



**Erratum: Elastic rate coefficients for Li+H<sub>2</sub> collisions in the calibration of a cold-atom vacuum standard [Phys. Rev. A **99**, 042704 (2019)]**

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We found an error in our computation of the thermally averaged total rate coefficients for the collision of a room-temperature hydrogen dimer H<sub>2</sub> with an ultracold lithium sensor atom. We incorrectly accounted for the nuclear spin degeneracy and omitted the factor  $1/\sqrt{\pi}$  in the normalization over the Boltzmann distribution. Our corrected predictions for the thermally averaged rate coefficient for a 300-K H<sub>2</sub> gas and a 1- $\mu$ K Li gas are  $3.13(6) \times 10^{-9}$  cm<sup>3</sup>/s and  $3.18(6) \times 10^{-9}$  cm<sup>3</sup>/s for H<sub>2</sub>+<sup>6</sup>Li and H<sub>2</sub>+<sup>7</sup>Li, respectively, where the number in parentheses is the one-standard-deviation uncertainty in the last significant digit. Moreover, the temperature dependence of the corrected rate coefficients near 300 K is significantly smaller than in our original article.

Figure 1(a) shows corrected thermalized rate coefficients  $\sum_{v'j'} L_{v'j',vj}(T_{\text{Li}}, T_{\text{H}_2})$  as functions of H<sub>2</sub> temperature  $T_{\text{H}_2}$  with  $T_{\text{Li}} = 1 \mu\text{K}$  for the <sup>6</sup>Li isotope computed with coupled-channels calculations using our best ground-state potential-energy surface (PES) of the LiH<sub>2</sub> trimer. Here, H<sub>2</sub> is prepared in one of the rotational states  $j = 0, 1, \dots, 4$  of the  $v = 0$  vibrational level of its  $X^1\Sigma_g^+$  electronic state. For H<sub>2</sub> temperatures less than 450 K only these five rotational states have significant population. Also shown in Fig. 1(a) is the corrected thermalized total rate coefficient  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$ , which is a weighted sum of  $L_{v'j',vj}(T_{\text{Li}}, T_{\text{H}_2})$ . The state-to-state rate coefficients  $L_{v'j',vj}(T_{\text{Li}}, T_{\text{H}_2})$  and thermalized total rate coefficient  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$  are defined in Appendix B of our original article.

Figure 1(b) shows corrected thermalized rate coefficients  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$  as functions of H<sub>2</sub> temperature based on four determinations of the LiH<sub>2</sub> electronic potential-energy surface. These electronic potentials are labeled by TZ, QZ, 5Z, and  $\infty$ Z and correspond to increasing accuracy in the determination of the electronic potential-energy surface. Our most accurate potential has label  $\infty$ Z.

From Fig. 1(b) we observe that  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$  is close to linear near room-temperature H<sub>2</sub> and is well represented by Taylor expansion,

$$K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2}) = \mathcal{K}_0 + \mathcal{K}_1 (T_{\text{H}_2} - T_{\text{ref}}), \quad (1)$$

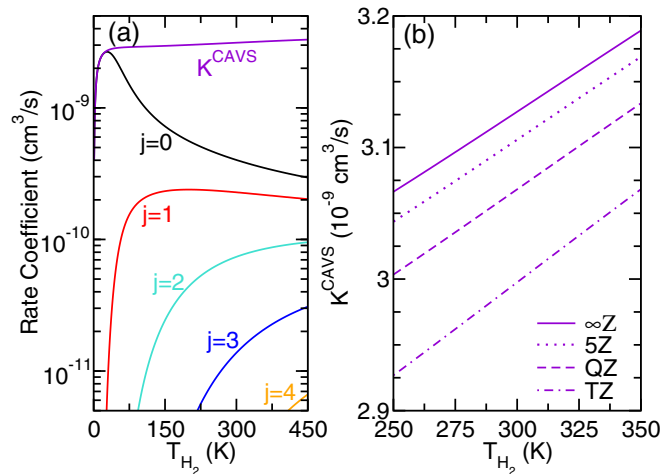


FIG. 1. (a) Rate coefficients  $\sum_{v'j'} L_{v'j',vj}(T_{\text{Li}}, T_{\text{H}_2})$  for rovibrational states  $v = 0, j = 0, 1, \dots, 4$  of H<sub>2</sub> and  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$  as functions of the H<sub>2</sub> temperature with <sup>6</sup>Li cold sensor atoms at  $T_{\text{Li}} = 1 \mu\text{K}$  using our most-accurate  $\infty$ Z PES. (b) Thermalized  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$  as a function of  $T_{\text{H}_2}$  around room temperature. The dashed-dot, dashed, dotted, and solid lines correspond to rate coefficients based on the TZ, QZ, 5Z, and  $\infty$ Z PESs.

TABLE I. Expansion coefficients  $\mathcal{K}_0$  and  $\mathcal{K}_1$  of the thermalized total rate coefficient  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$  for near room-temperature hydrogen molecules and  $1 \mu\text{K}$   ${}^6,{}^7\text{Li}$  sensor atoms with  $T_{\text{ref}} = 300 \text{ K}$ . The uncertainty  $\sigma(K^{\text{CAVS}})$  is found by error propagation with correlation coefficient  $r(\mathcal{K}_0, \mathcal{K}_1) = 1$ .

Sensor atom	$\mathcal{K}_0$ ( $\text{cm}^3/\text{s}$ )	$\mathcal{K}_1$ ( $\text{cm}^3/\text{s/K}$ )
${}^6\text{Li}$	$3.13(6) \times 10^{-9}$	$1.24(8) \times 10^{-12}$
${}^7\text{Li}$	$3.18(6) \times 10^{-9}$	$1.21(8) \times 10^{-12}$

with expansion coefficients  $\mathcal{K}_i$  and  $T_{\text{ref}} \equiv 300 \text{ K}$ . The corrected values and one-standard-deviation uncertainties for the  $\mathcal{K}_i$  can be found in Table I for both  $\text{H}_2+{}^6\text{Li}$  and  $\text{H}_2+{}^7\text{Li}$ . Uncertainties of  $K^{\text{CAVS}}(T_{\text{Li}}, T_{\text{H}_2})$  are based on differences from calculations with the QZ and  $\infty\text{Z}$  PESs (see also our original article). The Taylor expansion reproduces the coupled-channels result to about 0.1% for a  $\pm 50\text{-K}$  region around  $T_{\text{H}_2} = T_{\text{ref}}$  for each of the potentials. The dependence on the Li temperature up to  $100 \mu\text{K}$  is negligible.

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