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

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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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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[1] 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[2,3] and experiments.[4–6] 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.[7]

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

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