

Response to Reviewer 2 Comments

Thank you for such valuable questions and recommendations that allowed us to strengthen this work. Below are the responses to yours comments and recommendations:

Point: The present manuscript aims to find lipophilicity of some organophosphate pesticides, with the help of theoretical techniques. They have employed continuum solvation model to simulate solvent environment and estimate distribution coefficients and compare with experimental results. Also, they have shown that some methods (which takes dispersion effects into account) provide satisfactory results. Calculations and employed models are quite routine and I could find no interesting results or conclusion. Performance and applications of DFT methods are well understood and conclusions about these methods are trivial. Therefore, I do not recommend publication of this manuscript.

Response: The methods considered in the article were not previously applied to the determination of the lipophilicity of pesticides and there was no assessment of their accuracy and characteristics of the computing resources used. Such works may be of great interest to the agro-industry and ecology for predicting the properties of new substances. The conclusions are supplemented and highlighted in yellow.

Other points:

1- The authors have stated that initial structures were chosen with respect to symmetry criteria. Most of the considered molecules possess no symmetry. What symmetry criteria are chosen? Moreover, symmetry-based sampling does not necessarily give rise to most minimum structure. Alternatively, the authors should at least (but not limited to) perform a conformational search.

Response 1:

There was a typo in the text. Geometric optimization of molecules was carried out without symmetry restrictions. Conformational search was not carried out, since the molecules are relatively small. The corresponding changes have been made to the manuscript of the article.

2- The authors have mixed different definitions up, rising phrases with no physical meaning:

What is "functional basis sets"? functional and basis set are two distinct mathematical objects.

What is "ab-initio density functional theory methods"? None of DFTs in this manuscript are ab-initio.

Response 2:

We agree with your remark. Corrections have been made to the text of the manuscript (and highlighted in yellow).

Absence of imaginary frequencies in the calculated IR spectra? Can an imaginary frequency exist in spectrum? Do the authors mean imaginary frequency in harmonic vibrational frequency analysis?

Response 3: An imaginary frequency cannot exist in the real experimental spectrum. In the calculated IR spectrum, there can be any imaginary frequency, even a very small one. This shows that the structure is incorrect, and its total energy and other properties based on energy and geometry will be incorrect.