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Erratum: “Several Levels of Theory for Description of Isotope Effects in Ozone: Effect of Resonance Lifetimes and Channel Couplings”

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Erratum: “Several levels of theory for description of isotope effects in ozone: Effect of resonance lifetimes and channel couplings” [J. Chem. Phys. **149**, 164302 (2018)]

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The notions of *isotopomer* and *isotopologue* were used inconsistently throughout the paper.¹ The correct use of these concepts is clarified here. Consider ozone molecules substituted with rare isotope ¹⁸O. In this case, one could define symmetric and asymmetric *isotopomers* for singly and doubly substituted *isotopologues*, as summarized in Table I:

TABLE I. Definitions of isotopomers and isotopologues in ozone.

Isotopologues	Symmetric isotopomers	Asymmetric isotopomers
Singly-substituted	¹⁶ O ¹⁸ O ¹⁶ O	¹⁶ O ¹⁶ O ¹⁸ O, ¹⁸ O ¹⁶ O ¹⁶ O
Doubly-substituted	¹⁸ O ¹⁶ O ¹⁸ O	¹⁸ O ¹⁸ O ¹⁶ O, ¹⁶ O ¹⁸ O ¹⁸ O

Indeed, different *isotopomers* are isotopic isomers that can be found in different parts of the global potential energy landscape. The rotational-vibrational states of both symmetric and asymmetric *isotopomers* of the same *isotopologue* are computed at once. Namely, if the global potential energy surface is used, the states of ¹⁶O¹⁸O¹⁶O, ¹⁶O¹⁶O¹⁸O, and ¹⁸O¹⁶O¹⁶O (all *isotopomers* of singly-substituted *isotopologue*) are computed all together in one run. The states of ¹⁸O¹⁶O¹⁸O, ¹⁸O¹⁸O¹⁶O, and ¹⁶O¹⁸O¹⁸O are computed in the second run but also together (all *isotopomers* of doubly-substituted *isotopologue*).

The definitions of isotopomer and isotopologue can be found in Ref. 2.

¹A. Teplukhin, I. Gayday, and D. Babikov, “Several levels of theory for description of isotope effects in ozone: Effect of resonance lifetimes and channel couplings,” *J. Chem. Phys.* **149**, 164302 (2018).

²V. I. Minkin, “Glossary of terms used in theoretical organic chemistry,” *Pure Appl. Chem.* **71**, 1919–1981 (1999).

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