

Correction to: An accurate set of H3O+ – H2 collisional rate coefficients for non-LTE modelling of warm interstellar clouds

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Advance Access publication 2023 November 15 Correction to: An accurate set of $H_3O^+ - H_2$ collisional rate coefficients

for non-LTE modelling of warm interstellar clouds

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Key words: errata, addenda – astrochemistry – molecular data – molecular processes – radiative transfer – methods: laboratory: molecular - ISM: molecules.

We have discovered errors in our recent paper Demes et al. (2022). Indeed, the supplementary material contains some incorrect theoretical data due to a software bug in the calculations of high energy cross sections. The cross sections for para-H₃O⁺ collision with ortho-H₂ are affected at total energies above 800 cm⁻¹. Consequently, most of the high temperature rate coefficients for the para-H₃O⁺ + ortho-H₂ nuclear spin configurations are affected too. At kinetic temperatures lower than $T_{\rm kin} = 100$ K the impact due to the correction of the cross sections is usually very minor: the average relative change in the magnitude of the rate coefficients is less then 0.5 per cent including all transitions in the analysis and the largest state-to-state change is below 4 per cent. These corrections are much smaller than the global accuracy of the collisional data (25-30 per cent) estimated by Demes et al. (2022). While the average relative difference for the rate coefficients at temperatures 150, 200, and 300 K are also low (0.5, 1.5, and 5.1 per cent, respectively), some specific transitions are significantly impacted. In particular, the largest state-specific correction at 150 K is about 15 per cent, while at 200 and 300 they reach \sim 41 and \sim 71 per cent, respectively. Except for some particular cases, the magnitude of the rate coefficients decreased after the corrections have been made in the cross section calculations. Large corrections (i.e. those above the global accuracy of the data) are almost entirely related to high-lying states (with $j_k^{\epsilon} \geq 5_5^+$, see table A1 in the Appendix of the original paper).

Regarding the radiative transfer modellings, the corrected data have a moderate impact, except for some specific transitions. Thus, most of the radiation temperatures (T_R) reported by Demes et al.

(2022) are well-reproduced with the corrected rate coefficients. At lower kinetic temperatures (50 and 100 K), the largest correction in the ratios $T_{\rm R}^{\rm curr.work}/T_{\rm R}^{\rm LAMDA}$ (see fig. 6 in the original paper) is less than 0.5 per cent and on average less than 0.1 per cent. At 200 and 300 K we found slightly larger impact due to the corrections, up to ~ 8 per cent for specific transitions with a mean of 0.5-4.0 per cent, depending on the temperature, H₂ and column densities. It is worth to mention however that at 10^6 cm⁻³ molecular and $N = 10^{16}$ cm⁻² column densities we found two strongly impacted transitions with larger changes in the T_R -ratios. In particular, after the corrections they decrease by ~ 37 per cent for the 364 GHz $3_2^+ \rightarrow 2_2^-$ transition, while for the 4241 GHz $4_1^- \rightarrow 3_1^+$ transition at 300 K the T_R -ratio decreases by a factor of \sim 40. This strong impact is however due to the large opacity of the line (> 100) which makes the convergence of RADEX difficult.

We would like to emphasise that the changes found due to the subsequent corrections do not affect the general discussion or the conclusion of the original paper. The corrected magnitude of the cross sections, rate coefficients, and radiation temperatures fully supports the original findings of the paper and only gives quantitative corrections. The updated set of collisional data is made available within the current supplementary material online as well as through the EMAA, LAMDA, and BASECOL databases.

Since the corrections of the data affected some values plotted in fig. 6 of the original paper, we provide the updated figures in the present notice as Fig. 1.

The authors apologize for any inconvenience due to the possible use of the incorrect supplementary data.

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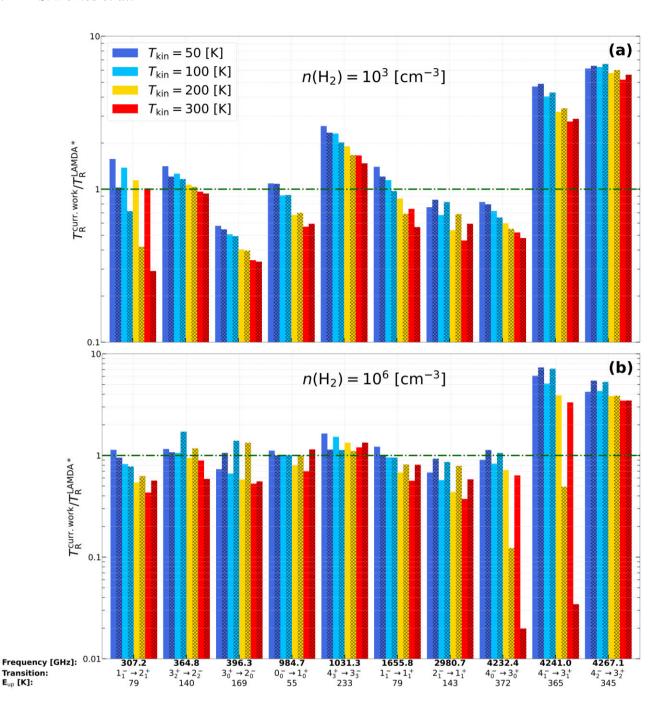


Figure 1. [Correction to fig. 6 originally published by Demes et al. (2022)] The relative ratio of radiation temperatures at 50, 100, 200, and 300 K kinetic temperatures for the majority of the observed radiative H_3O^+ transitions calculated for diffuse [panel (a), $n(H_2) = 10^3$ cm⁻³] and dense [panel (b), $n(H_2) = 10^6$ cm⁻³] molecular cloud conditions. The $T_R^{\text{curr.work}}$ data is computed from our new set of rate coefficients, while the $T_R^{\text{LAMDA}^*}$ set is calculated based on the corresponding collisional data from the LAMDA data base. The colour bars correspond for radiative transfer calculations in the optically thin environments ($N = 10^{13}$ cm⁻³), while the hatch-filled bars show the same quantities, but for optically thick regions ($N = 10^{16}$ cm⁻³).

REFERENCE

Demes S., Lique F., Faure A., van der Tak F. F. S., 2022, MNRAS, 518, 3593

SUPPORTING INFORMATION

Supplementary data are available at MNRAS online.

H3O+ - H2 RADEX input with rate coefficients.zip

H3O+ - H2 collisional cross sections.zip

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