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](https://aip.scitation.org/doi/10.1063/1.5079540) 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](https://aip.scitation.org/doi/10.1063/1.5079540#t1):

**TABLE I.** Definitions of isotopomers and isotopologues in ozone.

|  |  |  |
| --- | --- | --- |
| **Isotopologues** | **Symmetric isotopomers** | **Asymmetric isotopomers** |
| Singly-substituted | 16O18O16O | 16O16O18O,18O16O16O |
| Doubly-substituted | 18O16O18O | 18O18O16O,16O18O18O |

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](https://aip.scitation.org/doi/10.1063/1.5079540).

# REFERENCES

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2. V. I. Minkin, “Glossary of terms used in theoretical organic chemistry,” Pure Appl. Chem. **71**, 1919–1981(1999). <https://doi.org/10.1351/pac199971101919>,