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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Structure-activity relationship for the estimation of OH-oxidation rate constants of carbonyl compounds in the aqueous phase" *by* J. F. Doussin and A. Monod

Anonymous Referee #1

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General

This is a heavily awaited continuation of the SAR application for OH reactions in the aqueous phase extending the treated reactions to those of carbonyl compounds. This work is very important and needs to be published urgently. I would like to congratulate the authors to this very important contribution. Below I am listing just a few comments on minor issues which should be trated prior to acceptance.

Details

Page 15950, line 23: These are not always chain reactions but often reaction se-

quences (only)

P. 15951, l. 3: 'Carbonyls': I would like to suggest to always address the compounds in question as 'carbonyl compounds' instead of only 'carbonyls' because in chemistry the latter term is often used to describe metal complexes of CO.

P 15960, l.15: Setting up an SAR estimation for elcetron transfers might be a good future project, especially for radical other than OH

P 15964, l. 14ff: As nice as the method is, it might be good to call for some care in its application - just as in all predictions. Maybe the authors could introduce a note on this in the concluding section: In one case of another, the predicted rate constant might be strongly different from a correctly measured one. This should always be kept in mind and critical rate constant should at best be investigated experimentally. Maybe the authors could add a remark in this direction.

Furthermore, in the 'Conclusions' section I am missing an outlook to other aqueous phase radicals. I think it might be very interesting to extend these correlations to NO3 or SO4-.

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 15949, 2013.