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Addition/Correction

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Correction to "High-Accuracy Theoretical Thermochemistry of Atmospherically Important Sulfur-Containing Molecules"

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Because of a data processing error, our previously published[1] heat of formation values for the radical S_2COH at both 0 and 298.15 K are incorrect. This erratum does not affect either the entropy data of the radical, $S^\circ_{298}(S_2COH)$, or any other parts of the discussion and the final conclusions published in the original article. Nevertheless, the correction of the enthalpy results is necessary.

Page 7828: In the last row of Table 2, the correct values for $\Delta_f H^\circ_0(S_2COH)$ and $\Delta_f H^\circ_{298}(S_2COH)$ are 20.1 ± 4.6 and 15.1 ± 4.6 kJ/mol, respectively.

Page 7830: In Table 3 of the original article, the correct thermodynamical parameters for reaction $CS_2 + OH \rightleftharpoons S_2COH$ are as follows: $\Delta_r H^\circ_{298} = -138.9$ kJ/mol, $\Delta_r G^\circ_{298} = -101.8$ kJ/mol, $K = 2.80 \times 10^{-2}$, and $f = 2.4$.

Page 7831: In the first sentence of the second paragraph, the $\Delta_f H^\circ_0$ and $\Delta_f H^\circ_{298}$ values for S_2COH are also incorrect. The sentence with the correct results is as follows: "Our results for the C- and S-adducts of CS_2OH are $\Delta_f H^\circ_0(S_2COH) = 20.1 \pm 4.6$ kJ/mol, $\Delta_f H^\circ_{298}(S_2COH) = 15.1 \pm 4.6$ kJ/mol, $\Delta_f H^\circ_0(SCSOH) = 111.4 \pm 5.0$ kJ/mol, and $\Delta_f H^\circ_{298}(SCSOH) = 108.9 \pm 5.0$ kJ/mol."

REFERENCES

(1) Nagy, B.; Szakács, P.; Csontos, J.; Rolik, Z.; Tasi, G.; Kállay, M. High-Accuracy Theoretical Thermochemistry of Atmospherically Important Sulfur-Containing Molecules. *J. Phys. Chem. A* **2011**, *115*, 7823−7833.

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