



Contents lists available at ScienceDirect

Ecotoxicology and Environmental Safety

journal homepage: www.elsevier.com/locate/ecoenv

Abiotic transformation of radiolabelled 6-PPD and 6-PPDQ in water and in presence of nitrogen/air/ozone and light

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ARTICLE INFO

Key words:

Tire abrasion
Leaching
Persistence
Photolysis
Aging

ABSTRACT

N-(1,3-Dimethylbutyl)-N'-phenyl-p-phenylenediamine (6-PPD) and one of its oxidation products, 6-PPD quinone (6-PPDQ) are environmental contaminants released from tire and road wear particles (TRWP). The abiotic transformation of both compounds by hydrolysis and in contact with atmosphere with and without oxygen species and simulated sunlight was studied, following relevant portions of OECD-guidelines 111 and 316, and using radiolabelled test substances. This allowed for mass balances including transformation products, those identified by liquid chromatography-mass spectrometry and those remaining unidentified. 6-PPD was effectively degraded by hydrolysis at neutral and basic pH (DT50 5 – 12 h at 25°C), with 4-HDPA being the major reaction intermediate. 6-PPDQ remained below 0.2% of the applied radioactivity (AR) of 6-PPD, except at very acidic conditions and low temperature (10°C) with an intermediate yield of 7.5% AR. In contact with atmosphere 6-PPD was transformed by direct photolysis (DT50 14 h). Direct reaction with ozone was slow (DT50 3.5 d) but degradation by OH-radicals (ozone/light) was very fast (DT50 3.7 h). A diverse set of products was formed; 6-PPDQ was determined in some cases, with a maximum intermediate yield of 1.3% AR and decreasing again with ongoing oxidation of 6-PPD (to levels ≤ 0.6% AR with ongoing oxidation). 6-PPDQ is not susceptible to pure hydrolysis (DT50 > 1000 d at pH 7, mean 490 d in 13 natural waters) and very limited to direct photolysis (DT50 56 d). On the contrary, reactivity towards reactive oxygen species (air/ozone and light) is in the same range as for 6-PPD (DT50 2 – 7 h). Oxidative transformation of 6-PPDQ proceeds via opening of the quinone-ring, with 20–50% AR recorded as CO₂ within 2 d. For 6-PPDQ oxidation in the presence of light only 50 – 80% of AR could be recovered. This study with ¹⁴C-labelled test substances provides solid information on the abiotic transformation of both, 6-PPD and 6-PPDQ, and supports environmental risk assessment.

1. Introduction

The abrasion of tires on roads generates tire and road wear particles (TRWP) which are an important proportion of non-exhaust emissions of automotive traffic, with abrasion rates ranging from 50 to 200 mg/km for passenger cars and 1000–1500 mg/km for trucks (Baensch-Baltrusch et al., 2020). TRWP have received growing attention with the debate on microplastic emission and occurrence in the environment; the attention grew further by the assignment of the “urban runoff mortality syndrome” in Coho Salmon (*Oncorhynchus kisutch*) to the quinone of the antioxidant of N-(1,

3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6-PPD) (Tian et al., 2021). While not all fish are equally sensitive to 6-PPDQ (Montgomery et al., 2023), lab experiments have also recorded detrimental effects of leachates of tire particles on other aquatic organisms (Day et al., 1993; Marwood et al., 2011). Concentrations of 6-PPD and 6-PPDQ found in the environment, from road environment to marine sediments, have been reviewed recently (Müller et al., 2025). Consequently, 6-PPD and 6-PPDQ both are under regulatory scrutiny in Canada, the US and Europe (CEPA, 2025; ECHA, 2025; NTP, 2025).

Experiments with tire particles have shown, however, that both compounds are prone to abiotic as well as biotic transformation

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<https://doi.org/10.1016/j.ecoenv.2026.120082>

Received 5 January 2026; Received in revised form 23 March 2026; Accepted 26 March 2026

Available online 2 April 2026

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reactions: namely sunlight exposure was effective in degrading 6-PPD from cryo-milled tire tread (CMTT) as well as from TRWP (Fohet et al., 2023; Weyrauch et al., 2023). The dissolved organic carbon content of leachates can be strongly reduced by microbial activity, indicating mineralization of many compounds leached from tire particles (Foscari et al., 2024). Analyses of tire-related compounds in aging and leaching studies with CMTT or TRWP turned out to be difficult to understand as the concentration of chemicals in leachates as well as in extracts are influenced by competing processes of leaching and transformation (Weyrauch et al., 2023). For that reason, dedicated studies with pure chemicals (in aqueous solution or as a solid film) have been performed to obtain information on their stability.

Hydrolysis of 6-PPD has been studied in aqueous solution and a half-life at neutral pH of 4.8–5.2 h was reported (Di et al., 2022). 4-HDPA was shown to be a major hydrolysis product of 6-PPD (Unice et al., 2015). These results were generally confirmed in a recent study (Xu et al., 2025). Further information on the stability in aqueous solution was provided from abiotic control experiments of biodegradation studies: the stability of 6-PPD in these abiotic systems was almost as short as when incubated with microorganisms (Han et al., 2025). Contradictory results are available on the stability of 6-PPDQ in aqueous solution: Some studies reported rapid degradation with a half-life of 33 h (Hiki et al., 2021) and 18–54% loss of 6-PPDQ within 24 h (Brinkmann et al., 2022) (Lo et al., 2023), while others reported half-lives of 15–16 days at neutral pH (Di et al., 2022) or no measurable loss over 5 d (Yan et al., 2024).

The reaction of 6-PPD with ozone was investigated to learn about the processes that transform 6-PPD in contact with an oxidizing atmosphere such as in tire rubber (Seiwert et al., 2022; Tian et al., 2021). 6-PPD was shown to be highly reactive and this was subsequently confirmed by other studies (Hu et al., 2022; Rossomme et al., 2023; Xie et al., 2024; Zhao et al., 2023). It was concluded from a recent mechanistic study that 6-PPDQ formation from 6-PPD is due to the direct attack of ozone to the aromatic ring (Rossomme et al., 2023). While the ozonation of 6-PPD was studied repeatedly, only one report is available on 6-PPDQ, showing that it is also quite reactive to ozone (Seiwert et al., 2022).

Products of hydrolytic and oxidative transformation of 6-PPD have been analyzed by liquid chromatography-high resolution-mass spectrometry (LC-HRMS) and larger numbers of transformation products (TPs) were detected and tentatively identified: 26 (Seiwert et al., 2022), 17 (Zhao et al., 2023), 10 (Xie et al., 2024) and 9 TPs (Hu et al., 2022). Transformation products of 6-PPDQ are less well known and reported for only one study with ozone (Seiwert et al., 2022).

Obviously, one of the important aspects in transformation studies with 6-PPD is the extent to which 6-PPDQ is formed. In water, where hydrolysis is the major reaction, 6-PPDQ was only found in pH 4 water solution (Di et al., 2022) and was not detected at neutral pH in several studies (Han et al., 2025) (Yan et al., 2024). For the reaction of 6-PPD with ozone gas yields of 8–10% of 6-PPDQ have been reported (Hu et al., 2022; Xie et al., 2024). Lower values of around 1% were found for 6-PPD in tire particles (Hu et al., 2022).

Quantitative half-life data are essential for a solid environmental exposure assessment as well as for regulatory purposes. In addition, it is strongly recommended to consider the products of transformation processes for an in-depth environmental risk assessment (Zahn et al., 2024). One of the challenges in such transformation studies is the lack of reference compounds of transformation products, hampering their detection and identification and preventing their quantification. In the case of 6-PPD and 6-PPDQ, six known TPs are commercially available (4-HDPA, ADPA, NO-DPA, N-formyl-6-PPD, 6-QDI and 4-DBAP). Therefore, many studies that do detect TPs use signal intensities of LC-MS analyses for a so-called *semi-quantification*. The error in this approach remains unknown and may well be huge (Zahn et al., 2024).

The use of radiolabeled test compounds is a well-established approach to circumvent this limitation, as all TPs that keep the labeling can be quantified by radioactivity detection, even if their identity is

unknown. Radiolabelling also allows to conclude on the extent of mineralization (formation of carbon dioxide) of labelled compounds. For that reason radiolabelling is employed in simulation tests to assess the biodegradability of test compounds before being placed onto the market and it is integrated into many related OECD guidelines (Strotmann et al., 2023). Performing studies according to standardized procedures, e.g. OECD guidelines, ensures data quality and allows to compare quantitative data with other studies or for other chemicals. Transformation studies on 6-PPD and 6-PPDQ following OECD-guidelines and using radiolabeled compounds are not currently available.

The work described uses [¹⁴C]-labelled 6-PPD and 6-PPDQ to study their abiotic transformation with mass balancing, addressing the following open questions: What is the half-life of 6-PPD and 6-PPDQ in water at acidic, neutral and basic pH, when photolytic and oxidative processes are excluded? Does this correspond to the half-lives in natural surface waters under the same experimental conditions? Which transformation products are formed upon hydrolysis? What is the half-life of 6-PPD and 6-PPDQ in oxidizing (air, ozone) and non-oxidizing (nitrogen) atmospheres in the dark and under sunlight exposure? Which transformation products are quantitatively important? Answers to these questions should be instrumental for the environmental risk assessment of both compounds.

2. Materials and methods

2.1. Test specimen and samples

[¹⁴C]-labelled 6-PPD (CAS number 793–24–8) and 6-PPDQ (CAS number 2754428–18–5) was obtained from Pharmaron UK Ltd (Cardiff, UK) and was stored frozen (nominally –20°C) in the dark. Both compounds had a radiochemical purity of 97–98% (own analyses). In 6-PPD and 6-PPDQ the central phenyldiamine-ring was [¹⁴C]-labelled (Table S1).

Surface water samples were collected from 13 sites in the US and in England. Five sites were located around Seattle, State of Washington, USA (Table S2). The samples were of diverse quality in terms of pH (5.3–8.7, median 7.8), suspended solids (3–1953 mg/L, median 5 mg/L), hardness (27–5750 mg/L CaCO₃, median 185 mg/L CaCO₃) and salinity (0–31 ppt) (Table S7). Samples were filtered through 212 µm sieve and sterilized by autoclaving.

2.2. Experiments

Single kinetic experiments were performed with [¹⁴C]-labelled 6-PPD and 6-PPDQ. In all experiments duplicate samples were taken and analyzed over a time course defined in preliminary experiments. The studies have been designed to meet the relevant portions of the guidelines, namely OECD 111 for hydrolysis (OECD, 2004) and OECD 316 for experiments in contact with gases and light (OECD, 2008).

2.2.1. Experiments in water

Test concentrations of 0.5 µg/mL for 6-PPD and 0.1 µg/mL for 6-PPDQ (less than 50% of the water solubility) were used. Stability in three sterile buffered solutions (0.01 M, pH 4, 7, 9) at three temperatures (10, 25 and 50°C) was investigated in the dark (Table S3). In addition, stability was also studied in 13 surface waters (pH range 5.3–8.7) at three temperatures (10, 25 and 50°C). All surface waters and buffers were sparged with nitrogen prior to sterilization (121°C for 25 min). More experimental details are provided in the SI in section 1.2.

At predefined time intervals (Table S4) a glass vessel was removed and duplicate weighed aliquots (ca 150 µL) taken to quantify the radioactivity by LSC. Other aliquots (750 µL) were taken for analysis by radio-HPLC and HPLC/MS-MS. They were kept under nitrogen, over up to approximately 30 days until experiment completion

2.2.2. Experiments in contact with gases

[¹⁴C]-labelled 6-PPD and 6-PPDQ were applied to the base of glass test vessels (*ca* 1.00 µg/cm²) with a quartz glass lid and irradiated with simulated sunlight (Atlas Suntest CPS+, Atlas Materials Testing Technology, Bicester, UK) under a flow of nitrogen, air or air with ozone (Figure S1) at 30, 70 or 100 ppb at 20 ± 2°C for predefined intervals (Table S5). Nitrogen and ambient air were dried by a gas drying cartridge before use. Control experiments were performed in contact with the gases in the dark. More experimental details are provided in the SI, section 1.3.

Products in the reaction vial were taken up in acetonitrile, acetonitrile/water and water (extract 1, 2 and 3) and analysed separately. The off-gases of each experiment were directed through two NaOH traps (trap 1 and 2) to collect carbon dioxide (Figure S1). For selected samples, effluent air from the second NaOH trap was passed through a catalytic oven set at 600°C and then through further NaOH traps (trap 3 and 4). Radioactivity in all fractions was determined.

2.3. Analysis

Total radioactivity of samples was measured by liquid scintillation counting (LSC). All samples were analyzed for the test compound and transformation products by reversed-phase liquid chromatography (water/acetonitrile gradient with 0.01% formic acid) with UV (230 nm) and radioactivity detection (radio-LC). All results given as percent values refer to the applied radioactivity (AR) of the respective experiment. More details on the analytical methods are provided in the SI in section 1.4.

Identification of transformation products was conducted by LC-MS/MS analysis using the same chromatographic conditions, with electrospray ionization operated in positive and negative mode (Table S6). Non-labelled reference compounds were available for 6-PPD, 6-PPDQ, 4-aminophenol, N-phenyl-p-phenyleneamine, aniline and 4-HDPA (Table S1).

Instability during frozen sample storage was observed in some cases. For example, in the hydrolysis experiments with 6-PPDQ, products initially detected by radio-HPLC were not detected after thawing for LC-MS analysis.

2.4. Calculation of kinetic constants

All kinetic calculations are based on the radio-LC data of the parent compound. The rate of transformation of 6-PPDQ in contact with water

was modelled using single first-order (SFO) kinetics using CAKE (Computer Assisted Kinetic Evaluation) software (Tessella Ltd, Abingdon, Oxfordshire, UK). For all other experiments calculation of pseudo-1st order rate constants was done by linear regression analysis using the logarithmic linearization of the AR data with an intensity not lower than 5% AR. All half-life data are denoted as DT50 for dissipation time for 50%.

For some experiments in contact with gases a clear slow-down of the reaction kinetics was visible. In those cases, only the initial 3 – 4 data points were used. Such a slow-down may be explainable from the fact that this was a heterogenous reaction between a gas and a solid film of 6-PPD or 6-PPDQ; its uppermost layer was directly exposed to the gas phase while deeper layers were more difficult to reach by the oxidant. This agrees with previous observations (Hu et al., 2022; Huang et al. 2001). At least 3 data points were kept for the rate calculation.

Full details of all experiments and analyses are provided as supporting information.

3. Results

3.1. Hydrolytic transformation in water

The hydrolysis of 6-PPD and 6-PPDQ was studied at acidic, neutral and basic conditions as foreseen in OECD guideline 111. In addition, it was studied with the same experimental approach in 13 surface waters with different pH, salinity and suspended solids content, and different concentration of total N, total P and dissolved organic carbon (Table S7). These surface waters were included to explore to which extent results obtained under standardized conditions can be extrapolated to natural waters of a more complex and more diverse composition.

3.1.1. 6-PPD hydrolysis

3.1.1.1. Transformation products and pathway. The analysis of the aqueous solution of 6-PPD (in buffer as well as in 13 surface waters) over the course of the 30 d of experimental duration resulted in the detection of more than 20 signals in the LC-radioactivity chromatograms. Of these, a number of 12 could be detected also by LC-MS and structure proposals be elaborated (Table S8, Table S9).

These identified compounds are arranged, among them 6-PPD and 4-HDPA, in Fig. 1. Some molecular formulas indicate sulfonated compounds of 6-PPD as well as of 4-HPDA. Their formation process as well as the origin of the sulfur for the formation of these TPs is not clear. Due to

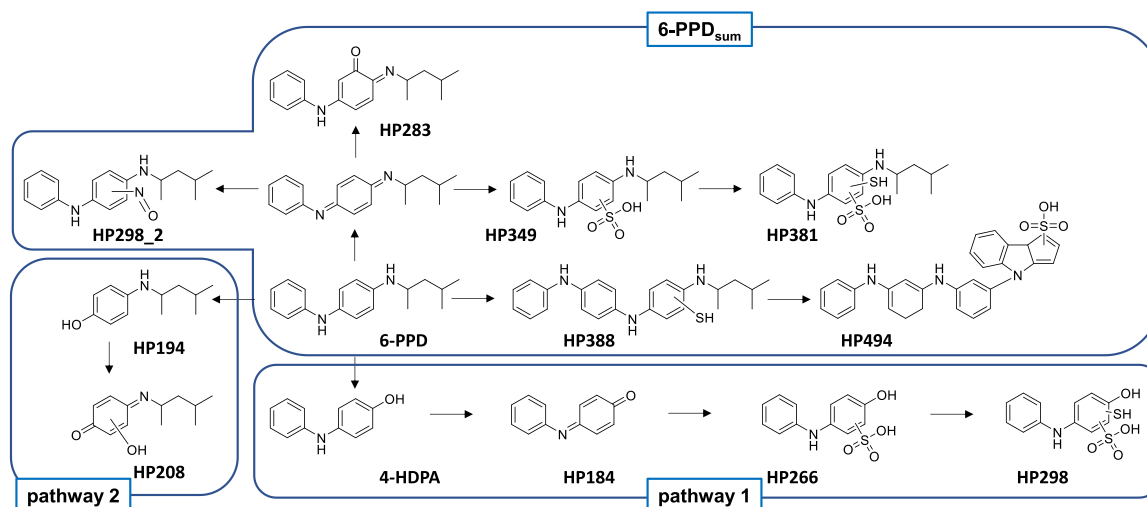


Fig. 1. Structure proposals of transformation products of 6-PPD in water at pH 7 and above under the exclusion of oxygen. (mass spectrometric information provided in Tables S8 and S9).

Table 1
Hydrolysis half-lives of 6-PPD_{sum} and of 6-PPD assuming pseudo-first-order kinetics.

	DT50 (10°C) (h)	DT50 (25°C) (h)	DT50 (50°C) (h)	k (25°C) (1/s)
6-PPD_{sum}				
pH 4	545	58.8	0.70	$3.2755 \cdot 10^{-6}$
pH 7	41.5	5.4	n.d. ¹⁾	$35.8796 \cdot 10^{-6}$
pH 9	56.8	12.1	n.d. ¹⁾	$15.9583 \cdot 10^{-6}$
surface waters – median (25 / 75 %ile)	37.9 (27.9 / 61.7)	7.55 (7.08 / 8.15)	n.d. ¹⁾	$25.5226 \cdot 10^{-6}$ $23.645 \cdot 10^{-6}$ $27.2109 \cdot 10^{-6}$
6-PPDQ				
	DT50 (10°C) (d)	DT50 (25°C) (d)	DT50 (50°C) (d)	k (25°C) (1/s)
pH 4	> 1000 ²⁾	> 1000 ²⁾	65.3	< 0.0080 10^{-6}
pH 7	> 1000 ²⁾	> 1000 ²⁾	31.6	< 0.0080 10^{-6}
pH 9	> 1000 ²⁾	467	5.5	0.0172 10^{-6}
surface waters – median (25 / 75 %ile)	> 1000 ²⁾	466 (242 / 759)	21.6 (16.6 / 32.6)	0.0200 10^{-6} $0.0125 \cdot 10^{-6}$ / $0.0311 \cdot 10^{-6}$

1) Reaction too fast to derive half-life data (see Methods section for details)

2) Reaction too slow to derive half-life data

the ¹⁴C-labelling, these compounds were not only detected but their concentration and contribution to the total AR could be determined. Although these sulfonated TPs were quite prominent in some samples, they occurred as intermediates, only.

The most important transformation of 6-PPD in water is the hydrolytic cleavage of the 1,3-dimethylbutylamine moiety to form 4-HDPA. Correspondingly, 4-HDPA and the further TPs derived from it (pathway 1 in Fig. 1), were the major TPs in all experiments. The hydrolytic cleavage of the aniline group (pathway 2 in Fig. 1), forming 4-[(1,3-dimethylbutyl)amino]-phenol (4-DBAP, HP194), was less favourable and was observed only in single experiments (Figure S3).

Formation of 6-PPDQ remained below the limit of detection (< 0.2% AR) in all experiments at 25°C and 50°C and all experiments at pH 7 and pH 9 as well as in the surface waters at their native pH. Only in pH 4 buffer incubated at 10°C was formation of 6-PPDQ via HP283 observed (maximum 7.4% AR at 1 d; Table S11). At this acidic pH and low temperature, the base-catalyzed hydrolysis of 6-PPD to 4-HPDA was so slow that no 4-HPDA was observed; however, the corresponding quinone, OP184, and OP298 were detected. Correspondingly, the half-life of 6-PPD was highest under these conditions (DT50 of 545 h/8.6 d; Table 1), leaving enough time for the oxidative transformation of 6-PPD to 6-PPDQ. This was, likely, enabled by traces of oxygen that remained in the system despite sparging with nitrogen.

The few literature reports looking into the formation of 6-PPDQ from 6-PPD in water reported 6-PPDQ to remain below LOQ (Yan et al., 2024), or to occur only at pH 4 (Di et al., 2022). This agrees well with this study using radio-labeled 6-PPD, witnessing that 6-PPDQ is not formed to a significant extent from 6-PPD upon hydrolysis.

3.1.1.2. Speed of transformation in water and effects of temperature and pH. To ease the subsequent kinetic analysis, all compounds with the intact 6-PPD structure were summed (6-PPD_{sum}), as well as all products formed by hydrolysis of the alkylamine-moiety (HDPA-pathway, pathway_1) and all products formed by hydrolysis of the aniline moiety (pathway_2). Half-lives derived from this summation can be considered conservative, as the half-life of 6-PPD alone would have been lower than that of 6-PPD_{sum}.

The decrease in concentration of 6-PPD_{sum} in water was well-described by pseudo-first-order kinetics at 25°C and 10°C, down to a remaining 6-PPD_{sum} concentration of around 5% AR. 6-PPD_{sum} stability was highest at pH 4 (DT50 of 59 h d at 25°C) and decreased by about one order of magnitude towards pH 7 (DT50 of 5.4 h at 25°C), while it seemed to slightly increase again in the pH 9 buffer (Table 1). This trend suggests a base-catalyzed hydrolysis of 6-PPD as the primary transformation reaction, possibly supported by the deprotonation of the tertiary amine moiety with a pK_a of 6.41 (Xu et al., 2025). At 50°C the transformation of 6-PPD was too fast to derive half-life data for pH 7 and

pH 9 (Table 1).

Half-lives were also determined in a set of 13 sterilized surface waters (pH 5.3 – 8.7), with a median DT50 of 6-PPD_{sum} of 7.6 h at 25°C (Table 1). This median value corresponds well with the data obtained from the buffered systems for the pH-range 7–9. In accordance with this, the pH-dependence of the half-lives in the surface waters followed the trend seen for the buffer systems, with a marked decrease from acidic pH values towards pH 7 (namely at 10°C) (Fig. 2a). The difference in the four surface waters of similar pH was quite small at 25°C (6.4 – 8.2 h for pH 8.1 – 8.2) but was more pronounced at lower temperature (28 – 62 h at 10°C).

Among the 13 waters were three with elevated salinity (20 – 31 ppt); 6-PPD_{sum} half-lives in these waters ranged from 7.7 to 8.2 h at 25°C and were, thus, not different from those of the freshwater samples. This suggests a similar half-life of 6-PPD in marine waters compared to

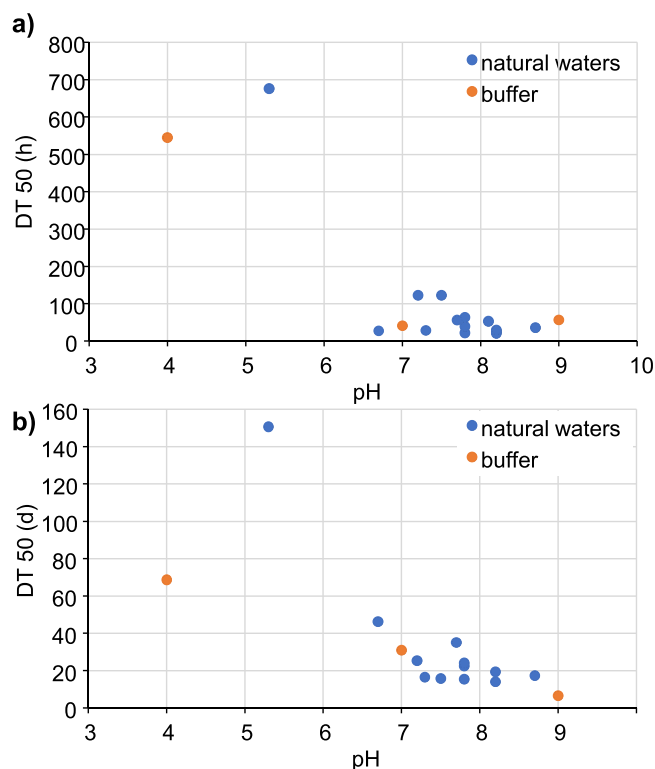


Fig. 2. Hydrolysis half-lives vs. pH in buffered systems and in natural surface waters (n = 13). A) for 6-PPD at 10°C, in hours; b) for 6-PPDQ at 50°C, in days. (the outlier sample (pH 5.3) had an extremely high DOC (23 mg/L)).

freshwater systems. The median DT50 of 6-PPD of 7.6 h at 25°C in sterile surface water under the exclusion of oxygen clearly indicates the fast hydrolysis of 6-PPD in aqueous systems.

Half-lives for 6-PPD in water hydrolysis have been reported, but not all followed standardized OECD protocol or excluded oxygen; moreover, experimental details are not always reported completely (temperature, pH) or the natural waters characterized. For synthetic waters (at neutral pH) one study reported a DT50 for 6-PPD below 1 h (Yan et al., 2024), while others were in the range of 5–10 h (Di et al., 2022; Han et al., 2025; Xu et al., 2025).

The half-lives determined in this study (Table 1) are at the upper end of this range. Shorter half-lives may be found in studies which allow contact of the aqueous solution with air (oxygen), enabling parallel oxidative transformation of 6-PPD (see below). Concerning the pH-dependence this study substantiates the trend reported in a previous study in which a DT50 decrease from 57–61 h at pH 4 to 4.8–5.2 h at pH 7 at 25°C was reported (Di et al., 2022).

3.1.1.3. Product distribution. The ¹⁴C-labelling of the 6-PPD used in these experiments allowed to provide full mass balances including transformation products for which no reference compounds are available and unidentified transformation products detected only by LC-radioactivity analysis. The recovery of AR was almost 100% (Fig. 3). In the buffered systems, hydrolysis to 4-HPDA was the dominant initial transformation. The products of this pathway accounted for 75–80% AR at day 5 for pH 7 and 9. With increasing reaction time also 4-HPDA was transformed to unidentified TPs (sum_unk) which accounted for 63% AR at 10°C on day 30 (Fig. 3a). All these unidentified TPs exhibited very short retention times in RPLC, indicating a significantly higher polarity compared to 6-PPD and 4-HPDA.

For the median composition of the surface waters, the unidentified TPs did not exceed 20% after 30 d at 10°C and HDPA-related TPs (pathway 1) still dominated with 80% AR (Fig. 3a). This indicates a slower transformation of 4-HPDA in the surface waters compared to the buffer systems. At 50°C, however, complete conversion of HDPA-related TPs was reached within 30 d and the early-eluting polar TPs comprised 100% of the AR. It is reasonable to assume that a large proportion of such highly polar TPs are prone to aerobic microbial mineralization under non-sterile conditions.

Other studies on the transformation of radiolabeled 6-PPD in water are not available, but for non-labelled 6-PPD. With respect to the hydrolysis mechanism, it has been noticed earlier that pathway 1 (via 4-HPDA) is preferred over pathway 2 (Di et al., 2022; Unice et al., 2015; Xu et al., 2025).

3.1.2. 6-PPDQ hydrolysis

The reactions of 6-PPDQ in water were studied with the same experimental and analytical approach as for 6-PPD.

3.1.2.1. Speed of hydrolysis and effects of temperature and pH. The reactivity of 6-PPDQ in sterile water and under the exclusion of oxygen is markedly lower than that of 6-PPD. At 25°C, only 0–3% of 6-PPDQ was transformed within 30 d, resulting in half-lives from > 1000 d to 467 d in the pH range 4–9 (Table 1). Therefore, kinetic data are best compared at 50°C. Half-life data in the surface waters compare well to those found for the buffer systems with a median of 466 d at 25°C and 22 d at 50°C. Transformation of 6-PPDQ increases with increasing pH, in the buffer solutions as well as for the 13 surface waters (Fig. 2b), suggesting a base-catalyzed hydrolysis of 6-PPDQ as the initial step of transformation. However, in the natural waters also other factors than pH influenced the kinetics: for the four surface waters of pH 8.1–8.2 the DT50 of 6-PPDQ varied from 118 to 352 d at 25°C.

Also for 6-PPDQ hydrolysis no effect of salinity was obvious: the half-lives of 6-PPDQ in the three saline surface waters (20–31 ppt) at 50°C varied from 136 d to > 1000 d (Table S12) which is in the range of the remaining samples. The DOC of most surface waters ranged from 0.6 to 5.3 mg/L (median 1.55 mg/L). The sample with an extremely high DOC of 23 mg/L exhibited the longest half-life of 6-PPDQ at 50°C of 154 d compared to a half-life in the range of 50–55 d expected from its pH (Fig. 2b).

The transformation of 6-PPDQ in aqueous solution has been studied less often than that of 6-PPD and no reports for radiolabeled 6-PPDQ are available. No hydrolysis products have been reported, either. Half-lives reported for abiotic transformation at neutral pH and room temperature differ widely, from 33 h to 43 d (Di et al., 2022; Han et al., 2025; Hiki et al., 2021). All these half-life values are orders of magnitude shorter than the half-life of > 1000 d found in this study at 25°C and pH 7 (Table 1). One study reported less than 5% hydrolysis over 5 days in sterilized surface water (Yan et al., 2024). This difference, as well as the differences between the other studies, may well be due to different degree of sterility, variable extent of contact with air or oxygen and also to temperature effects. Note that in this study the half-life of 6-PPDQ decreased from > 1000 d at 25°C to 32 d at 50°C and pH 7 (Table 1), indicating that the effect of temperature is strong. This outlines the need of performing hydrolysis experiments under fully standardized conditions as in this study.

It has also been shown that aerobic microbial degradation of 6-PPDQ is fast, resulting in a half-life of around 3 d (Han et al., 2025) at room temperature. On this basis one may conclude that abiotic hydrolysis of 6-PPDQ in the environment is, likely, less important than other processes like biodegradation.

3.1.2.2. Transformation products. LC-radioactivity analyses revealed 8 chromatographic signals, which were not fully separated. Attempts to detect and identify these TPs by LC-MS were not successful and all signals remained unidentified. As in the case of 6-PPD, however, most TPs eluted very early in RPLC, reflecting their high polarity. At 50°C, the

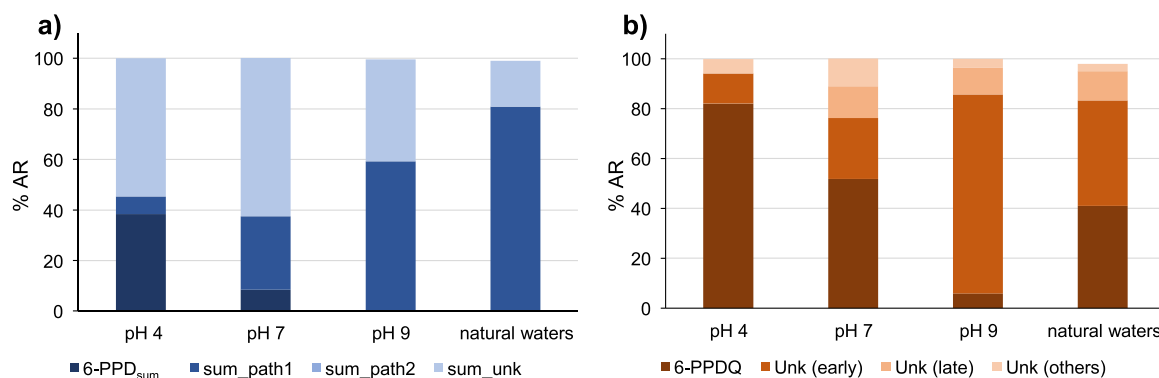


Fig. 3. Balance of the added radioactivity (AR) for 6-PPD and 6-PPDQ. a) for 6-PPD at 10°C after 30d; b) for 6-PPDQ at 50°C after 30 d. (early: RT 3.0–6.0 min), (late: RT 38.6–40.0 min).

only temperature with strong transformation, up to 15% of the TP determined after 30 d were late eluting compounds that may have been formed by radical coupling.

In the surface waters, late eluting compounds accounted for up to 30% AR in single waters, but were not relevant for the median composition (< LOD). This suggests that some components of natural waters may couple with 6-PPDQ or a radical species formed from it to products of higher molecular weight and lower overall polarity. The difference in the proportion of these potential coupling products may reflect differences in the concentration of these reactants in the different surface waters. The DOC content was not linked to this phenomenon, however.

3.1.2.3. Product distribution. The product distribution determined by LC with radioactivity detection in the 13 surface waters after 30 d at 50°C differed clearly (Figure S5). Beyond 6-PPDQ, most AR was found in five other signals, each reaching values around 20% AR in some of the waters. While these compounds could not be identified, the diversity of products suggest that the pathway of 6-PPD hydrolysis is strongly affected by other organic or inorganic components of the waters. There was no obvious difference in the composition of the hydrolysis products between freshwater and seawater samples.

Literature does not provide information on the identity of hydrolysis products of 6-PPDQ. This is, likely, due to the limited extent to which 6-PPDQ hydrolyses and the limited stability of these products, making it challenging to detect and to identify these products. Owing to the very long hydrolysis half-lives of 6-PPDQ compared to oxidative transformation reactions (see below) hydrolysis products of 6-PPDQ are not expected to be of much relevance in the environment.

3.2. Transformation in presence of gases and light

3.2.1. 6-PPD

3.2.1.1. Speed of transformation. In the dark the half-lives of 6-PPD in contact with nitrogen and air were quite similar (DT50 16–17 d; Table 2), indicating that the direct reaction of 6-PPD with oxygen (21% in air) gas is slow. A markedly shorter DT50 was found for 30 ppb ozone (3.5 d).

Sunlight greatly speeds up the transformation, even in absence of oxygen species (Table 2). In nitrogen atmosphere, the half-life of 6-PPD was more than an order of magnitude lower than in the dark (DT50 of 0.6 d instead of 16 d), indicating that direct photolytic transformation of 6-PPD is an effective process. Correspondingly, presence of oxygen (air) instead of nitrogen did not speed up 6-PPD transformation significantly (DT50 of 0.5 d).

In the presence of 30 ppb ozone in air the half-life was further reduced by a factor of 4 (0.15 d). This shows that oxidation by reactive oxygen species (likely OH-radicals) formed from ozone upon sunlight photolysis does add markedly to the direct photolytic transformation of 6-PPD. Interestingly, higher ozone dosages (70 ppb, 100 ppb) led to an

increase in the half-life compared to 30 ppb. This may be due to the fact that the dry atmosphere limits OH-radical formation so that higher ozone dosages are not more effective but rather scavenge some of the OH-radicals (Jans, 2000). Ozone concentrations of 30–70 ppb are environmentally most relevant (UBA, 2025).

3.2.1.2. Transformation products. By LC-MS/MS analysis two transformation products were confirmed with reference compounds (4-HDPA and 6-PPDQ) and structure proposals elaborated for further 8 monomeric products and 9 oligomeric TPs (Table S13, Table S14) (Fig. 4). Basically, 6-PPD was transformed along five pathways: a) hydrolytic cleavage to 4-HPDA, (b) oxidation to the quinone diimine (QDI, OP267), leading to OP283 and other products, and (c) N-oxidation to OP285 and beyond (d) formation of 6-PPDQ, which was explained by asymmetric Criegee addition followed immediately by a further oxidation by a second ozone molecule (Rossomme et al., 2023) (e) Additionally, oxidative coupling of different oxidation products of 6-PPD with 6-PPD was observed, which were likely formed by intramolecular reactions of radical intermediates or quinones occurring in 6-PPD oxidation. It is assumed that such dimers are found only because pure solid 6-PPD was reacted here; they are expected to be less relevant in real situations when 6-PPD is more diluted (as in the rubber matrix of TRWP). These same products were determined for all reaction conditions.

The transformation of solid 6-PPD with ozone gas and light has been studied repeatedly, and large numbers of products have been reported. Of the products in Fig. 4 all except OP208 and OP281 have been reported previously (Hu et al., 2022; Li et al., 2023; Seiwert et al., 2022; Xie et al., 2024; Zhao et al., 2023), including dimerization products (m/z 464) (Xie et al., 2024; Zhao et al., 2023). Many factors may explain the differences in the spectrum of transformation products between these studies, among them experimental conditions (concentration of 6-PPD and ozone, humidity of the gas phase, spectrum and irradiance of the light) as well as differences in the analytical procedures.

3.2.1.3. Product distribution. A good recovery of AR (85 – 98%) was achieved for the dark experiments with 6-PPD, with no significant contribution of carbon dioxide (Fig. 5a). Most of the AR remained as 6-PPD in the case of nitrogen, air, and 70 and 100 ppb of ozone (70 – 85% AR). For the experiment with 30 ppb ozone only 42% AR remained as 6-PPD after 11 d, while a similar percentage was determined as transformation products (other in extract).

For the experiments with simulated sunlight with the strong extent of 6-PPD transformation the recovery was systematically lower (40 – 78%), even though the experimental setup included NaOH traps in the off-gas line to collect carbon dioxide and volatile organic compounds after catalytic oxidation. Recovery of AR can decrease in the course of oxidative opening of ring-labelled compounds. Low molecular weight compounds formed from such reactions are often difficult to recover. Alternative trapping media may have improved the recovery of AR but were not employed in this work.

Table 2

Half-lives of 6-PPD_{sum} and of 6-PPDQ in contact with different gases in the dark and under simulated sunlight according to pseudo-first-order kinetics. (data normalized to OECD summer sunny day and Tokyo Spring Sunlight given in Table S16 and Table S19).

	nitrogen	air	30 ppb ozone in air	70 ppb ozone in air	100 ppb ozone in air
6-PPD					
Dark (d)	15.8	17.2	3.5	14.3	27.0
Light (d)	0.59	0.46	0.15	0.61	0.54
Light (h)	14.2	11.0	3.7	14.8	13.0
OECD (h)	15.5	12.3	3.9	17.8	13.7
6-PPDQ					
Dark (d)	> 100 ¹⁾	> 100 ¹⁾	7.9	> 100 ¹⁾	> 100 ¹⁾
Light (d)	56	0.28	0.09	0.11	0.45
Light (h)	1342	6.7	2.1	2.7	10.8
OECD (h)	1458	7.5	2.2	3.3	11.4

1) Reaction too slow to derive half-life data.

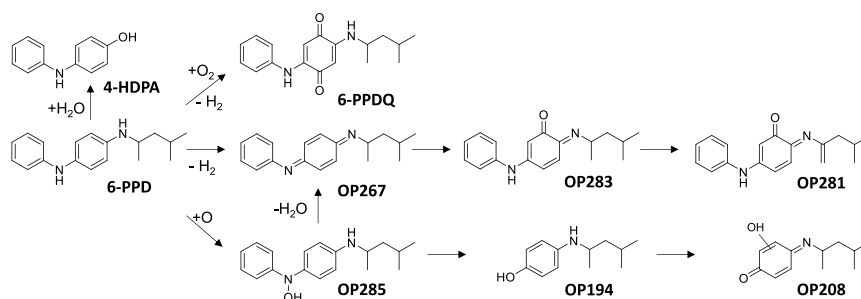


Fig. 4. Tentatively identified transformation products of 6-PPD in oxidative environment. Dimerization products not included. (mass spectrometric information provided in Tables S13 and S14).

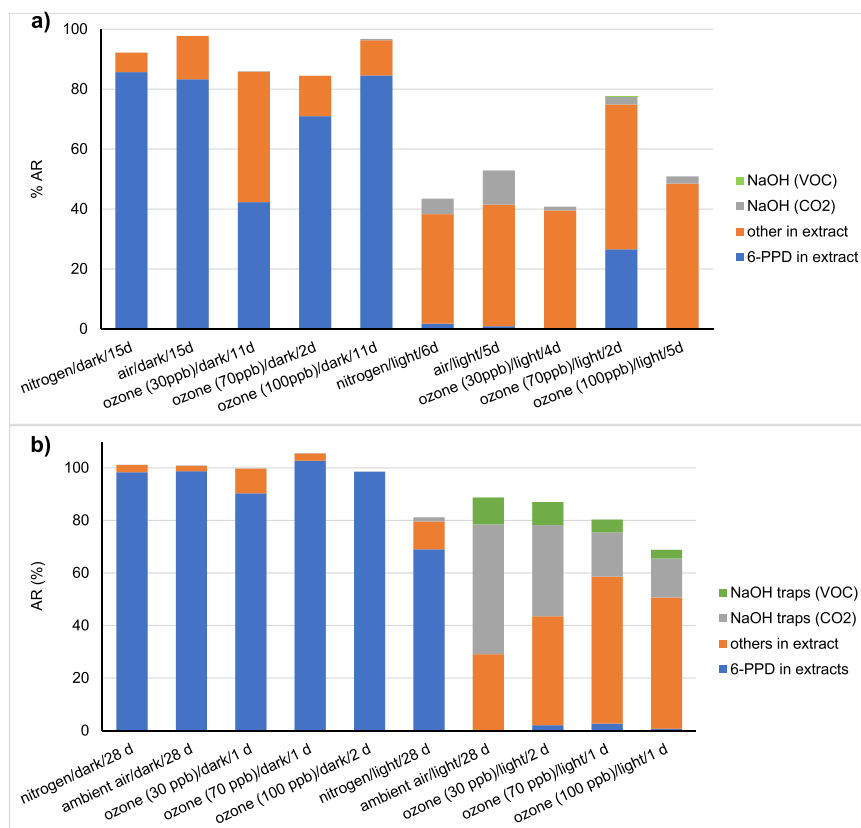


Fig. 5. Balance of added radioactivity (AR) for the reactions in contact with gases, in the dark and under simulated sunlight; a) of 6-PPD, b) of 6-PPDQ. Note the different test durations (d).

After 5–6 d of sunlight exposure no 6-PPD remained in contact with nitrogen, air or ozone but around 40–50% AR was determined as transformation products in the reaction chamber (Fig. 5a). The proportion of AR determined as carbon dioxide reached 11% for air after 5d and 20% for 30 ppm ozone after 11 d.

The amount of 6-PPDQ formed from 6-PPD that was found at the end of each of the experiments was $\leq 0.6\%$ AR in all cases (Table S15). In some experiments with oxygen and ozone the intermediate concentration of 6-PPDQ reached 1.0–1.3% AR, as long as larger proportions of 6-PPD were present (50–30% AR). Beyond that point in time, the 6-PPDQ concentration decreased. This reflects the reactivity of 6-PPDQ towards oxygen and ozone (see below) that prevents its accumulation under these conditions.

Only limited quantitative data is available in literature on transformation products of 6-PPD except for 6-PPDQ, 4-HDPA and 4-DBAP (Di et al., 2022) for which reference compounds are available. This

study with the radiolabeled 6-PPD provides the first full quantification.

3.2.2. 6-PPDQ

3.2.2.1. Speed of transformation. 6-PPDQ was stable in the dark with most tested gases, so that half-lives could not be determined (Table 2). Only with 30 ppb ozone a clear decrease was recorded within 2 d, resulting in a half-life of 8 d (Fig. 5b). Sunlight exposure greatly reduced the stability of 6-PPDQ in all cases. A half-life of 56 d in nitrogen under sunlight exposure indicates that direct photolysis takes place to some extent but is orders of magnitude less important than for 6-PPD (DT50 of 0.5 h). This agrees to studies in aqueous solution (Redman et al., 2023; Seiwert et al., 2022).

However, 6-PPDQ is highly reactive in presence of air or ozone with simulated sunlight: its half-life then ranges from 2 h to 11 h and is even a little shorter than that of 6-PPD under the same conditions (4–15 h)

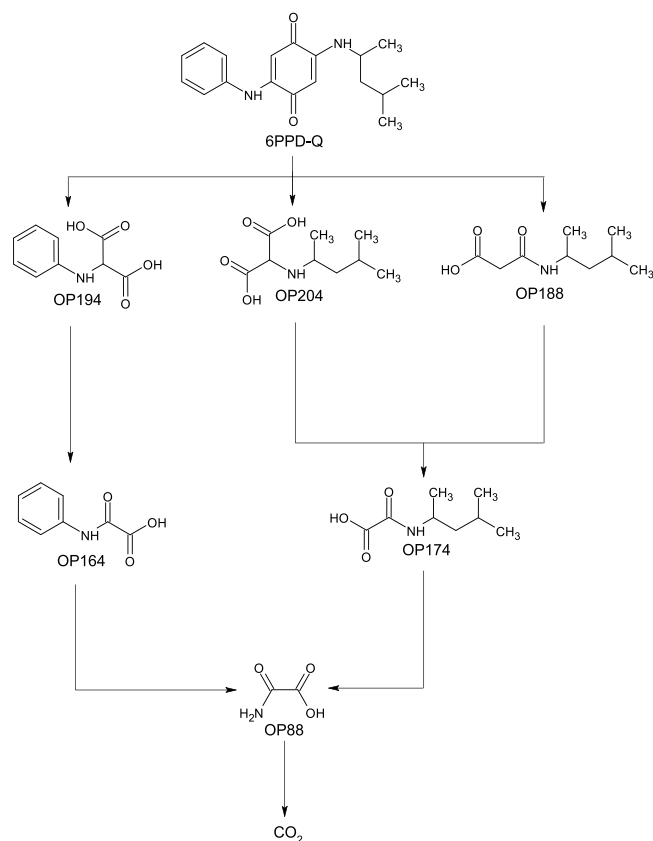


Fig. 6. Proposed structures of transformation products of 6-PPDQ in contact with gases and simulated sunlight. (mass spectrometric information provided in Tables S17 and S18).

(Table 2). This explains, why the extent of formation of 6-PPDQ from 6-PPD is limited and 6-PPDQ is only detectable as long as sufficient 6-PPD is present to allow for a rapid formation of new 6-PPDQ (see above).

3.2.2.2. Transformation product. Structure proposals were elaborated for 6 transformation products based on LC-MS analysis (Fig. 6; Table S17, Table S18). The pathway constructed from them shows three initial transformation products (OP194, OP204, OP188), all of which originate from the oxidative opening of the quinone ring. Via two further products (OP164, OP174) they lead to the highly oxidized OP88 (2-amino-2-oxoacetic acid) and, eventually, to carbon dioxide.

The oxidative transformation of 6-PPDQ has been studied far less often than that of 6-PPD. In those studies available (partially in aqueous solution and using a high-energy mercury lamp instead of a xenon lamp), oxidative opening of the quinone ring has been shown to be the major initial oxidation reaction and OH-radicals the major drivers of oxidation (Redman et al., 2023; Seiwert et al., 2022; Wang et al., 2024). The transformation products detected in this study do not agree to those previously reported, except for OP204 (Seiwert et al., 2022). The radiolabeling in this study may have allowed to detect transformation products that otherwise would have been overlooked. Detection of transformation products in LC-MS is strongly dependent on the analytical conditions.

3.2.2.3. Product distribution. Recovery of total AR was high for all dark experiments where the extent of 6-PPDQ transformation was limited; it decreased to 70 – 90% in the experiments with simulated sunlight (Fig. 5b). The effect of direct photolysis on 6-PPDQ (in nitrogen) was limited, strong transformation was visible in presence of air and ozone, with hardly any 6-PPDQ remaining after 1 – 2 d.

However, 6-PPDQ was not quantitatively transformed into CO₂

during the experiments: 20 – 50% of AR was determined as CO₂, while 30 – 60% remained as transformation products in the reaction vial (Fig. 5b). In the cases with the strongest transformation (air/light/28 d and ozone 30ppb/light/2 d) formation of VOCs was visible and comprised 9 – 10% AR. For these two experiments, 44 – 60% AR occurred as volatiles, in inorganic (CO₂) and organic form (VOCs). No quantitative data on oxidation products of 6-PPDQ are reported in literature, with which the results reported here could be compared.

4. Conclusions

This study provides the first results on the abiotic transformation of 6-PPD and 6-PPDQ under standardized conditions and using radiolabeled test compounds. It yields the following results:

- 6-PPD is susceptible to hydrolysis with DT50 at 25°C and neutral pH of 5 d in buffer and median 7.6 d in the 13 surface waters studied. The major initial product is 4-HDPA, which is transformed further to unknown products. 6-PPD stability increase at lower temperature and lower pH; only then intermediate formation of 6-PPDQ was observed with a yield of 7.5% AR.
- 6-PPDQ is not prone to hydrolysis: the DT50 under sterile conditions and exclusion of oxygen and light at 25°C at pH7 exceeded > 1000 d in buffer and showed a median of 409 d in surface waters at native pH. At 50°C and pH 9 the DT50 was 467 d. Hydrolysis is not expected to play a major role in the environmental fate of 6-PPDQ as oxidation processes have been shown to be much faster.
- 6-PPD reacts directly with (traces of) oxygen (DT50 16 d) and faster with ozone gas (DT50 of 3.5 d with 30 ppb ozone). Direct sunlight photolysis results in a half-life of 14 h, while indirect photolysis of 6-PPD with reactive oxygen species is much fast with a DT50 of 3.7 h in presence of 30 ppb ozone and sunlight. 6-PPDQ was formed in some of the experiments up to intermediate 1.3% AR, decreasing to some level of 0.6% at the end of the experiment.
- 6-PPDQ is less reactive to oxygen and ozone in the dark than 6-PPD (DT50 range: 3.5 – 27 d). Direct photolysis was slow (DT50 56 d). As soon as light and air/oxygen or light and ozone are present, the half-life of 6-PPDQ decrease to values similar to 6-PPD. Roughly 40% AR was determined as carbon dioxide and VOCs) with 30 ppb ozone and light after 2d; another 40% AR were determined as very polar products. For that reason, no significant 6-PPDQ formation occurs when 6-PPD reacts with ozone and light. Oxidative transformation of 6-PPDQ proceeds via opening products of the quinone-ring, with 20–50% AR recorded as CO₂.

In summary 6-PPD is susceptible to abiotic transformation with water as well as with light and oxygen species. Its transformation product 6-PPDQ is resistant to hydrolysis and direct photolysis; it is highly reactive in presence of reactive oxygen species (indirect photolysis in presence of oxygen or ozone) and typically found in a proportion of ≤ 1%. The occurrence of 6-PPDQ as reaction product from 6-PPD in the environment is expected to be relevant when 6-PPD reacts with oxygen species in the dark and in absence of water or microorganisms.

The outcomes of this study support the environmental risk assessment of 6-PPD and 6-PPDQ.

CRedit authorship contribution statement

Sara Bennett: Writing – review & editing, Funding acquisition. **Rory Mumford:** Supervision, Methodology, Investigation. **Pete Yeomans:** Supervision, Methodology, Investigation, Conceptualization. **Bettina Seiwert:** Writing – review & editing, Writing – original draft, Visualization, Formal analysis. **Thorsten Reemtsma:** Writing – review & editing, Writing – original draft, Visualization, Project administration, Funding acquisition, Formal analysis.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Thorsten Reemtsma reports financial support was provided by World Business Council for Sustainable Development. Sara Bennett reports financial support was provided by World Business Council for Sustainable Development. Thorsten Reemtsma reports a relationship with World Business Council for Sustainable Development that includes: funding grants. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

TR and BS gratefully acknowledge funding by Tire Industry Project (TIP), a global, voluntary initiative led by CEOs from 10 major tire companies, operating under the World Business Council for Sustainable Development (WBCSD, Geneva, Switzerland). The work presented was performed independently by Smithers and was funded by the Tire Industry Project. The study's design, execution and interpretation were carried out exclusively by the authors.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.ecoenv.2026.120082](https://doi.org/10.1016/j.ecoenv.2026.120082).

Data availability

Data will be made available on request.

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