**Response to the Reviewers' Comments on Manuscript FPE-D-18-00388**

To: Prof. Ioannis Economou

Editor

Fluid Phase Equilibria

Dear Prof. Economou:

Thank you for your message forwarding the reviewer’s comments on our manuscript entitled “Evaluation of the SAFT-γ Mie force field with solvation free energy calculations”. We have carefully addressed all comments, which required us to make changes in the text. To facilitate your evaluation, we have attached an annotated version in which we crossed out in red all removed text and incorporated new content in blue.

We hope the revised version of our manuscript is suitable for publication in this journal.

Sincerely yours,

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| Charlles R. A. Abreu  Assistant Professor  Federal University of Rio de Janeiro | Isabela Quintela Matos  Ph.D. Student  Cornell University |

**Reviewer #1: FPE-D-18-00388R1**

**Reviewer:**

**This is not a justification to use or not a value or to select some. In fact, the acentric factor can be calculated from the experimental data of vapor pressure as the authors used in fig. 2**

Our answer:

In fact, the piece of information which I were not able to find, despite all our effort, is the liquid density of phenanthrene at Tr = 0.7.

**Reviewer:**

**From a statistical point of view, the author's statement is right. However, from a Thermodynamic point of view, there are three different effects that cannot be fitted only using vapor pressure. This is a thermodynamic fact rather than a statistical issue. The author should try to calculate the enthalpy of vaporization to see the performance of the proposed molecular parameters. The main idea is to provide molecular parameters that can be used for prediction.**

Our answer:

To try to settle the question of which parameters are better for phenanthrene, we carried out a whole new set of molecular dynamics, expanded ensemble simulations and calculated the solvation free energies of phenanthrene in all different solvents using the parameters suggested by the reviewer. The new results were included in Tables 2 and 5 of the revised manuscript, and discussions were included in the text. Please find the inclusions highlighted in blue in the provided annotated manuscript.

**Reviewer:**

**The authors claim that the public (not publicly) information is not available, therefore, the used other information. This is not a valid reason, In fact, in the previous review, this information was included. An also described some points out of the scope of this work.**

**In any case, the goal of this work is not a procedure to find molecular parameters. The main point is to use them to calculate solvation energy. Therefore, it must be necessary that the used molecular parameters display a thermodynamic consistency.**

Our answer:

Even though we disagree with the statement that these data are public, we used the information provided by the reviewer regarding the density of phenanthrene at Tr = 0.7. The results obtained with these parameters are shown in Tables 2 and 5 of the revised manuscript.