

Erratum: Rotational relaxation of H₂S by collision with He (Astronomy & Astrophysics (2020) 638 (A31) DOI: 10.1051/0004-6361/202037821)

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Abstract

This is a corrigendum to Denis-Alpizar & Stoecklin (2020). Owing to an interface error in the implementation of the potential energy surface in the Newmat dynamics code, the cross sections and rate coefficients presented in Figs. 3, 4, and 5 and discussed in Sect. 3.2 of Denis-Alpizar & Stoecklin (2020), regarding the dynamics, appear to be significantly wrong and are replaced by the new Figs. 1, 2, and 3, respectively. The new cross sections and rate coefficients are of the same order of magnitude as the previous ones, but the sorting and the structures of the curves associated with different transitions are hardly comparable to the previous ones. As is detailed below, the main conclusions of our original manuscript remain, however, unchanged. The ($K_c = 0$) propensity rule mentioned in our original manuscript, which results from the fact that H₂S is a near oblate symmetric top, remains visible in Figs. 1 and 2 and it still becomes increasingly rigorous as j and the collision energy both increase. The transitions towards the levels the closest in energy to the initial one and associated with the lowest ($j = 0$ or 1) also give the largest cross sections, as noted previously. Conversely, the conservation of the parity index is not observable anymore for the lowest values of j , but it still appears to give the largest cross sections as j and the collision energy both increase. The comparison of our new results with the only experimental data available for this system appear to be quite a bit more satisfactory than before. Indeed, our calculated value for the depopulation rate coefficient rate of the 110 level of H₂S at 11.1K is now about 1.75 times larger ($3.06 \cdot 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) than the one reported by Ball et al. (1999) ($1.75 \cdot 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), while our previous value was three times larger than the one from their experiment. It is also interesting to see that the value ($4.0 \cdot 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) which can be obtained from the results of Dagdigian (2020) for the collision of H₂S with H₂ ($5.6 \cdot 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) by using the mass scaling (Formula present) is also in fair agreement with our results. If we now revisit in Fig. 3 the comparison we made previously between the H₂S + He and H₂O + He collisional systems, the temperature dependences are now seen to be similar for these two systems while they used to differ in our previous (Figure present) calculations. This result can be understood by reminding readers that the well depths of the two associated potential energy surfaces (PESs) are very close, while the ratio of the reduced masses of the two systems nearly equals one. Conversely, the magnitudes and the propensity rules are still quite different for some of the transitions as a result of both the differences in the angular anisotropies of the two PESs and in the rotational constants, H₂S being a nearly oblate symmetric top while H₂O is a good example of an asymmetric top intermediate case. The important conclusion of our uncorrected manuscript stating

that (Figure present) mass scaled HeH₂O data cannot be used to obtain those for He+H₂S then remains correct. The comparison, in the upper and lower panels of Fig. 3, of the rotational de-excitation rate coefficients of H₂S by collision with He from the initial states 2 2 1 and 2 2 0 of H₂S with those recently published by Dagdigan (2020) for the collisions with H₂ leads to similar conclusions as in our original paper. The rate coefficients for the two systems are still seen to differ both in the law variation as a function of temperature and in the propensity rules. Moreover, they now also differ more in magnitude than they previously did, and the explanations of these discrepancies remain the same: the well depth of the H₂?H₂S complex (146.8 cm⁻¹) calculated by Dagdigan (2020) is five times deeper than the one of He?H₂S, while the relative masses of the former is about a half of the later. The general conclusion of our paper is then unchanged. The scaling law based on the square root of the inverse ratio of the relative masses is not a good option to predict the rate coefficients for the collisions of H₂S with pH₂ (Figure present) from those with He, while the excitation rate coefficients with He need to be included in the modeling of the rotational excitation of H₂S. The new rates will soon be made available in the Basecol and Lambda database.