

**Erratum: “Core hole screening and decay rates of double core ionized first row hydrides” [J. Chem. Phys.138, 164304 (2013)]**

L. Inhester, G. Groenhof, and H. Grubmüller

Citation: *The Journal of Chemical Physics* **141**, 069902 (2014); doi: 10.1063/1.4892983

View online: <http://dx.doi.org/10.1063/1.4892983>

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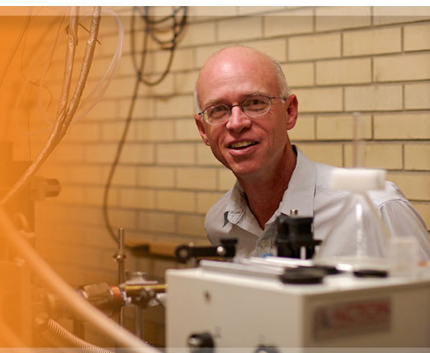
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## Erratum: “Core hole screening and decay rates of double core ionized first row hydrides” [J. Chem. Phys. **138**, 164304 (2013)]

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(Received 31 July 2014; accepted 1 August 2014; published online 12 August 2014)

[<http://dx.doi.org/10.1063/1.4892983>]

We discovered a sign error in our implementation of the (correct) expression for the exchange interaction between the Auger electron and the bound electrons (Eq. (2)). As a consequence, the Auger rates reported in the aforementioned article<sup>1</sup> are not correct. We have corrected the error in our implementation and recomputed the single and double core Auger rates for all molecules. After correcting the sign of the exchange potential the computed Auger decay rates are slightly smaller. The deviation to previously published values is slightly larger, but still comparable to the deviations between the two theoretical works<sup>2,3</sup> and experiments.<sup>4-6</sup> Since both single and double core Auger rates were overestimated, the conclusions we draw, which were concerned with the ratio between the double and single-core Auger rates, remain unaltered. Therefore, with this correction Tables I–III and Figure 1 of the original article need to be replaced by the tables and the figure in this erratum. The tables and figures can be found in the supplemental material.<sup>7</sup>

<sup>1</sup>L. Inhester, G. Groenhof, and H. Grubmüller, “Core hole screening and decay rates of double core ionized first row hydrides,” *J. Chem. Phys.* **138**, 164304 (2013).

<sup>2</sup>P. Kolorenč and V. Averbukh, “K-shell Auger lifetime variation in doubly ionized Ne and first row hydrides,” *J. Chem. Phys.* **135**, 134314 (2011).

<sup>3</sup>F. Larkins, “Influence of core hole screening on molecular Auger rates and inner-shell lifetimes,” *J. Electron Spectrosc. Relat. Phenom.* **67**, 159 (1994).

<sup>4</sup>T. X. Carroll, N. Berrah, J. Bozek, J. Hahne, E. Kukk, L. J. Sæthre, and T. D. Thomas, “Carbon 1s photoelectron spectrum of methane: Vibrational excitation and core-hole lifetime,” *Phys. Rev. A* **59**, 3386 (1999).

<sup>5</sup>H. M. Köppe, B. S. Itchkawitz, A. L. D. Kilcoyne, J. Feldhaus, B. Kempgens, A. Kivimäki, M. Neeb, and A. M. Bradshaw, “High-resolution c 1 s photoelectron spectra of methane,” *Phys. Rev. A* **53**, 4120 (1996).

<sup>6</sup>R. Sankari, M. Ehara, H. Nakatsuji, Y. Senba, K. Hosokawa, H. Yoshida, A. D. Fanis, Y. Tamenori, S. Aksela, and K. Ueda, “Vibrationally resolved O 1s photoelectron spectrum of water,” *Chem. Phys. Lett.* **380**, 647 (2003).

<sup>7</sup>See supplementary material at <http://dx.doi.org/10.1063/1.4892983> for Tables I–III and Figure 1.

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