

The second version of the manuscript has improved by adding more graphics to the manuscript and to the supplementary material and the information about another detailed study by Roman et al. (2021) on the IR spectra and further fundamental properties of the nitrocatechols of the present study.

The abstract might mention the two reference compounds for the relative rate technique and to add the upper limits of photolysis (and lower limits of photolytic lifetimes) for the two catechols with isolated nitro groups (4NCat and 4M5NCat) at 365 nm and the photolytic rate constants of these compounds at 254 nm of this excellent photochemical study.

The estimated quantum yields should be treated with caution: The charge transfer band of nitroaromatics is known to undergo a considerable redshift by the change from gas-phase to solution and in thin film; water is expected to provide largest shifts, see Reichardt, C., Solvents and solvent effects in organic chemistry, 2nd ed., VCH-Verlagsgesellschaft, Weinheim (1999). There might also be an influence on the oscillator strength.

Suggested further corrections:

L. 10: => insert "at lasi" here and possibly omit "for the first time"

L. 12: => and a total

L.12: you might wish to mention the two photolytic sources of OH radicals and the two reference compounds here

L. 14: omit "For the investigated compounds" but start the sentence with The photolysis...

L. 29: put references into chronological order

L. 31: => ring opening and fragmentation.

L. 34: put references into chronological order

L. 35: dimethylphenols trimethylphenols

L. 37: to the Master

L. 50, 52-55, 62: put cumulated references into chronological order

L. 61: aerosols, the

L. 65: seem to => may

L. 80: from => at

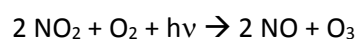
L. 84: Gas-phase..

L. 87: and a temperature

L. 90: a stream

L. 92: Teflon-blade

L. 104: the ozone formation might be explained by adding the reaction:



L. 107: $\rightarrow 2 \text{OH}$

L. 108: photodissociate

L. 115: time with respect

L. 119, 120: referent => reference

L. 131: nitrocatechols, their

L. 140: nitrocatechols were

L. 145: have => has

L. 150-154: use subscripts

L. 159: have => has

L. 175: has => have

L. 179: omit about in the first place and replace it by "it was" in the second one

L. 184: The four digits of precision are not justified; I would suggest errors of 0.7 and 0.5

L. 188: give wavenumber here

L. 193-208: Such a discussion of collision theory is not required nor useful without information about size distribution and particle number density and aerosol surface area, including the geometric surface area of the chamber. How the loss of OH might affect the relative rate and photolysis constants remains unclear. The precision of the OH velocity (L. 196) as an average of a broad distribution and even more so the discussion of Henry's law constants appear to be meaningless in view of the linearity and the zero intercept of figure 1-4 and the small intercept of the photolysis results in figure S1 and S2. The wall reaction k_4 might be an appropriate topic here - and how the numbers in L. 199 are calculated. To which experiment/figure do they refer? L. 212 of?

L. 220: atoms

L221: reveals a H-bond between

L. 224: H-bonds

L. 230-231: change color of text to black

L. 233: structures

L. 234: This suggest that

L. 239: To the first one => position(?).

L. 240: group to its

L. 243: reactivities

L. 246: orders

L. 254: radicals

L. 255: that the H-atom ...than the abstraction..

L. 2r57: gas-phase

L. 279: radicals

- L. 283: If the OH group
- L. 290: considered to be
- L. 294: analysis, that
- L. 296: reaction pathways
- L. 328: $\tau \Rightarrow \sigma$
- L. 363: behavior
- L. 369: using the Kwok
- L. 370: observations, revisions for the
- L. 372: presents such a correlation
- L. 373: presents.....substituent interactions
- L. 376-378: reflects...for the nitrophenols.....reduced.....spread.....the correlation lines of interest.
- L. 383: H-bond on the rate coefficient values...rising from $r =$
- L. 385: ...we believe...
- L. 392: nitronaphthalenes... methylnitronaphthalenes...
- L. 395: area might...
- L. 401 and 403: 3-nitroctechol compounds
- L. 404: in 4-nitr- or 5-nitrocatechols, the.....while in the 3-nitrocatechols case..
- L. 408: atmospheric degradation process
- L.631-645: The sum $k_3 + k_4$ forces the straight lines through the origin and should be given in the figure captions of figs. 1-4; this should be the case for the photolysis experiments in figures S1 and S2 as well, where k_4 could be given, neglecting any wall loss of the reference compounds.
- L. 666-669: Legend 8A \Rightarrow Figure 8A (and so on)

A space should be added between the Σ and the σ in fig 8A and fig. 8B. Minor ticks might be more useful on the ordinate axes (see below) instead of half orders of magnitude.

Fig. 8D: electrofilic \Rightarrow electrophilic

The linear scales of figures 8C and 8D do not provide an overview about the present limitations of SAR calculation. This led me to provide the data of 8C in a double logarithmic diagram (using e.g. Sigmaplot) with compound names, where deviations by a factor of two are marked by dashed lines.

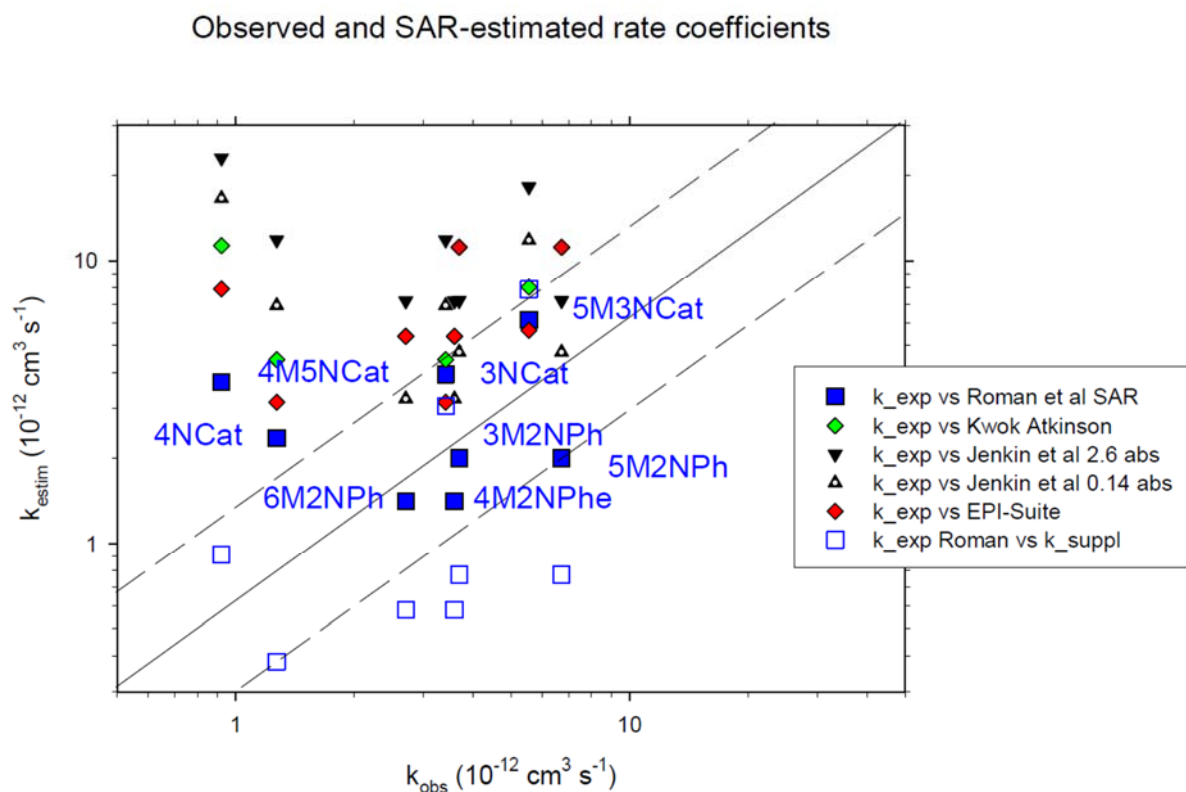
Table 1: Referent \Rightarrow Reference

The precision of the stated lifetimes is unreasonable, and the very simple formula (an oversimplification for good reasons) used for its calculation should be given in the footnote

Table 2: Unreasonable precision of lifetimes, which are simply the inverse of the rate constants here in still inconvenient units. These are different for daylight hours and nighttime and for different seasons and latitudes.

Supplementary material

The UV-VIS absorbance spectra of 3NCAT and 5M3NCAT in aqueous solution are a valuable information about the absorption bands responsible for photolysis. It might be more instructive to use a logarithmic scale for the absorbance and to display them in separate diagrams together with the spectrum of the lamps. The conversion of the molar extinction into molecular absorption cross sections on the right ordinate is misleading and should be restricted to table TS1, where the conversion factor could be given as a footnote. That table should extend to 500 nm in order to cover the full range of the measurements. This will unravel the band shapes and demonstrate the proper background subtraction/purity of the compounds. A reference to tabulated data of the emission spectrum over the same spectral range would be useful.



Suggested illustration of the present status of SARs