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Correction to “Isotope Effect in D₂O Negative Ion Formation in Electron Transfer Experiments: DO–D Bond Dissociation Energy”

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 Article Recommendations

 Supporting Information

In a recent Letter,¹ a set of minor inconsistencies have been found in the main body text and in the [Supporting Information](#) files; these are now thoroughly corrected. Thus, we highlight the sections where these changes apply.

■ MAIN MANUSCRIPT BODY TEXT

Abstract: The DO–D bond dissociation energy has been reported to be 5.41 ± 0.10 eV, while considering EA(O) in the original manuscript. However, EA(OD) should be used instead, thus leading to a bond dissociation energy of 5.28 ± 0.20 eV.

Page 5365, left column, second paragraph; “From the appearance...” is reorganized and reads as follows:

Taking the values in [Table S4](#) together with the BDE, the enthalpy of reaction can be obtained from $\Delta H_r(\text{OH}^-) = D(\text{H}-\text{OH}) - \text{EA}(\text{OH}) = 3.34$ eV. In the charge transfer process, if we add the potassium ionization energy, OH⁻ is expected at 7.68 eV. The reactions threshold was obtained assuming no excess energy (E^\ddagger), yet momentum conservation of the dissociating partners may impact on the lighter fragment kinetic energy, thus shifting the energy to a higher value. We note a difference of ~ 1.1 eV for the energy loss data, which is certainly plausible given the kinetic-energy release distribution of H⁻ in [Figure S3](#). Thus, from the appearance energy (AE) in the H₂O energy loss spectrum ([Figure 2](#)) at $\Delta E \approx 8.8$ eV, one can obtain the HO–H bond dissociation energy (BDE) by taking the potassium ionization energy and the data from [Table S4](#),² i.e., $D(\text{HO}-\text{H}) = \text{AE}(\text{OH}^-) - \text{IE}(\text{K}) + \text{EA}(\text{OH}) - E^\ddagger$, yielding therefore $D(\text{HO}-\text{H}) = 5.19 \pm 0.20$ eV which is in good agreement with the values 5.15 eV (118.81 ± 0.07 kcal/mol)³ and 5.17 eV.⁴ Following the same approach for D₂O, the energy loss spectrum shows a threshold feature at $\Delta E \approx 9.0$ eV. We obtain for the first time the DO–D bond dissociation energy to be $D(\text{DO}-\text{D}) = 5.28 \pm 0.20$ eV. In D₂O the DO–D energy value is slightly higher than the O–D bond dissociation energy (5.176 eV⁵), which is in agreement with its analogue H₂O.

Page 5366, right column, last paragraph; “Electronic state spectroscopy...” reads as follows:

The electronic state spectroscopy of H₂O/D₂O was thoroughly discussed from the experimental K⁺ energy loss spectra obtained, from which the DO–D bond dissociation energy has been obtained for the first time to be 5.28 ± 0.20 eV.

■ SUPPORTING INFORMATION

Enthalpies of formation ($\Delta_f H_g^\circ$) in reactions 2a.1–2b.2 and 4a.1–4b.2 are actually enthalpies of reaction (ΔH_r). [Table S2](#) decimal places for O⁻ and OH⁻ from H₂O have been corrected; they now read 12.08 ± 0.20 and 7.80 ± 0.20 .

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.jpcllett.3c02406>.

Revised Supporting Information file ([PDF](#))

■ REFERENCES

- (1) Kumar, S.; Hoshino, M.; Kerkeni, B.; García, G.; Limão-Vieira, P. Isotope Effect in D₂O Negative Ion Formation in Electron Transfer Experiments: DO–D Bond Dissociation Energy. *J. Phys. Chem. Lett.* **2023**, *14*, 5362–5369.
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- (3) Ruscic, B.; Wagner, A. F.; Harding, L. B.; Asher, R. L.; Feller, D.; Dixon, D. A.; Peterson, K. A.; Song, Y.; Qian, X.; Ng, C. Y.; et al. On the Enthalpy of Formation of Hydroxyl Radical and Gas-Phase Bond Dissociation Energies of Water and Hydroxyl. *J. Phys. Chem. A* **2002**, *106*, 2727–2747.
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