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The original version of this Article contained errors in the reference list, in which reference [80] “Aquilante, F. et al. Molcas 8: new capabilities for multiconfigurational quantum chemical calculations across the periodic table. *J. Comput. Chem.* 37, 506–541 (2016)” was incorrectly given as [81], reference [81] “Ponder, J. W. & Richards, F. M. Tinker molecular modeling package. *J. Comput. Chem.* 8, 1016–1024 (1987)” was incorrectly given as [82], reference [82] “Fdez Galván, I. et al. OpenMolcas: from Source Code to Insight. *J. Chem. Theory Comput.* 15, 5925–5964 (2019)” was incorrectly given as [83], and reference [83] “Briand, J. et al. Coherent ultrafast torsional motion and isomerization of a biomimetic dipolar photoswitch. *Phys. Chem. Chem. Phys.* 12, 3178–3187 (2010)” was incorrectly given as [80]. This has been corrected in the PDF and HTML versions of the Article.

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