

## ***Interactive comment on “Development of a protocol for the auto-generation of explicit aqueous-phase oxidation schemes of organic compounds” by P. Bräuer et al.***

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### **1 General comments**

The paper presents an interesting extension of existing auto-generation mechanisms to include aqueous-phase reactions. The work is novel, and fits well within the scope of ACP. Thorough literature review work is presented, evaluating data and rate constant prediction methods, carefully discussing the limitations and rationalising the choices made for the new CAPRAM/GECKO-A protocol. The new mechanism is also evaluated against experimental chamber data. Overall, the paper is well-structured, though

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rather long. I would recommend trying to shorten the manuscript before publication by scanning for any obviously repeated concepts and superfluous content, as well as carefully reviewing the grammar and ensuring all sentences are easy to parse (I cannot guarantee to have caught all typos, grammatical mistakes, and unclear sentences, but the ones I have are highlighted below – there are also some excess commas in places; please proofread the article again carefully). However, it is definitely suitable for publication in ACP subject to revision.

### **2 Specific comments**

While I have found the written text (despite the reservations above) for the most part easy to follow, I believe some of the figures used are quite difficult to read and interpret, and would benefit from replotting.

This applies in particular to Figure 1, where I am struggling to see what the different boxplots represent. Figures 3, 4, 5, 7, S1, S3, S4, S5, S6 and S7 would benefit from using different symbols as markers rather than just different colours, as some of the colours are quite difficult to distinguish. Figure 8 could be made clearer by using more significantly different markers (rather than crosses with different orientations). The figures showing simulation data can only be understood in conjunction with careful reading of the main text, and would benefit from more detailed descriptions in their labels.

I would try to move more of the detail into the ESM, as the main text is currently very long. For example, at present, sections discussed at length in the ESM are still discussed in a lot of detail in the main text (e.g page 2 and page 7), when referencing the ESM should be enough. The text also feels unnecessarily long when sections are introduced carefully, and then go on to repeat the context mentioned previously.

The new “advanced” Evans-Polanyi correlation strikes me as unusual, in that it can no

C2

doubt usefully scale with molecular size – but it would intuitively seem to me that we are losing most of the useful information that the individual bond enthalpies provide by lumping them into one sum. There ought to be a “better” way of accounting for more than the weakest bond than using the sum of BDEs, and perhaps this will be something that can be further improved in the future.

### 3 Technical corrections

p1, line 19: change “was” to “were” for consistency with plural usage of “data” elsewhere

p1, line 30: add “The” at start of sentence

p1, line 39: add “a” before “supplementary tool”

p1, line 40: change “understanding” to “understand”

p2, line 3-4: review sentence

p2, line 36-39: review sentence

p3, line 1-3: review sentence (singular/plural inconsistency)

p3, line 9-11: review sentence

p3, line 12: rephrase to “kinetic data available in the literature”

p3, line 13: get rid of last “reactions”

p3, line 17: add “The” at start of sentence

p3, line 29: review choice of word “actuality”

p3, line 31: add “The” at start of sentence

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p4, line 11: add “The” at start of sentence

p4, line 13: review use of word “disqualify” (should be in passive voice)

p4, line 22: add “the” best results

p4, line 32: review use of word “disqualifies” (as above), and remove first “are”

p4, line 33: “functional predication”?

p5, line 1: Arrhenius expression is presented as a mixture of logarithmic and normal form, making it incorrect; also, odd to refer to the atoms as weak, rather than bonds

p5, line 23: rephrase “are resulting”

p6, line 4/5: mistakenly referring to  $R^2$  value as correlation coefficient

p6, line 7: placement of brackets should include “molecules”?

p6, line 14: “are” should be “is” in both cases, or else get rid of “a” at the end of the previous line

p7, line 32: “suggest” should say “suggested”

p8, line 3/4/5: review choice of word “increment” here (appears three times in total)

p8, line 7: add “the” literature

p8, line 12: “phosphorous” should say “phosphorus” and would link with hyphen to “containing” for consistency

p8, line 28: “introduce” should say “introduced”

p8, line 34: add “The” at start of sentence

p9, line 7: change comma before “however” to a semicolon

p9, line 28: add comma after “therefore”

C4

p10, line 15/16: change "Figure" to "Figures" or "show" to "shows"; add hyphen to "first"

p11, line 13: check bracket placement/reference towards end of line; also, correct the spelling of "submicron"

p11, line 17: following what?

p11, line 20: add "level of" detail

p12, line 15: format LHS properly

p12, line 22/23: revisit start of sentence

p13, line 8: add "The" at start of first sentence

p13, line 17/18: review sentence

p13, line 29: add "The" at start of first sentence

p13, line 34: add "the" best estimate

p14, line 28: change comma before "however" to semicolon, add comma before "especially"

p14, line 39: change "little" to "few" and add "the" before "literature"

p15, line 13/14: review sentence

p16, line 7: "define" should say "defined"

p16, line 24: either remove "a" or change "constants" to "constant"

p16, line 38: another singular/plural inconsistency at the start of the sentence

p17, line 9: change "with" to "as"

p17, line 23: "gem-dial" should say "gem-diol"

p17, line 24: change "radicals" to "radical" or "this type" to "these types"

#### C5

p17, line 29: again a singular/plural inconsistency

p17, line 34: "braking" should say "breaking"

p17, line 35: maybe hyphenate "subversion" throughout, or change the word, as this has a different meaning, usually

p17, line 41/42: review sentence

p18, line 1: ditto re "subversions"

p18, line 3-9: rephrase and fix grammar issues

p18, line 10: add "a" new module, change "to"

p18, line 22: change article... In "the" next step

p19, line 39: add article before "reaction product"

p20, line 5: add article before "reaction product"

p20, line 7: remove "with"

p21, line 4: add article before "reaction product"

p21, line 5: change "with" to "at"

p21, line 7: change "has also" to "also has" and add comma before "decreasing"

Inconsistent use of hyphenation of gas-phase/aqueous-phase throughout this section – standardise

p22, line 20: add "The" at start of sentence, and "those" before seen

p22, line 25: change "are" to "is"

p22, line 27: change "a" to "and"

p22, line 38: add "off" between "levelling" and "of"

#### C6

p23, line 9: "let" should say "led"

p32, in Table 3, entry for "Monomolecular decay of alkoxy radicals": "breaking" not "braking" and "an", not "and"

p32, in Table 3, entry for "Decomposition of acyloxy radicals": "breaking" not "braking"

p33, Table 4 caption: review use of articles; as stands, add "the" before "start"; correct "UC" to "UV"

p40, Figure 7 caption (line 3): "there" should say "their"

p41, Figure 8 caption (line 4): "cross" should say "crosses"

p41, Figure 8 caption (line 5): add "an" outlier

ESM, p15, p18, p20, p21, p22, p23: throughout (including the labels of Tables S3, S5, S6, S7),  $R^2$  is mistakenly referred to as the correlation coefficient

ESM, p18, line 5: review "tropospheric relevant organics compounds"

ESM, p18, line 12: change "prove" to "proof"

ESM, p18, line 17: review commas

ESM, p18/19, line 21/1: review sentence

ESM, p19, Figure S2 caption (line 6): when referring to subfigure c likely should be referring to subfigure d, and when referring to subfigure d should be referring to subfigure e

ESM, p20, line 4/5 and beyond: unsure what is going on here – where is the start of the sentence? This whole paragraph repeats the same exact content already described earlier in different words

ESM, p20, line 5: insert "it"

ESM p20, line 10: Figure S4 is not the figure described – should this refer to Figure

C7

S8?

ESM, p20, line 23: "Figure S2d" should say "Figure S2e"

ESM, p25, Table S9, p27, Table S10, p28 Tables S11 and S12: please check the units; I can understand those in Table S8, even though it would perhaps make more sense to say  $C$  itself is dimensionless (etc.) unless the division by its units is also added into the equation; for these other tables, the volume part of the units does not seem to add up correctly

ESM, p26, Figure S6 caption (line 6): correct the spelling of "respective"

ESM, p30, Figure S9 caption (line 7): "give" should say "given"

ESM, p31, Figure S10 caption: expand "orig"

ESM, p33, Figure S14 caption: correct the spelling of "investigating"

ESM, p34, line 3: "these type", inconsistent use of singular/plural

ESM, p34, line 4: correct the spelling of "initialised"

ESM, p34, line 9: insert "the" only reaction pathway

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Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2018-1318>, 2019.