

***Interactive comment on “Technical Note:
Estimating fusion properties for polyacids” by
S. Compernelle et al.***

Anonymous Referee #2

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The authors present a simple model for prediction of some thermo-chemical properties of polyacids and test it against experimental values. Results are statistically compared with other approaches.

I can recommend publication only after a major revision and reconsideration.

- General comments.

This work may certainly be interesting. Aerosol scientists need methods for estimating thermo-chemical properties of organic compounds commonly found in atmospheric particles.

The following points should be addressed to render the manuscript helpful.

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1. The dataset is limited. The number of compounds could be implemented with some monocarboxylic and tricarboxylic acids. Moreover, the authors use one single reference per compound and property (Table 1). Please justify this choice, or implement with other datasets. One could otherwise consider the good performance of the model as purely accidental, based on similar compounds and on one, specific experimental result.

2. The model, for the general reader, may appear arbitrary in its construction. What are the reasons for choosing that set of variables (τ , n_{OH} , and n_{CO}): physico-chemical or purely statistical? Did the authors try different combination of variables and took at the end the best choice justified by a satisfactory statistical PRESS approach?

3. Table 6 should be extended to all the other suitable compounds and properties and include the experimental and producer's values for comparison (where available). It may be merged with Table 1 and/or 2, for instance.

4. There is a lack of graphical visualization of the results (6 tables and no figure). For instance, one graph with estimations versus experimental results would be desirable.

- Specific comments.

Suggested Title: “Technical Note: Estimating fusion properties of a series of polyacids”.

Introduction. The authors do not mention experimental methods. The reader cannot distinguish high T methods from ambient T, or bulk from particles.

7536, 2. The statement is too strong. There is experimental evidence, and theoretical support, that multi-component OA is likely to be liquid, or partially liquid.

7536, 25. Reformulate. I would mention the possibility of solid stable/liquid metastable state of those compounds in a condensed phase.

7537, 2. “Very prone to error”. This is in principle true, but actually there are also examples of amazing agreement. Succinic acid (you cite Ribeiro and DaSilva, 2001) is

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one example. Reformulate.

7537, Eq1 - and 7538, line 4. The authors do not talk about ΔC_p . This is critical to get the correct liquid state vapor pressure from the solid state, since ΔC_p can vary from zero up to ΔS . Can the authors say something (briefly) on the best choice of ΔC_p based on their estimate of the other fusion properties?

7538 Eq3,4,5. How did you calculate the STD? Please reformulate lines 19-22.

Section 5. Too short. Expand or move it before.

Table 2. Please add a column with producer's values: they are often used for back of the envelope calculations, but can differ substantially among different experimental methods.

- Minor/Technical comments.

7539, 3. Roughly speaking(?)

7541, 14. As is well known (?)

7543, 1. Table 3? You probably mean Table 4.

7543, 3. This should of course not be a surprise(?)

7543, 10. no way (?)

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 7535, 2011.