Reviewer's comment:

"However, I still want to kindly remind the authors that some potential readers might not be very familiar with the terminologies in your field, especially for journals like ACP, which cover a wide range of topics. Therefore, more patient and detailed explanations in the manuscript and supplementary materials would always be very helpful for a broad range of future readers. Specifically, many experimentalists might not be well-versed in all the details of quantum computation. Without more detailed clarifications, the application and implication of your work might be limited. In addition, the initial submission contained many typos and numerical errors, which have been corrected. However, in the latest version (the one attached in R5), there are still several obvious typos, e.g., in the abstract, line 14, there are two periods at the end of the sentence; but in the conclusion, line 340, that sentence ends without a period."

We have added a supportive paragraph to the SI in part 4. Computed data for norpinonic acid.

In this study, computational methods were used to confirm the proper localization of all isomers, transition states and intermediates. The procedure was performed in several steps. In the first step, the isomeric structures of the deprotonated MBTcA (anion structures) were optimized. This was followed by scan-type calculations by varying in incremental steps the interatomic distances, which allow tracking the chemical transformation and identifying the transition state on the path. Once the transition state has been found, the next step was to optimise the transition states, whose verification was based on vibration analysis (one of the vibrations for the transition state must be negative) and IRC (Intrinsic Reaction Coordinate) calculations to check whether form the transition state the reaction can lead to the substrate (reverse) and to the product (forward) structures. Calculations were carried out using three different functionals to find the one that most closely approximates the experimental results. The optimised isomers and transition states for each of the fragmentation steps were then subjected to energy analysis, where it was shown that the Gibbs free energy difference most closely matched the experimental results. The use of computational methods makes it possible to analyse and distinguish isobaric structures of the same molecular mass but different geometries, which is not possible using only experimental methods. In addition, quantum chemical modeling techniques allows to draw mechanistic picture, including the identification of the transition state structures and key intermediates that are not structurally detectable in the experiment (Elm J, Ayoubi D, Engsvang M, Jensen AB, Knattrup Y, Kubečka J, et al. Quantum chemical modeling of organic enhanced atmospheric nucleation: A critical review. WIREs Comput Mol Sci. 2023; 13(5):e1662. https://doi.org/10.1002/wcms.1662).