3 Chemical Properties

This section reviews the modeled and measured physicochemical properties of 6PPD and 6PPD-quinone. This information is needed to inform analytical field and lab methods, best management practices, and remediation actions. In general, more research is needed to verify the characteristics of tire contaminants.

This section is a review of the current knowledge of physicochemical properties, sources, and transport for 6PPD and 6PPD-q in the environment. This is an emerging and ongoing area of research, and widespread sampling for 6PPD and 6PPD-q has yet to begin. In addition, the presence of 6PPD in many products, transformation to 6PPD-q, and the leaching characteristics of both are not yet clear (see Section 8.2: Occurrence, Fate, Transport, and Exposure to 6PPD and 6PPD-q). Although other emerging contaminants that originate from tires are known to occur in the environment, the scope of this document is limited to discussion of 6PPD and its transformation product 6PPD-q.

A summary of the physicochemical characteristics of 6PPD and 6PPD-q is provided in Table 3-1. Studies highlighted in the table were performed with an isolated 6PPD-q standard in a lab setting and not with field-collected samples (for example, stormwater or tire leachate) unless otherwise specified. Therefore, the physicochemical properties of 6PPD-q may be different in the environment.

Table 3-1. Properties of 6PPD and 6PPD-q

Property	6PPD	6PPD-q	Reference
Molecular Formula	$C_{18}H_{24}N_2$	$C_{18}H_{22}N_2O_2$	(Tian et al. 2022 [BICQHLBC] Tian, Zhenyu, Melissa Gonzalez, Craig A. Rideout, et al. 2022. “6PPD-Quinone: Revised Toxicity Assessment and Quantification with a Commercial Standard.” Environmental Science & Technology Letters, ahead of print, January 11. https://doi.org/10.1021/acs.estlett.1c00910. Tian et al. 2021 [X88WFG3P] Tian, Zhenyu, Haoqi Zhao, Katherine T. Peter, et al. 2021. “A Ubiquitous Tire Rubber–Derived Chemical Induces Acute Mortality in Coho Salmon.” Report. Science 371 (6525): 185–89. https://doi.org/10.1126/science.abd6951. PubChem 2021 [H3YIMDP9] PubChem. 2021. “N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine.” January. https://pubchem.ncbi.nlm.nih.gov/compound/13101.)
CAS Number	793-24-8	2754428-18-5	CompTox: 6PPD, 6PPD-q
SMILES	CC(C)CC(C)NC1=CC=C(C=C1)NC2=CC=CC=C2	CC(C)CC(C)NC1=CC(=O)C(=CC1=O)NC2=CC=CC=C2	CompTox: 6PPD, 6PPD-q
Molecular Name	N-(1,3-Dimethylbutyl)-N′-phenyl-p-phenylenediamine	2-((4-Methylpentan-2-yl)amino)-5-(phenylamino)cyclohexa-2,5-diene-1,4-dione	(Hu et al. 2023 [BFCNSBLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber-Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. PubChem 2021 [H3YIMDP9] PubChem. 2021. “N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine.” January. https://pubchem.ncbi.nlm.nih.gov/compound/13101.)
Molecular Weight	268.402 g/mol	298.39 g/mol	CompTox: 6PPD, 6PPD-q
Solubility	500 – 2,000 µg/L at 50°C	38 +/- 10 µg/L	(Hu et al. 2023 [BFCNSBLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber-Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. OSPAR Commission 2006 [SVMKJMTX] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.)
Physical State	Solid (brown or violet)	Solid (from dark red/deep yellow red/dark orange to black)	CompTox: 6PPD, 6PPD-q
Melting Point	49.2°C	66.0°C	CompTox: 6PPD, 6PPD-q
Boiling Point	163–165°C	341°C	CompTox: 6PPD, 6PPD-q
Vapor Pressure	3.35×10^{-6} Pa at 25°C (estimated)	2.11×10^{-5} Pa at 25°C (estimated)	CompTox: 6PPD, 6PPD-q
Dissociation constant	pKa=6.7 at 20°C	pKa=9.14 (estimated)	CompTox: 6PPD, 6PPD-q
Octanol-Water Partition Coefficient, log(K_{ow})	4.68	4.3 ± 0.02	(Hu et al. 2023 [BFCNSBLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber-Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. PubChem 2021 [H3YIMDP9] PubChem. 2021. “N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine.” January. https://pubchem.ncbi.nlm.nih.gov/compound/13101.)
Organic Carbon-Water Partition coefficient (K_{oc}).	K_{oc}: 11,000 L/kg	K_{oc}: 2400 L/kg	CompTox: 6PPD, 6PPD-q
Organic Carbon-Water Partition Coefficient, log(K_{oc})	4.84	3.928	(USEPA 2023 [8EAETLJA] USEPA. 2023. Estimation Programs Interface SuiteTM for Microsoft® Windows, v 4.11 (EPISuite). V. v 4.11. Released. https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface. OSPAR Commission 2006 [SVMKJMTX] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.);
Bioaccumulation	Low to moderate bioaccumulation (see Section 3.5 for study details)	Limited information & data available (see Section 3.5 for study details)	CompTox: 6PPD, 6PPD-q (Nair et al. 2023 [8V5ES4MI] Nair, Pranav, Jianxian Sun, Linna Xie, et al. 2023. “In Process: Synthesis and Toxicity Evaluation of Tire Rubber–Derived Quinones.” Preprint. Chemistry, June 20. https://doi.org/10.26434/chemrxiv-2023-pmxvc. Fang et al. 2023 [FFFKR3MY] Fang, Chanlin, Liya Fang, Shanshan Di, et al. 2023. “Characterization of N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine (6PPD)-Induced Cardiotoxicity in Larval Zebrafish (Danio Rerio).” Science of the Total Environment 882 (July): 163595. https://doi.org/10.1016/j.scitotenv.2023.163595. Hiki and Yamamoto 2022 [VQE4EZWI] Hiki, Kyoshiro, and Hiroshi Yamamoto. 2022. “The Tire-Derived Chemical 6PPD-Quinone Is Lethally Toxic to the White-Spotted Char Salvelinus leucomaenis pluvius but Not to Two Other Salmonid Species.” Environmental Science & Technology Letters 9 (12): 1050–55. https://doi.org/10.1021/acs.estlett.2c00683. Grasse et al. 2023 [WJHX578U] Grasse, Nico, Bettina Seiwert, Riccardo Massei, Stefan Scholz, Qiuguo Fu, and Thorsten Reemtsma. 2023. “Uptake and Biotransformation of the Tire Rubber-Derived Contaminants 6-PPD and 6-PPD Quinone in the Zebrafish Embryo (Danio rerio).” Environmental Science & Technology 57 (41): 15598–607. https://doi.org/10.1021/acs.est.3c02819. Zhang et al. 2023 [3FCHDX8N] Zhang, Shu-Yun, Xiufeng Gan, Baoguo Shen, et al. 2023. “6PPD and Its Metabolite 6PPDQ Induce Different Developmental Toxicities and Phenotypes in Embryonic Zebrafish.” Journal of Hazardous Materials 455 (August): 131601. https://doi.org/10.1016/j.jhazmat.2023.131601.)
Sorption	Readily sorbs to organics and soils	Readily sorbs to organics and soils; high sorption losses are observed during sampling and lab analysis	(Hu et al. 2023 [BFCNSBLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber-Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. OSPAR Commission 2006 [SVMKJMTX] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.)

Half-life	Less than 1 day (aerobic conditions and dissolved)	Days (aerobic conditions and dissolved) to weeks; characteristics suggest more persistent if bound to soils/ organics	(DTSC 2022 [2M3ZBZ4F] DTSC. 2022. Product-Chemical Profile for Motor Vehicle Tires Containing N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine (6PPD) from the California Department of Toxic Substances Control (DTSC). https://dtsc.ca.gov/wp-content/uploads/sites/31/2022/05/6PPD-in-Tires-Priority-Product-Profile_FINAL-VERSION_accessible.pdf. OECD 2004 [FCJPCPVW] OECD. 2004. SIDS Initial Assessment Report for N-(1,3-Dimethylbutyl)-N´-Phenyl-1,4-Phenylenediamine (6PPD), Organisation for Economic Co-Operation and Development (OECD). https://hpvchemicals.oecd.org/UI/handler.axd?id=5e1a446c-5969-479c-9270-7ced8726952e. Hu et al. 2023 [BFCN5BLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber-Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. OSPAR Commission 2006 [SVMKJM7X] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.) (Section 3.2)
Stability in Water	Abiotic half-life less than a day under most conditions; faster degradation in biologically active water	Half-life=33 hours in 23°C tap water; approx. 25+/-10% loss over 47 days at pH 5, 7, and 9	(Hu et al. 2023 [BFCN5BLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber-Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. Hiki et al. 2021 [WZF69GXC] Hiki, Kyoshiro, Kenta Asahina, Kota Kato, et al. 2021. “Acute Toxicity of a Tire Rubber–Derived Chemical, 6PPD Quinone, to Freshwater Fish and Crustacean Species.” Environmental Science & Technology Letters 8 (9): 779–84. https://doi.org/10.1021/acs.estlett.1c00453. Johannessen et al. 2022 [E9K7U5U3] Johannessen, Cassandra, Paul Helm, Brent Lashuk, Viviane Yargeau, and Chris D. Metcalfe. 2022. “The Tire Wear Compounds 6PPD-Quinone and 1,3-Diphenylguanidine in an Urban Watershed.” Archives of Environmental Contamination and Toxicology 82 (2): 171–79. https://doi.org/10.1007/s00244-021-00878-4. OSPAR Commission 2006 [SVMKJM7X] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.)

Notes: µg/L=micrograms per liter, g/mol=grams per mole, L/kg=liter per kilogram

3.1 Solubility

Solubility

- 6PPD is more soluble than 6PPD-q in water (mg/L vs. ug/L).
- 6PPD-q preferentially binds to organic matter and can sorb to containers, so it has some hydrophobic properties.
- Conversely, 6PPD-q is sufficiently soluble to be transported by water until it is captured by an organic medium.

One notable characteristic is the solubility of 6PPD and 6PPD-q. 6PPD needs to be unbound and mobile in the rubber of tires. The migration rate from inside the tire to the outside layer where it will react with ozone is vital to its performance (Huntink, N.M. and Datta, R.N. 2003 [RTIIEIBC] Huntink, N.M., and Datta, R.N. 2003. “A Novel Slow Release Antidegradant for the Rubber Industry—Part 1: Migration Behavior of Newly Developed Anti-Ozonant Compared to Conventional Antidegradants.” Kautschuk Gummi Kunststoffe 56 (6): 310–15. Razumovskii and Batashova 1970 [JRUTALHF] Razumovskii, S. D., and L. S. Batashova. 1970. “Mechanism of Protection against Ozone by N-Phenyl-N′-Isopropyl-p-Phenylenediamine.” Rubber Chemistry and Technology 43 (6): 1340–48. https://doi.org/10.5254/1.3547334.). The solubility of 6PPD in water is between 0.5 and 2 mg per liter (mg/L) (Hiki et al. 2021 [WZF69GXC] Hiki, Kyoshiro, Kenta Asahina, Kota Kato, et al. 2021. “Acute Toxicity of a Tire Rubber–Derived Chemical, 6PPD Quinone, to Freshwater Fish and Crustacean Species.” Environmental Science & Technology Letters 8 (9): 779–84. https://doi.org/10.1021/acs.estlett.1c00453. DTSC 2022 [MK5W6W3J] DTSC. 2022. The Impact of California’s Brake Pad Law: Report to the Legislature. Department of Toxic Substances Control and State Water Resources Control Board. https://dtsc.ca.gov/wp-content/uploads/sites/31/2023/08/Brake-Pad-Legislative-Report-Accessible.pdf. ECHA 2022 [Z9UAAF4F] ECHA. 2022. “6PPD: 1,4-Benzenediamine, N1-(1,3-Dimethylbutyl)-N4-Phenyl- Registration Dossier - European Chemicals Agency (ECHA).” December 2. https://echa.europa.eu/registration-dossier/-/registered-dossier/15367/1/2. Seiwert et al. 2020 [XRNTFZ69] Seiwert, Bettina, Philipp Klöckner, Stephan Wagner, and Thorsten Reemtsma. 2020. “Source-Related Smart Suspect Screening in the Aqueous Environment: Search for Tire-Derived Persistent and Mobile Trace Organic Contaminants in Surface Waters.” Analytical and Bioanalytical Chemistry 412 (20): 4909–19. https://doi.org/10.1007/s00216-020-02653-1.). Although isolated 6PPD-q is modeled to be more soluble, testing a 6PPD-q commercial standard has shown that it is much less soluble than 6PPD, with reported solubilities ranging from 0.04–0.07 mg/L (Hu et al. 2023 [BFCN5BLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber–Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. DTSC 2022 [MK5W6W3J] DTSC. 2022. The Impact of California’s Brake Pad Law: Report to the Legislature. Department of Toxic Substances Control and State Water Resources Control Board. https://dtsc.ca.gov/wp-content/uploads/sites/31/2023/08/Brake-Pad-Legislative-Report-Accessible.pdf.).[5] This has consequences on the toxicity and transport of these compounds in aquatic environments, as well as analytical methods, where they are often dissolved in other solvents such as methanol or acetonitrile before use in the lab. 6PPD-q preferentially binds to organic matter and can sorb to containers, so it has some hydrophobic properties (Hu et al. 2023 [BFCN5BLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber–Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H.).

3.2 Half-life

Half-life

- 6PPD-q is more stable than 6PPD in water (half-life of weeks vs. less than 1 day).
- More research is needed to understand the half-life under variable conditions and formations.

6PPD and 6PPD-q also have different stabilities. In water, 6PPD has a half-life of less than a day under aerobic conditions (OECD 2004 [FCJPCPVW] OECD. 2004. SIDS Initial Assessment Report for N-(1,3-Dimethylbutyl)-N´-Phenyl-1,4-Phenylenediamine (6PPD), Organisation for Economic Co-Operation and Development (OECD). https://hpvchemicals.oecd.org/UI/handler.axd?id=5e1a446c-5969-479c-9270-7ced8726952e.), whereas 6PPD-q has been shown to be relatively stable in water. The half-life for 6PPD-q has been reported to range from 33 hours at 23°C in dechlorinated tap water (Hiki et al. 2021 [WZF69GXC] Hiki, Kyoshiro, Kenta Asahina, Kota Kato, et al. 2021. “Acute Toxicity of a Tire Rubber–Derived Chemical, 6PPD Quinone, to Freshwater Fish and Crustacean Species.” Environmental Science & Technology Letters 8 (9): 779–84. https://doi.org/10.1021/acs.estlett.1c00453.) to longer than 47 days (approximately 25% degradation) (DTSC 2022 [2M3Z8Z4F] DTSC. 2022. Product-Chemical Profile for Motor Vehicle Tires Containing N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine (6PPD) from the California Department of Toxic Substances Control (DTSC). https://dtsc.ca.gov/wp-content/uploads/sites/31/2022/05/6PPD-in-Tires-Priority-Product-Profile_FINAL-VERSION_accessible.pdf . Hu et al. 2023 [BFCN5BLS] Hu, Ximin, Haoqi (Nina) Zhao, Zhenyu Tian, Katherine T. Peter, Michael C. Dodd, and Edward P. Kolodziej. 2023. “Chemical Characteristics, Leaching, and Stability of the Ubiquitous Tire Rubber–Derived Toxicant 6PPD-Quinone.” Environmental Science: Processes & Impacts 25 (5): 901–11. https://doi.org/10.1039/D3EM00047H. OSPAR Commission 2006 [SVMKJM7X] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029. ECHA 2021 [Y79Z3ZWV] ECHA. 2021. “Substance Infocard: N-1,3-Dimethylbutyl-N’-Phenyl-p-Phenylenediamine. European Chemicals Agency (ECHA).” April 7. https://echa.europa.eu/substance-information/-/substanceinfo/100.011.222.). The half-lives of 6PPD and 6PPD-q have been shown to change with temperature and pH and also be affected by sunlight and biological processes (Qian et al. 2023 [KRT88TMQ] Qian, Yiguang, Ziyu Chen, Jiahui Wang, et al. 2023. “H/D Exchange Coupled with 2H-Labeled Stable Isotope–Assisted Metabolomics Discover Transformation Products of Contaminants of Emerging Concern.” Analytical Chemistry 95 (33): 12541–49. https://doi.org/10.1021/acs.analchem.3c02833. Hiki et al. 2021 [WZF69GXC] Hiki, Kyoshiro, Kenta Asahina, Kota Kato, et al. 2021. “Acute Toxicity of a Tire Rubber–Derived Chemical, 6PPD Quinone, to Freshwater Fish and Crustacean Species.” Environmental Science & Technology Letters 8 (9): 779–84. https://doi.org/10.1021/acs.estlett.1c00453. Redman et al. 2023 [YJE933XT] Redman, Zachary C., Jessica L. Begley, Isabel Hillestad, et al. 2023. “Reactive Oxygen Species and Chromophoric Dissolved Organic Matter Drive the Aquatic Photochemical Pathways and Photoproducts of 6PPD-Quinone under Simulated High-Latitude Conditions.” Environmental Science & Technology 57 (49): 20813–21. https://doi.org/10.1021/acs.est.3c05742.). More research is needed to predict stability under variable environmental conditions (for example, anaerobic, temperature, pH) and matrices (for example, air, water, soil, sediment).

3.3 Transformation Products and Processes

6PPD in Tires and Transformation to 6PPD-q

- Motor vehicle tires contain approximately 1–2% 6PPD (DTSC 2022 [2M3Z8Z4F] DTSC. 2022. Product-Chemical Profile for Motor Vehicle Tires Containing N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine (6PPD) from the California Department of Toxic Substances Control (DTSC). https://dtsc.ca.gov/wp-content/uploads/sites/31/2022/05/6PPD-in-Tires-Priority-Product-Profile_FINAL-VERSION_accessible.pdf.).
- The amount of 6PPD in tires decreases with age of the tire.
- 6PPD in solution transforms to 6PPD-q when exposed to ultraviolet radiation.
- 10% of the 6PPD transforms to 6PPD-q when exposed to ozone (Zhao et al. 2023 [ENE6F3HC] Zhao, Haoqi Nina, Ximin Hu, Zhenyu Tian, et al. 2023. “Transformation Products of Tire Rubber Antioxidant 6PPD in Heterogeneous Gas-Phase Ozonation: Identification and Environmental Occurrence.” Environmental Science & Technology 57 (14): 5621–32. https://doi.org/10.1021/acs.est.2c08690.).
- More research is needed to characterize additional PPDs and their transformation products.

The physicochemical properties that impact fate and transport of 6PPD and several transformation products from TRWP (fresh and weathered/aged) have been investigated under various benchtop leaching and sediment incubator conditions (Unice et al. 2015 [NS59BGK2] Unice, K. M., Jennifer Bare, Marisa Kreider, and Julie Panko. 2015. “Experimental Methodology for Assessing the Environmental Fate of Organic Chemicals in Polymer Matrices Using Column Leaching Studies and OECD 308 Water/Sediment Systems: Application to Tire and Road Wear Particles.” Science of the Total Environment 533 (July): 476–87. https://doi.org/10.1016/j.scitotenv.2015.06.053.). 6PPD-q was estimated to be 10% of the transformation products when 6PPD was exposed to gas-phase ozone in a column study with a total runtime of approximately 50 hours (Zhao et al. 2023 [ENE6F3HC] Zhao, Haoqi Nina, Ximin Hu, Zhenyu Tian, et al. 2023. “Transformation Products of Tire Rubber Antioxidant 6PPD in Heterogeneous Gas-Phase Ozonation: Identification and Environmental Occurrence.” Environmental Science & Technology 57 (14): 5621–32. https://doi.org/10.1021/acs.est.2c08690.). Ozonation of 6PPD to 6PPD-q has been found to depend on the ozone dose (Seiwert et al. 2022 [QDRRVWMW] Seiwert, Bettina, Maolida Nihemaiti, Mareva Troussier, Steffen Weyrauch, and Thorsten Reemtsma. 2022. “Abiotic Oxidative Transformation of 6-PPD and 6-PPD Quinone from Tires and Occurrence of Their Products in Snow from Urban Roads and in Municipal Wastewater.” Water Research 212: 118122. https://doi.org/10.1016/j.watres.2022.118122.). Other transformation products have been identified in roadway-impacted environmental samples, and 6PPD-q was found to further transform by ozone (Seiwert et al. 2022 [QDRRVWMW] Seiwert, Bettina, Maolida Nihemaiti, Mareva Troussier, Steffen Weyrauch, and Thorsten Reemtsma. 2022. “Abiotic Oxidative Transformation of 6-PPD and 6-PPD Quinone from Tires and Occurrence of Their Products in Snow from Urban Roads and in Municipal Wastewater.” Water Research 212: 118122. https://doi.org/10.1016/j.watres.2022.118122.). Unice et al. (Unice et al. 2015 [NS59BGK2] Unice, K. M., Jennifer Bare, Marisa Kreider, and Julie Panko. 2015. “Experimental Methodology for Assessing the Environmental Fate of Organic Chemicals in Polymer Matrices Using Column Leaching Studies and OECD 308 Water/Sediment Systems: Application to Tire and Road Wear Particles.” Science of the Total Environment 533 (July): 476–87. https://doi.org/10.1016/j.scitotenv.2015.06.053.) investigated 6PPD in all ages of TRWP (up to 3.3 years of simulated aging) where there was a decrease in mass detected as the age increased; the largest difference occurred between fresh (0 years) and 0.1 years of aging. As expected, there was limited leaching of 6PPD to water from the TRWP (i.e., low solubility) and a higher fraction that was released to sediment. This study was conducted prior to the discovery of 6PPD-q.

Rapid photodegradation has been observed when 6PPD (in solution) was exposed to light (especially in the ultraviolet wavelength, which is less than 400 nm) in lab water experiments (Li et al. 2023 [3EFLHAGA] Li, Chenguang, Yanlei Zhang, Shiqi Yin, et al. 2023. “First Insights into 6PPD-Quinone Formation from 6PPD Photodegradation in Water Environment.” Journal of Hazardous Materials 459 (October): 132127. https://doi.org/10.1016/j.jhazmat.2023.132127.). The photodegradation of 6PPD was observed to be accelerated under acidic conditions due to the increased absorption of long wavelength irradiation by ionized 6PPD. Li et al. (Li et al. 2023 [3EFLHAGA] Li, Chenguang, Yanlei Zhang, Shiqi Yin, et al. 2023. “First Insights into 6PPD-Quinone Formation from 6PPD Photodegradation in Water Environment.” Journal of Hazardous Materials 459 (October): 132127. https://doi.org/10.1016/j.jhazmat.2023.132127.) identified nine photodegradation products, as identified by ultra-high-performance LC quadrupole time-of-flight MS (UHPLC-QTOF-MS). Reported mechanisms involved in photodegradation include photoexcitation, direct photolysis, self-sensitized photodegradation, and O_2 oxidation (Li et al. 2023 [3EFLHAGA] Li, Chenguang, Yanlei Zhang, Shiqi Yin, et al. 2023. “First Insights into 6PPD-Quinone Formation from 6PPD Photodegradation in Water Environment.” Journal of Hazardous Materials 459 (October): 132127. https://doi.org/10.1016/j.jhazmat.2023.132127.). Sunlight has been shown to transform 6PPD in water to 6PPD-q with a molar yield of approximately 1.01% within 90 minutes at pH 7.0 under simulated sunlight irradiation (Zhou et al. 2023 [QGKYMZ6J] Zhou, Yangjian, Lacuo Yixi, Qingqing Kong, et al. 2023. “Sunlight-Induced Transformation of Tire Rubber Antioxidant N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine (6PPD) to 6PPD-Quinone in Water.” Environmental Science & Technology Letters 10 (9): 798–803. https://doi.org/10.1021/acs.estlett.3c00499.). Research suggests that the degradation of 6PPD-q by sunlight is temperature dependent. This is an area of active research, and the formation pathways and mechanisms of formation of these transformation products in the environment are still considered largely unknown. Evaluating the photodegradation pathway will help us understand the fate of 6PPD and 6PPD-q in the environment.

3.4 Volatility

Significant knowledge gaps exist concerning contaminants associated with TRWP that may be present in the gas phase (Johannessen et al. 2022 [RYBDCBV4] Johannessen, Cassandra, Amandeep Saini, Xianming Zhang, and Tom Harner. 2022. “Air Monitoring of Tire-Derived Chemicals in Global Megacities Using Passive Samplers.” Environmental Pollution 314

(December): 120206. https://doi.org/10.1016/j.envpol.2022.120206.). 6PPD and 6PPD-q have low vapor pressures (reported as 3.35×10^{-6} Pa and 2.11×10^{-5} Pa, respectively, at 25°C), which means these chemicals are unlikely to volatilize at typical conditions in the natural environment (Washington State Department of Ecology 2022 [K2CG7KTE] Washington State Department of Ecology. 2022. 6PPD in Road Runoff Assessment and Mitigation Strategies. Nos. 22-03–020. Environmental Assessment and Water Quality Programs. https://apps.ecology.wa.gov/publications/documents/2203020.pdf.). Due to the tendency for 6PPD to sorb to soil, sediments, and suspended particulates, 6PPD can be present on suspended particles in the air (OSPAR Commission 2006 [SVMKJM7X] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.). Based on an estimated Henry's Law constant of 7.43×10^{-4} at 25°C, 6PPD has moderate potential to volatilize from surface water (OSPAR Commission 2006 [SVMKJM7X] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.). Research summarized by OSPAR (OSPAR Commission 2006 [SVMKJM7X] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.) did not indicate gaseous emissions of 6PPD from tires, but it is unclear whether the absence of these emissions is due to lack of volatility from tires or rapid degradation of 6PPD after release.

3.5 Biological Uptake

The bioconcentration factor (BCF) for 6PPD is predicted to range from 617 to 801 (USEPA [NU4F8BLR] USEPA. n.d. "CompTox Chemicals Dashboard: 6PPD - Chemical Details." https://comptox.epa.gov/dashboard/chemical/details/DTXSID9025114.

OSPAR Commission 2006 [SVMKJM7X] OSPAR Commission. 2006. Hazardous Substances Series 4-(Dimethylbutylamino)Diphenylamine (6PPD) 2005 (2006 Update). Publication Number: 271/2006. https://www.ospar.org/documents?v=7029.), suggesting a low to moderate potential for bioaccumulation. For 6PPD-q, the bioconcentration factor has been predicted to be 20.9 (USEPA [H2B8TI2W] USEPA. n.d. "CompTox Chemicals Dashboard: 6PPD-Quinone - Chemical Details." https://comptox.epa.gov/dashboard/chemical/details/DTXSID301034849.), but more research is needed to confirm its bioavailability and bioaccumulation. For context, the USEPA's Sustainable Futures / P2 Framework Manual has defined the following levels of a chemical's bioaccumulation in *fish*: not bioaccumulative if BCF less than 1,000; bioaccumulative if BCF greater than or equal to 1,000; and very bioaccumulative if BCF greater than or equal to 5,000 (USEPA 2012 [METDU9H5] USEPA. 2012. 7. Estimating Persistence, Bioaccumulation, and Toxicity Using the PBT Profiler. EPA-748-B12-001. Sustainable Futures / P2 Framework Manual. https://www.epa.gov/sites/default/files/2015-05/documents/07.pdf.).

BCFs of 6PPD-q in rainbow trout were calculated at 2.9, 19, 25, and 17.2 liters per kg (L/kg) at water concentrations of 0.8, 3, 12, and 25 µg/L, respectively, and concentrations of 6PPD in tissue were similar at the same water concentrations (Nair et al. 2023 [9V5ES4MI] Nair, Pranav, Jianxian Sun, Linna Xie, et al. 2023. "In Process: Synthesis and Toxicity Evaluation of Tire Rubber–Derived Quinones." Preprint. Chemistry, June 20. https://doi.org/10.26434/chemrxiv-2023-pmxvc.). These BCF factors are 1 to 2 orders of magnitude lower than other contaminants with similar K_{ow} values, suggesting that 6PPD-q may be rapidly metabolized in rainbow trout (and other susceptible salmonids). Several studies have demonstrated moderate uptake of 6PPD and 6PPD-q in zebrafish from laboratory water, with uptake levels generally higher with 6PPD compared to 6PPD-q (Fang et al. 2023 [FFFKR3MY] Fang, Chanlin, Liya Fang, Shanshan Di, et al. 2023. "Characterization of N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine (6PPD)-Induced Cardiotoxicity in Larval Zebrafish (Danio Rerio)." Science of the Total Environment 882 (July): 163595. https://doi.org/10.1016/j.scitotenv.2023.163595. Grasse et al. 2023 [WJHX578U] Grasse, Nico, Bettina Seiwert, Riccardo Massei, Stefan Scholz, Qiuguo Fu, and Thorsten Reemtsma. 2023. "Uptake and Biotransformation of the Tire Rubber–Derived Contaminants 6-PPD and 6-PPD Quinone in the Zebrafish Embryo (Danio rerio)." Environmental Science & Technology 57 (41): 15598–607. https://doi.org/10.1021/acs.est.3c02819. Zhang et al. 2023 [3FCHDXBN] Zhang, Shu-Yun, Xiufeng Gan, Baoguo Shen, et al. 2023. "6PPD and Its Metabolite 6PPDQ Induce Different Developmental Toxicities and Phenotypes in Embryonic Zebrafish." Journal of Hazardous Materials 455 (August): 131601.

https://doi.org/10.1016/j.jhazmat.2023.131601.). Fang et al. (Fang et al. 2022 [69WA3QCX] Fang, Chanlin, Liya Fang, Shanshan Di, et al. 2022. "Not yet Peer Reviewed: Bioaccumulation of N-(1,3-Dimethylbutyl)-N′-Phenyl-p-Phenylenediamine (6PPD) and Its Potential Cardiotoxicity in Larval Zebrafish (Danio Rerio)." SSRN Scholarly Paper No. 4166691. Rochester, NY, July 19. https://papers.ssrn.com/abstract=4166691.) estimated accumulation factors for 6PPD in zebrafish larvae of 265 and 103

based on concentrations in water of 1.35 and 28.2 µg/L, respectively. Grasse et al. (Grasse et al. 2023 [WJHX578U] Grasse, Nico, Bettina Seiwert, Riccardo Massei, Stefan Scholz, Qiuguo Fu, and Thorsten Reemtsma. 2023. “Uptake and Biotransformation of the Tire Rubber–Derived Contaminants 6-PPD and 6-PPD Quinone in the Zebrafish Embryo (Danio rerio).” Environmental Science & Technology 57 (41): 15598–607. https://doi.org/10.1021/acs.est.3c02819.) estimated accumulation concentration factors of 6PPD and 6PPD-q in zebrafish embryo over 96 hours of exposure. Analytically determined exposure concentrations were 1.28 and 6.3 µg/L for 6PPD and 4.8, 11.3, and 20.9 µg/L for 6PPD-q. At 72 hours (when 6PPD reached steady state in all experiments), the concentration factors ranged from 142 to 2,447 for 6PPD. 6PPD-q never reached steady state; however, the concentration factors associated with the highest internal concentrations (at 48 hours) ranged from 75 to 216. The mean maximum concentration factor (135.8 ± 64.9) occurred between 24 and 48 hours before decreasing after 96 hours (55.5 ± 29.84). Overall, the decrease in internal concentration of 6PPD-q suggested that biotransformation reactions were occurring in the zebrafish embryos. Specifically, semi-quantification methods found that 50% of 6PPD and 95% 6PPD-q were detoxified through biotransformation in the zebrafish embryos within 96 hours of exposure, suggesting that zebrafish embryos have greater tolerance to 6PPD-q than other species (Grasse et al. 2023 [WJHX578U] Grasse, Nico, Bettina Seiwert, Riccardo Massei, Stefan Scholz, Qiuguo Fu, and Thorsten Reemtsma. 2023. “Uptake and Biotransformation of the Tire Rubber–Derived Contaminants 6-PPD and 6-PPD Quinone in the Zebrafish Embryo (Danio rerio).” Environmental Science & Technology 57 (41): 15598–607. https://doi.org/10.1021/acs.est.3c02819.).

Biological Uptake

- 6PPD is predicted to have a low to moderate potential for bioaccumulation.
- Research supports the biological uptake of both 6PPD and 6PPD-q.
- See Section 2: Effects Characterization and Toxicity for more information on the mode of action.
- More research is needed to confirm bioaccumulation of 6PPD-q.

Uptake studies published to date have occurred primarily in lab settings. Additional studies are needed to evaluate biological uptake for conditions outside the lab where variability in environmental (and stormwater) conditions over the range of concentrations measured in the field is considered and incorporated.

S.-Y. Zhang et al. (Zhang et al. 2023 [3FCHDXBN] Zhang, Shu-Yun, Xiufeng Gan, Baoguo Shen, et al. 2023. “6PPD and Its Metabolite 6PPDQ Induce Different Developmental Toxicities and Phenotypes in Embryonic Zebrafish.” Journal of Hazardous Materials 455 (August): 131601. https://doi.org/10.1016/j.jhazmat.2023.131601.) observed statistically significant accumulation of 6PPD and 6PPD-q in zebrafish embryos following exposures of 0.2 and 0.8 mg/L of each compound from 8 to 120 hours post fertilization, with 6PPD having a greater magnitude of accumulation. There was no statistically significant accumulation of either compound at an exposure concentration of 0.025 mg/L. With the exception of the minimum exposure concentrations in Fang et al. (Zhang et al. 2023 [3FCHDXBN] Zhang, Shu-Yun, Xiufeng Gan, Baoguo Shen, et al. 2023. “6PPD and Its Metabolite 6PPDQ Induce Different Developmental Toxicities and Phenotypes in Embryonic Zebrafish.” Journal of Hazardous Materials 455 (August): 131601. https://doi.org/10.1016/j.jhazmat.2023.131601.) and Grasse et al. (Grasse et al. 2023 [WJHX578U] Grasse, Nico, Bettina Seiwert, Riccardo Massei, Stefan Scholz, Qiuguo Fu, and Thorsten Reemtsma. 2023. “Uptake and Biotransformation of the Tire Rubber–Derived Contaminants 6-PPD and 6-PPD Quinone in the Zebrafish Embryo (Danio rerio).” Environmental Science & Technology 57 (41): 15598–607. https://doi.org/10.1021/acs.est.3c02819.), these experimental exposure levels were higher than those detected in surface water. Uptake has also been detected in lettuce in hydroponic solution in a laboratory (Castan et al. 2023 [3RBDETGD] Castan, Stephanie, Anya Sherman, Ruoting Peng, et al. 2023. “Uptake, Metabolism, and Accumulation of Tire Wear Particle–Derived Compounds in Lettuce.” Environmental Science & Technology 57 (1): 168–78. https://doi.org/10.1021/acs.est.2c05660.) and in fish purchased at a local market in China (Ji et al. 2022 [LDBNLUJS] Ji, Jiawen, Changsheng Li, Bingjie Zhang, et al. 2022. “Exploration of Emerging Environmental Pollutants 6PPD and 6PPDQ in Honey and Fish Samples.” Food Chemistry 396: 133640. https://doi.org/10.1016/j.foodchem.2022.133640.).

Another study assessed the toxicity and accumulation of 6PPD-q at environmentally relevant concentrations in three different fish species (Hiki and Yamamoto 2022 [VQE4EZWI] Hiki, Kyoshiro, and Hiroshi Yamamoto. 2022. “The Tire-Derived Chemical 6PPD-Quinone Is Lethally Toxic to the White-Spotted Char Salvelinus leucomaenis pluvius but Not to Two Other Salmonid Species.” Environmental Science & Technology Letters 9 (12): 1050–55. https://doi.org/10.1021/acs.estlett.2c00683.). The concentration of 6PPD-q in the target tissues (brain and gills) increased with exposure concentration in the most sensitive species tested (*S. leucomaenis pluvius*), yielding internal median lethal

concentration (ILC_{50}) estimates of "…4.0 µg/kg wet weight in brain and 6.2 µg/kg wet weight in gill for *S. leucomaenis pluvius*, while the tissue concentration of 6PPD-q in the two other non-surviving species (*S. curilus* and *O. masou masou*) exceeded the ILC_{50} value for *S. leucomaenis pluvius"* (Hiki and Yamamoto 2022 [VQE4EZWI] Hiki, Kyoshiro, and Hiroshi Yamamoto. 2022. "The Tire-Derived Chemical 6PPD-Quinone Is Lethally Toxic to the White-Spotted Char Salvelinus leucomaenis pluvius but Not to Two Other Salmonid Species." Environmental Science & Technology Letters 9 (12): 1050–55. https://doi.org/10.1021/acs.estlett.2c00683.).

As stated by Grasse et al. (Grasse et al. 2023 [WJHX578U] Grasse, Nico, Bettina Seiwert, Riccardo Massei, Stefan Scholz, Qiuguo Fu, and Thorsten Reemtsma. 2023. "Uptake and Biotransformation of the Tire Rubber–Derived Contaminants 6-PPD and 6-PPD Quinone in the Zebrafish Embryo (Danio rerio)." Environmental Science & Technology 57 (41): 15598–607. https://doi.org/10.1021/acs.est.3c02819.), "…[c]ross-species internal concentrations and biotransformation of [6PPD-q] provide an important contribution to the characterization of species-specific toxicity" and it "is still unknown whether toxicokinetics (TK) plays a role in the observed species-specific [6PPD-q] toxicity." The toxicological significance of any accumulation is currently unknown (see Section 8.1). See Section 2.3: Potential for Bioaccumulation and Adduct Formation in the toxicity section for more information about the mode of action.

3.6 Biodegradation

More research is needed to understand the biodegradation processes of tires, TRWP), and related contaminants. Whole tires, tire debris, and TRWP are all potential sources of 6PPD and 6PPD-q in the environment. Biodegradation of tire-related compounds, including 6PPD and 6PPD-q, may occur within the TRWP itself or in the environment after leaching (Calarnou et al. 2023 [2RFJ5BLH] Calarnou, Laurie, Mounir Traïkia, Martin Leremboure, et al. 2023. "Assessing Biodegradation of Roadway Particles via Complementary Mass Spectrometry and NMR Analyses." Science of the Total Environment 900 (November): 165698. https://doi.org/10.1016/j.scitotenv.2023.165698.). Some studies on the biodegradation of TWP or tire-related compounds have been done; however, these did not assess the leaching or biodegradation of 6PPD or 6PPD-q (Saifur and Gardner 2023 [9WDMIAY3] Saifur, Sumaiya, and Courtney M. Gardner. 2023. "Evaluation of Stormwater Microbiomes for the Potential Biodegradation of Tire Wear Particle Contaminants." Journal of Applied Microbiology 134 (5): lxad086. https://doi.org/10.1093/jambio/lxad086. Klun et al. 2023 [VS4VQ4A6] Klun, Barbara, Ula Rozman, and Gabriela Kalčíková. 2023. "Environmental Aging and Biodegradation of Tire Wear Microplastics in the Aquatic Environment." Journal of Environmental Chemical Engineering 11 (5): 110604. https://doi.org/10.1016/j.jece.2023.110604.).

A recent study by Foscari et al. (Foscari et al. 2024 [JBUK7E3P] Foscari, Aurelio, Bettina Seiwert, Daniel Zahn, Matthias Schmidt, and Thorsten Reemtsma. 2024. "Leaching of Tire Particles and Simultaneous Biodegradation of Leachables." Water Research 253 (April): 121322. https://doi.org/10.1016/j.watres.2024.121322.) evaluated biodegradation during and following leaching of suspended cryo-milled tire tread (CMTT). The first experiment (Phase I) simulated heterogeneous environmental conditions consisting of suspended CMTT, an aqueous phase (i.e., leaching), and microorganisms (i.e., biodegradation). The second experiment (Phase II) assessed just the biodegradation of the particle-free supernatant. To assess the impact of biotic versus abiotic degradation processes, Phase I experiments included test vessels without sludge, and the subsequent Phase II experiments included the supernatant of the sludge-free vessels. The authors concluded that microbial degradation of 6PPD was only observed in Phase I and suggested that abiotic transformation via hydrolysis was dominant in Phase II. In contrast, 6PPD-q showed a strong increasing trend in both sets of Phase I test vessels at the beginning of the study before leveling out in concentration, suggesting that an equilibrium was reached between 6PPD-q released or transformation of 6PPD to 6PPD-q. The equilibrium concentration was lower in the sludge test vessels, suggesting that microbial degradation was significant. Similarly, in Phase II, the sludge test supernatant had a faster decrease in concentration compared to the sludge-free test supernatant, but the observed decrease in concentration in the sludge-free test supernatant supported the impact of abiotic transformation of leached 6PPD-q. These study designs added to the experimental evidence that 6PPD-q is more stable than 6PPD.

6PPD-q has been shown to be formed in wetted soil from 6PPD, presumably by bacteria (Qian et al. 2023 [KRT88TMQ] Qian, Yiguang, Ziyu Chen, Jiahui Wang, et al. 2023. "H/D Exchange Coupled with 2H-Labeled Stable Isotope–Assisted Metabolomics Discover Transformation Products of Contaminants of Emerging Concern." Analytical Chemistry 95 (33): 12541–49. https://doi.org/10.1021/acs.analchem.3c02833.). Calarnou et al. (Calarnou et al. 2023 [2RFJ5BLH] Calarnou, Laurie, Mounir Traïkia, Martin Leremboure, et al. 2023. "Assessing Biodegradation of Roadway Particles via Complementary Mass Spectrometry and NMR Analyses." Science of the Total Environment 900 (November): 165698.

https://doi.org/10.1016/j.scitotenv.2023.165698.) investigated the biodegradation of TRWP (of which TWP is a component) and several tire-related compounds, including 6PPD-q. They found a significant decrease in 6PPD-q in the presence of *S. phaeofaciens* (NRRL 8092) (Calarnou et al. 2023 [2RFJ5BLH] Calarnou, Laurie, Mounir Traïkia, Martin Leremboure, et al. 2023. “Assessing Biodegradation of Roadway Particles via Complementary Mass Spectrometry and NMR Analyses.” Science of the Total Environment 900 (November): 165698. https://doi.org/10.1016/j.scitotenv.2023.165698.). Similarly, Xu et al. (Xu et al. 2023 [4P2E4JLJ] Xu, Qiao, Gang Li, Li Fang, et al. 2023. “Enhanced Formation of 6PPD-Q during the Aging of Tire Wear Particles in Anaerobic Flooded Soils: The Role of Iron Reduction and Environmentally Persistent Free Radicals.” Environmental Science & Technology, ahead of print, March 29. https://doi.org/10.1021/acs.est.2c08672.) suggested that the decrease of 6PPD-q in soil under wet conditions was attributable to biodegradation compared to anaerobic flooded conditions (Xu et al. 2023 [4P2E4JLJ] Xu, Qiao, Gang Li, Li Fang, et al. 2023. “Enhanced Formation of 6PPD-Q during the Aging of Tire Wear Particles in Anaerobic Flooded Soils: The Role of Iron Reduction and Environmentally Persistent Free Radicals.” Environmental Science & Technology, ahead of print, March 29. https://doi.org/10.1021/acs.est.2c08672.). Better understanding of the biodegradation and the fate of 6PPD and 6PPD-q is a major data gap, including validating laboratory study outcomes relative to observations, measurements, and other data from the natural and built environments.