

Erratum: Opposite Effects of the Rotational and Translational Energy on the Rates of Ion-Molecule Reactions near 0 K: The $D_2^+ + NH_3$ and $D_2^+ + ND_3$ Reactions [Phys. Rev. X **14**, 011034 (2024)]

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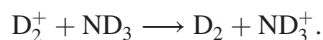


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In this paper, an error was found in a script used to calculate the state-averaged capture rate coefficients of the $D_2^+ + NH_3$ and $D_2^+ + ND_3$ reactions presented in Figs. 2 and 8 for comparison with the experimental results. The script erroneously contained $2J + 1$ weighting factors for the individual Stark states. Affected by this error are Figs. 2(c), 2(f), 8(b), and 8(d). The corrected versions of these figures are reproduced herein. The main consequence of this error is that the increase of the state-averaged capture rate coefficients with increasing rotational temperature becomes dominant at lower collision energies than reported. To highlight the increase of the state-specific capture rate coefficients with increasing rotational excitation, insets have been added in Figs. 2(e) and 2(f), which show the data for the $D_2^+ + ND_3$ reaction at low collision energies on an enlarged scale. The corrected figures are compatible with the calculated state-averaged capture rate coefficients of the $He^+ + NH_3$ and $He^+ + ND_3$ reactions presented in Figs. 4(c) and 4(d) of Ref. [1].

In addition, Eq. (3) [$D_2^+ + ND_3 \rightarrow D_2 + NH_3^+$] must be corrected to



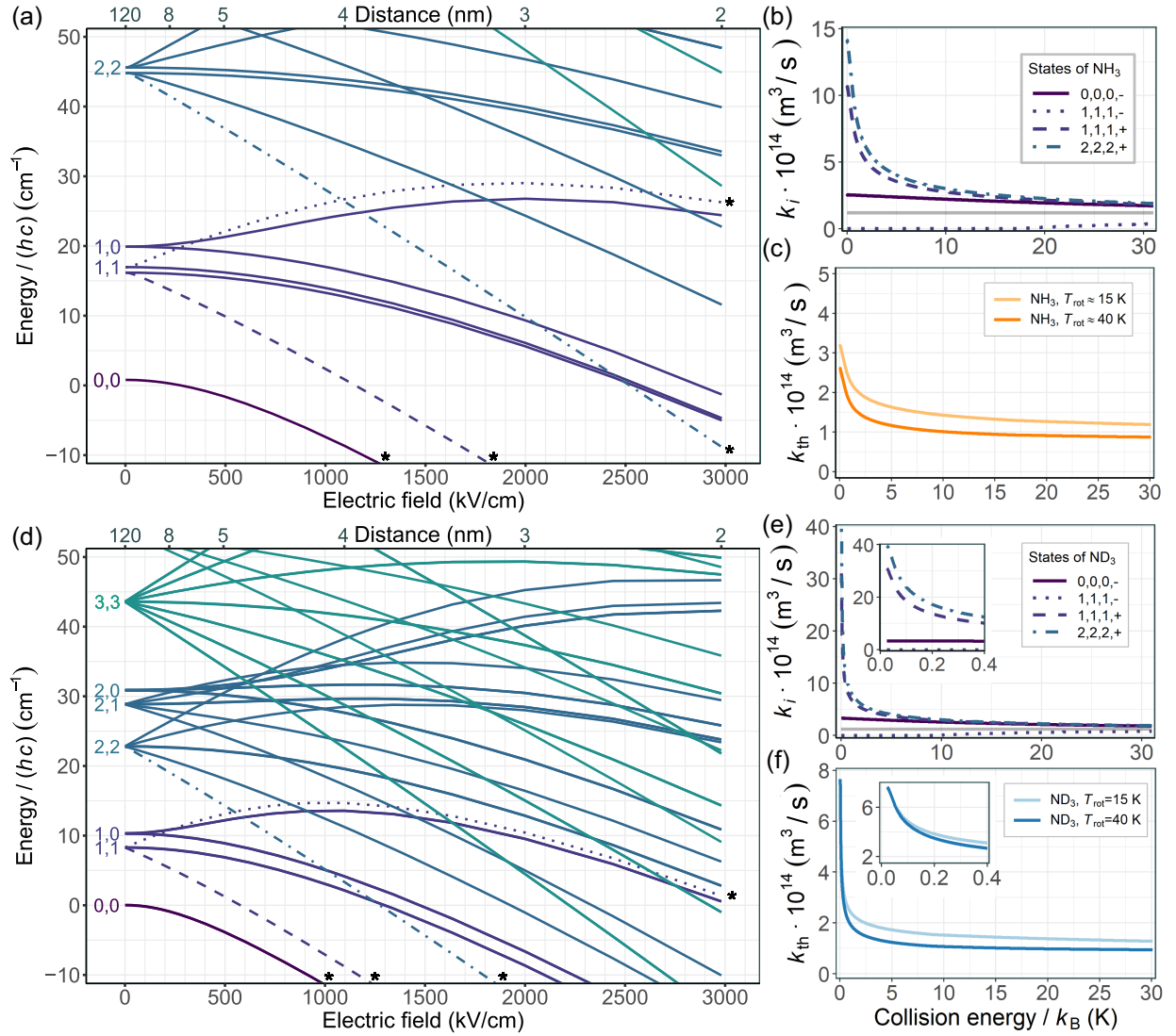


FIG. 2. Rotationally adiabatic capture model for NH_3 (a)–(c) and ND_3 (d)–(f). (a) Stark map of the rotational levels of NH_3 in the electric field of a pointlike ion at a given distance (top axis). The rotational states are labeled on the left by their quantum numbers (J, K) . (b) State-specific capture rate coefficients of the four states labeled with an asterisk in (a): $J = 0, K = 0, |M| = 0, p = -$ (solid, dark purple), $J = 1, K = 1, |M| = 1, p = +$ (dashed, indigo), $J = 1, K = 1, |M| = 1, p = -$ (dotted, indigo), and $J = 2, K = 2, |M| = 2, p = +$ (dash-dotted, teal). The Langevin rate coefficient is indicated by the gray horizontal line. (c) Averaged capture rate coefficients $k_{\text{th}}(E_{\text{coll}}, T_{\text{rot}})$ obtained using the calculated state-specific rate coefficients and the occupation probabilities of the rotational states for an expansion of pure NH_3 ($T_{\text{rot}} \approx 40$ K) (dark orange) and a seeded expansion (5%) in He ($T_{\text{rot}} \approx 15$ K) (light orange). (d)–(f) Same as (a)–(c) but for ND_3 .

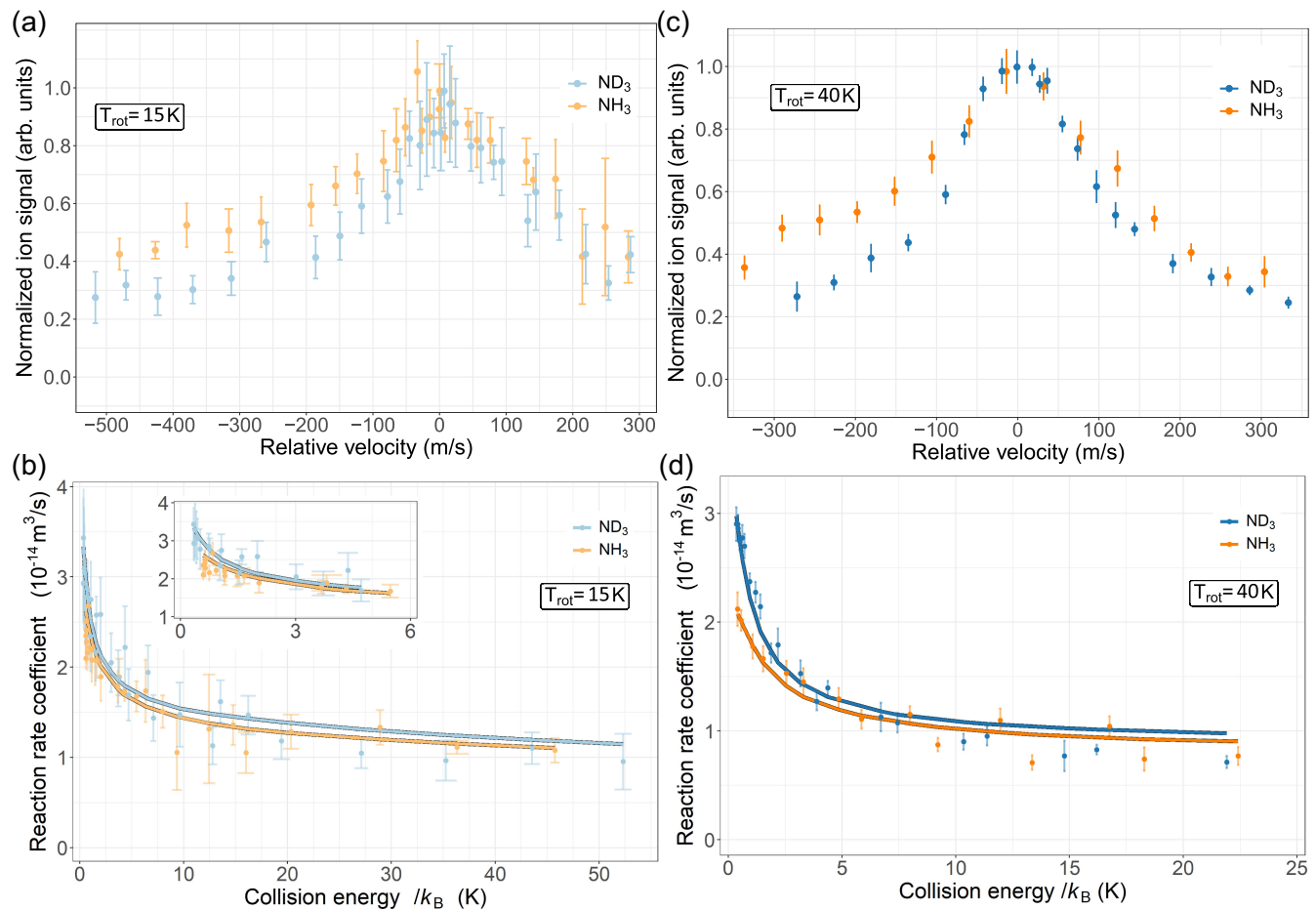


FIG. 8. Product-ion signals of the $D_2^+ + NH_3$ and $D_2^+ + ND_3$ reactions as measured for the seeded NH_3 and ND_3 samples (a) and for the pure NH_3 and ND_3 samples (c), given as a function of the nominal relative velocity. The experimental data (dots) are scaled by a global factor and compared to the calculated reaction rate coefficients averaged over the measured distributions of rotational states and collision energies $\rho(E_{coll}; v_f)$ (solid lines) for the seeded samples (b) and for the pure samples (d).

- [1] V. Zhelyazkova, F. B. V. Martins, J. A. Agner, H. Schmutz, and F. Merkt, *Multipole-moment effects in ion-molecule reactions at low temperatures: Part I—ion-dipole enhancement of the rate coefficients of the $He^+ + NH_3$ and $He^+ + ND_3$ reactions at collisional energies E_{coll}/k_B near 0 K*, *Phys. Chem. Chem. Phys.* **23**, 21606 (2021).