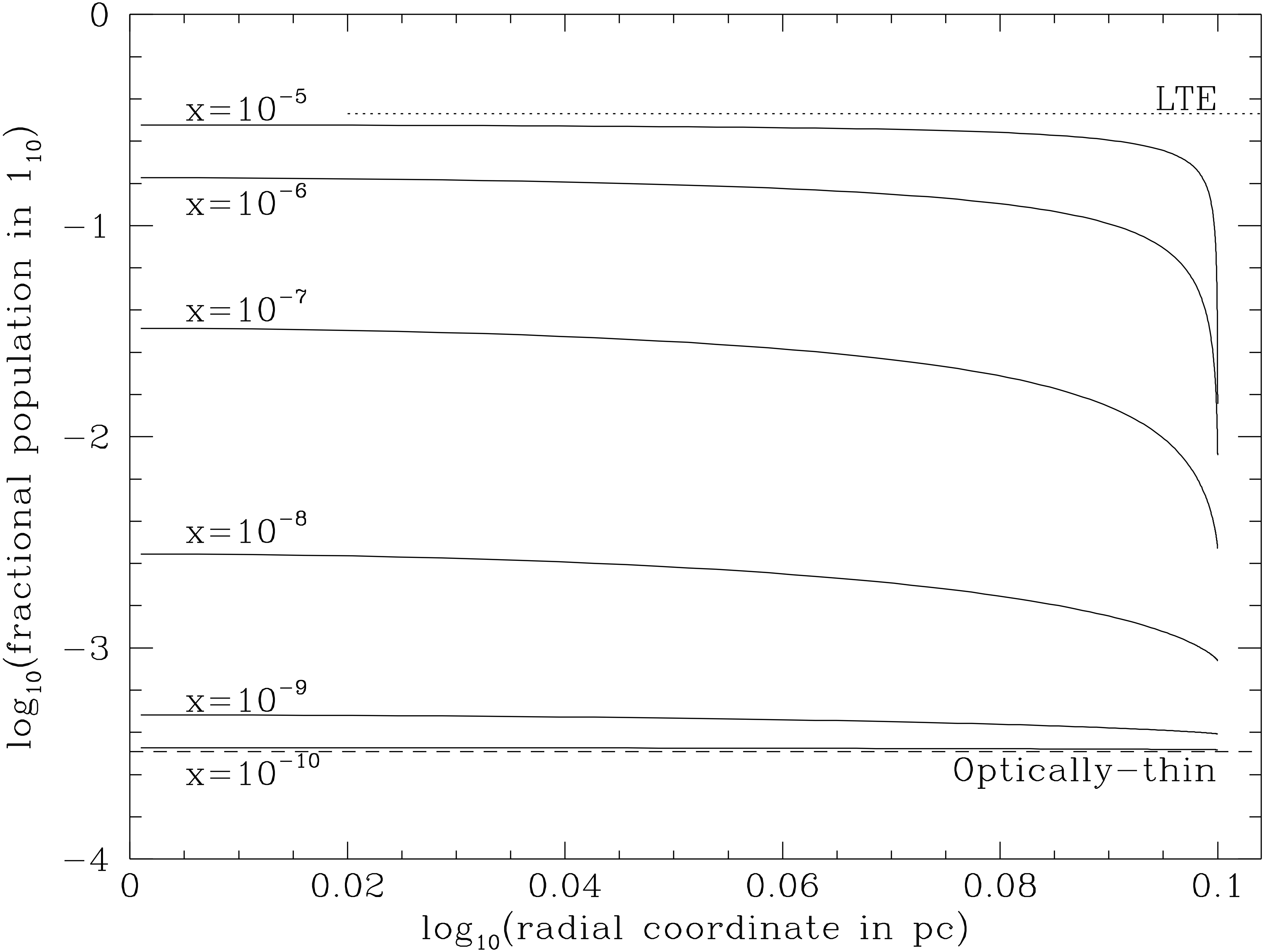
**Figure 4** shows the total line luminosity as a function of ortho-water abundance

For abundances in the range $10^{-9}$ - $10^{-7}$, **this computation provides a critical test of the ALI code**. In this range of abundance, the cloud has substantial line-center optical depth ($\tau_0$ ~ 0.6 - 60) but is not thick enough to thermalize the level populations. Thus collisional de-excitation is negligible and we expect a total luminosity

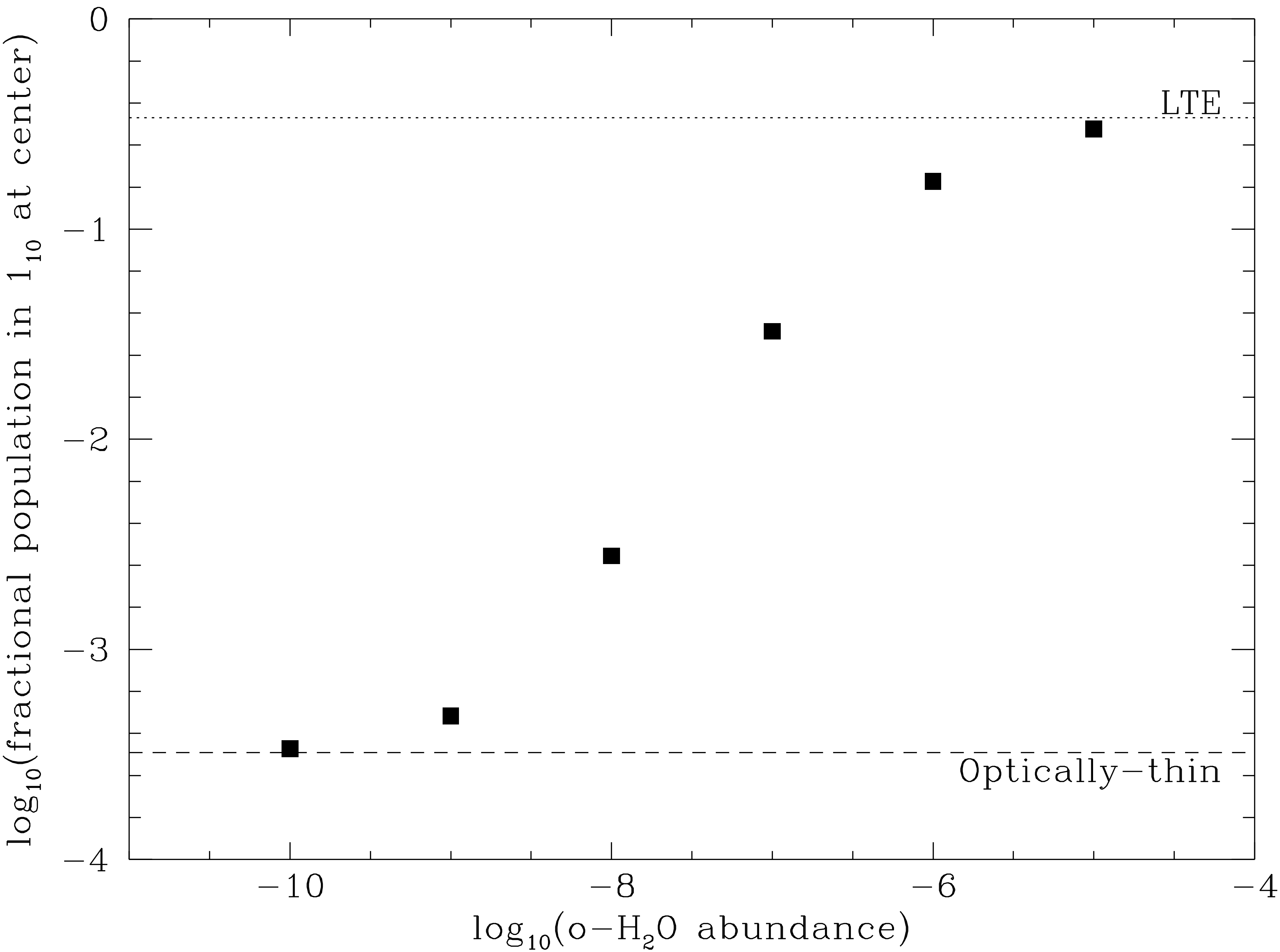
$$L = h\nu\, q_{12}\, n(o\text{-}H_2O)\, n(H_2)\; V = 5.09 \times 10^{26}\; [x(o\text{-}H_2O)/10^{-10}]\; \text{erg s}^{-1}$$

where V is the cloud volume and $q_{12}$ is the collisional excitation rate.

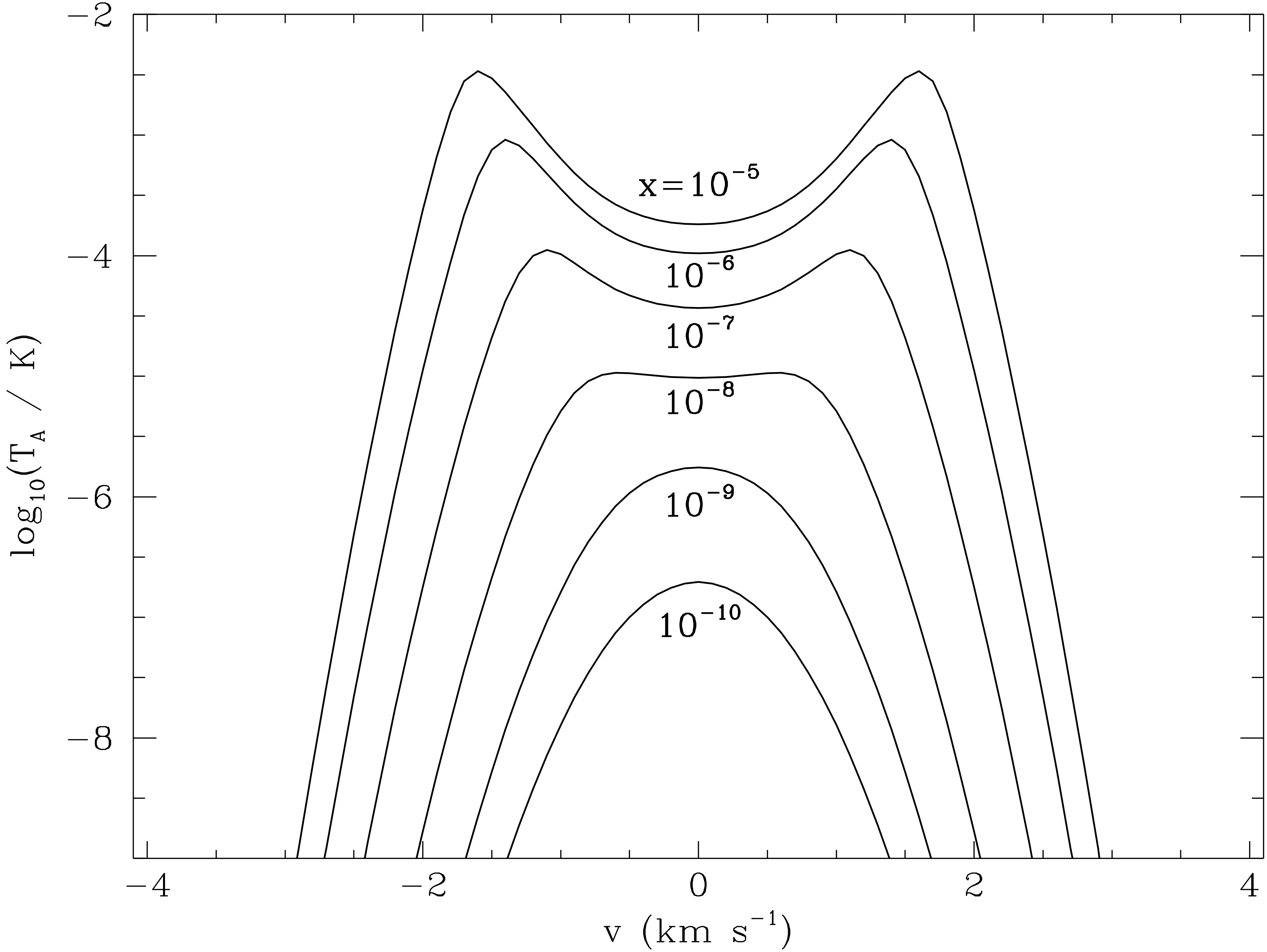
This luminosity is plotted as the dashed line in Figure 4. The agreement for $x(o\text{-}H_2O) \leq 10^{-7}$ is excellent and yields a stringent test of the model, demonstrating that the **results are correct for an optically-thick case in the which the level populations are subthermal but enhanced by radiative trapping**. For larger values of $x(o\text{-}H_2O)$, the level populations are thermalized in the interior and collisional de-excitation starts to quench the total emission rate.



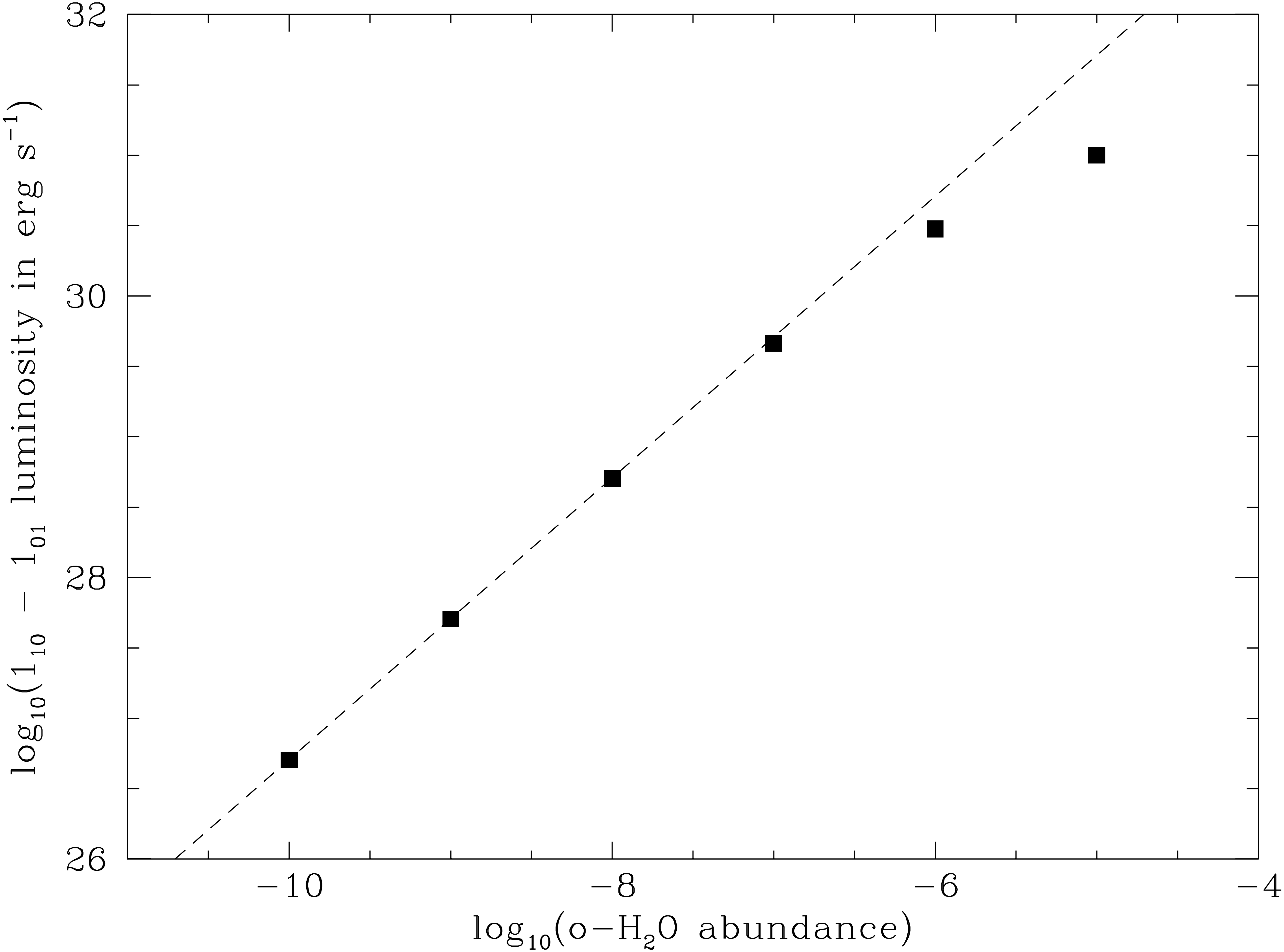
LTE
x=10^-5
x=10^-6
x=10^-7
x=10^-8
x=10^-9
x=10^-10
Optically−thin
log10(fractional population in 1_10)
log10(radial coordinate in pc)
0
−1
−2
−3
−4
0
0.02
0.04
0.06
0.08
0.1



0
−1
−2
−3
−4
−10
−8
−6
−4
LTE
Optically−thin
$\log_{10}$(fractional population in $1_{10}$ at center)
$\log_{10}$(o−$H_2O$ abundance)



x=10^−5
10^−6
10^−7
10^−8
10^−9
10^−10
−2
−4
−6
−8
log10(TA / K)
−4
−2
0
2
4
v (km s^−1)



32
30
28
26
−10
−8
−6
−4
$\log_{10}(1_{10} - 1_{01}$ luminosity in erg $s^{-1})$
$\log_{10}$(o−$H_2O$ abundance)