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Erratum

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Correction to Variational, Self-Consistent Implementation of the Perdew−Zunger Self-Interaction Correction with Complex Optimal Orbitals

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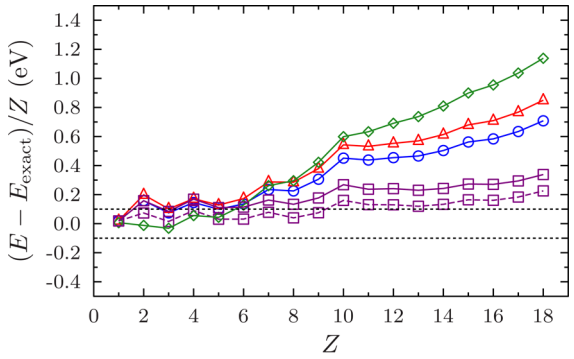
Figure 2b in our article[1] was by mistake identical to Figure 2c. The correct Figure 2b is shown below. We can add that



(b) PZ-SIC with real orbitals.

Figure 2. Effect of PZ-SIC on energy of atoms. The legend is the same as in the original manuscript.

we have subsequently made an implementation based on complex canonical orbitals and found that in the case of acrylic acid the restriction to real canonical orbitals had caused a significant error in the density matrix, and consequently, the energy as suggested by one of the reviewers. The other results presented in the article were not affected. The implementation with fully complex orbitals will be detailed in a later article.

REFERENCES

(1) Lehtola, S.; Jónsson, H. *J. Chem. Theory Comput.* **2014**, *10*, 5324−5337.

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