

Hazleton Lab. (1989) *Subchronic toxicity study in rats with paranitrophenol*. Sponsored by Monsanto Co., St. Louis, MO (HLA Study No. 241-221).

Herterich R, Herrmann R (1990) Comparing the distribution of nitrated phenols in the atmosphere of two German hill sites. *Environmental technology letters*, 11:961-972.

Hoechst AG (1977a) *Acute oral toxicity of p-nitrophenol in female SPF-Wistar rats*. Frankfurt/Main, Hoechst AG (unpublished report) (in German).

Hoechst AG (1977b) *Acute dermal toxicity of p-nitrophenol in female SPF-Wistar rats*. Frankfurt/Main, Hoechst AG (unpublished report) (in German).

Hoechst AG (1977c) *Skin and eye irritating effects of p-nitrophenol in rabbits*. Frankfurt/Main, Hoechst AG (unpublished report) (in German).

Hoechst AG (1980) *A mutagenicity screening of 408/80 A in bacteria (Ames test)*. Frankfurt/Main, Hoechst AG (unpublished report).

Hoover DG, Borgonovi GE, Jones SH, Alexander M (1986) Anomalies in mineralization of low concentrations of organic compounds in lake water and sewage. *Applied environmental microbiology*, 51:226-232.

Howe GE, Marking LL, Bills TD, Rach JJ, Mayer FLJ (1994) Effects of water temperature and pH on toxicity of terbufos, trichlorfon,

- 4-nitrophenol and 2,4-dinitrophenol to the amphipod *Gammarus pseudolimnaeus* and rainbow trout (*Oncorhynchus mykiss*).
Environmental toxicology and chemistry, 13:51-66.
- HSDB (1998) *Hazardous substances data bank*. Bethesda, MD, National Library of Medicine.
- Huang Q, Wang L, Han S (1995) The genotoxicity of substituted nitrobenzenes and the quantitative structure-activity relationship studies. *Chemosphere*, 30:915-923.
- Huang Q-G, Kong L-R, Liu Y-B, Wang L-S (1996) Relationships between molecular structure and chromosomal aberrations in *in vitro* human lymphocytes induced by substituted nitrobenzenes. *Bulletin of environmental contamination and toxicology*, 57:349-353.
- Huq AS, Ho NFH, Husari N, Flynn GL, Jetzer WE, Condie LJ Jr (1986) Permeation of water contaminative phenols through hairless mouse skin. *Archives of environmental contamination and toxicology*, 15:557-566.
- Hustert K, Mansour M, Parlar H, Korte F (1981) The EPA test - A method for the determination of the photochemical degradation of organic compounds in aquatic systems. *Chemosphere*, 10(9):995-998 (in German).
- International Research and Developmental Corporation (1983) *Range-finding teratology study in rats*. Sponsored by Monsanto Co., St. Louis, MO (IR-83-100).
- IPCS (1994) *Assessing human health risks of chemicals: derivation of*

guidance values for health-based exposure limits. Geneva, World Health Organization, International Programme on Chemical Safety (Environmental Health Criteria 170).

IPCS (1998) *International Chemical Safety Card - Mononitrophenols.* Geneva, World Health Organization, International Programme on Chemical Safety (ICSC 1342).

Japan Environment Agency (1979) *Chemicals in the environment. Monitoring of the general environment in Japan 1978.* Tokyo.

Japan Environment Agency (1980) *Chemicals in the environment. Monitoring of the general environment in Japan 1979.* Tokyo.

Japan Environment Agency (1995) *Chemicals in the environment. Monitoring of the general environment in Japan 1994.* Tokyo.

Jetzer WE, Huq AS, Ho NFH, Flynn GL, Duraiswamy N, Condie L Jr (1986) Permeation of mouse skin and silicone rubber membranes by phenols: relationship to *in vitro* partitioning. *Journal of pharmaceutical sciences*, 75:1098-1103.

Kavlock RJ (1990) Structure-activity relationships in the developmental toxicity of substituted phenols: *In vivo* effects. *Teratology*, 41:43-59.

Kawai A, Goto S, Matsumoto Y, Matsushita H (1987) Mutagenicity of aliphatic and aromatic nitro compounds. *Japanese journal of industrial health*, 29:34-54.

Kayser G, Koch M, Ruck W (1994) Simultaneous quantitative measurement of biodegradation and toxicity of environmental chemicals.

Vom Wasser, 82:219-232.

Koerdel W, Schoene K, Bruckert J, Pfeiffer U, Schreiber G, Rittmann D, Hochrainer D, Otto F, Spielberg T, Fingerhut R, Kuhnen-Clausen D, Koenig J (1981) *Assessment of the feasibility of test guidelines as well as the evidence of the base set of the law on chemicals*. Hanover, Fraunhofer Institute for Toxicology and Aerosol Research (in German).

Koerdel W, Kuhnen-Clausen D, Fabig W, Otto F (1984) *Evaluation of test guidelines for environmental chemicals*. Schmallenberg, Fraunhofer Institute for Environmental Chemistry and Ecotoxicology (in German).

Koop DR (1986) Hydroxylation of *p*-nitrophenol by rabbit ethanol-inducible cytochrome P-450 isozyme 3a. *Molecular pharmacology*, 29:399-404.

Koop DR, Laethem CL (1992) Inhibition of rabbit microsomal cytochrome P-450 2E1-dependent *p*-nitrophenol hydroxylation by substituted benzene derivatives. *Drug metabolism and disposition*, 20:775-777.

Kramer CR, Truemper I, Berger L (1986) Quantitative structure-activity relations for the autotrophic growth inhibition of synchrore *Chlorella vulgaris* suspensions by monosubstituted nitrobenzenes. *Biochemie und Physiologie der Pflanzen*, 181:411-420 (in German).

Kubinski H, Gutzke GE, Kubinski ZO (1981) DNA-cell-binding (DCB) assay

for suspected carcinogens and mutagens. *Mutation research*,
89:95-136.

Kuehn R, Pattard M, Pernak K-D, Winter A (1988) *Damaging effects of environmental chemicals in the Daphnia reproductive toxicity test as a basis for the evaluation of environmental hazards in aquatic systems*. Berlin, Institute for Water, Soil and Air Hygiene (in German).

Landrum PF, Crosby DG (1981) Comparison of the disposition of several nitrogen-containing compounds in the sea urchin and other marine invertebrates. *Xenobiotica*, 11:351-361.

Lang P-Z, Ma X-F, Lu G-H, Wang YI, Bian Y (1996) QSAR for the acute toxicity of nitroaromatics to the carp (*Cyprinus carpio*).
Chemosphere, 32:1547-1552.

Leone JA, Seinfeld JH (1985) Comparative analysis of chemical reaction mechanism for photochemical smog. *Atmospheric environment*, 19:437-464.

Leone JA, Flagan RC, Grosjean D, Seinfeld JH (1985) An outdoor smog chamber and modeling study of toluene-NO_x photooxidation.
International journal of chemical kinetics, 17:177-216.

León-González ME, Perez-Arribas LV, Santos-Delgado MJ, Polo-Diez LM (1992) Simultaneous flow-injection determination of *o* and *p*-nitrophenol using a photodiode-array detector. *Analytica Chimica Acta*, 258:269-273.

Leuenberger C, Czuczwa J, Tremp J, Giger W (1988) Nitrated phenols in rain: atmospheric occurrence of phytotoxic pollutants. *Chemosphere*, 17(3):511-516.

Levsen K, Behnert S, Priess B, Svoboda M, Winkeler H-D, Zietlow J (1990) Organic compounds in precipitation. *Chemosphere*, 21:1037-1061.

Levsen K, Behnert S, Musmann P, Raabe M, Priess B (1993) Organic compounds in cloud and rain water. *International journal of environmental analytical chemistry*, 52:87-97.

Lokke H (1984) Sorption of selected organic pollutants in Danish soils. *Ecotoxicology and environmental safety*, 8:395-409.

Luettker J, Levsen K (1994) Partitioning of phenol and nitrophenols in gas and liquid phase of clouds. In: Borrell PM, Borrell P, Cvitas T, Seiler W, eds. *Transport and transformation of pollutants in the troposphere*. Proceedings of EUROTRAC Symposium '94 Garmisch-Patenkirchen, 11-15 April 1994. Garmisch-Patenkirchen, SPB Academic Publishing bv / EUROTRAC International Scientific Secretariat (ISS); Fraunhofer Institute for Atmospheric Environmental Research, pp.1075-1078.

Luettker J, Scheer V, Levsen K, Wuensch G, Cape JN, Hargreaves KJ, Storeton-West RL, Acker K, Wieprecht W, Jones B (1997) Occurrence and formation of nitrated phenols in and out of cloud. *Atmospheric environment*, 31:2637-2648.

Machida M, Morita Y, Hayashi M, Awazu S (1982) Pharmacokinetic

- evidence for the occurrence of extrahepatic conjugative metabolism of *p*-nitrophenol in rats. *Biochemical pharmacology*, 31:787-791.
- Mansour M (1996) Abiotic degradation of pesticides and other organic chemicals in aquatic systems. *Pesticide outlook*, 7:9-10.
- Marquart HW, Sewekow B, Hamburger B, Harzdorf C, Hellbusch HD (1984) *Assessment of the feasibility and evidence of the test methods of levels I and II of the chemicals act. Part II.* Leverkusen, Bayer AG, pp. 1-128 (in German).
- Massey IJ, Aitken MD, Ball LM, Heck PE (1994) Mutagenicity screening of reaction products from the enzyme-catalyzed oxidation of phenolic pollutants. *Environmental toxicology and chemistry*, 13:1743-1752.
- McCann J, Choi E, Yamasaki E, Ames BN (1975) Detection of carcinogens as mutagens in the *Salmonella*/microsome test: assay of 300 chemicals. *Proceedings of the National Academy of Sciences of the United States of America*, 72:5135-5139.
- McCoy GD, Koop DR (1988) Biochemical and immunochemical evidence for the induction of an ethanol-inducible cytochrome P-450 isoenzyme in male Syrian golden hamsters. *Biochemical pharmacology*, 37:1563-1568.
- Means JL, Anderson SJ (1981) Comparison of five different methods for measuring biodegradability in aqueous environment. *Water, air, and soil pollution*, 16:301-315.
- Meerman JH, Nijland C, Mulder GJ (1987) Sex differences in sulfation and glucuronidation of phenol, 4-nitrophenol and

N-hydroxy-2-acetylaminofluorene in the rat *in vivo*. *Biochemical pharmacology*, 36:2605-2608.

Mussmann P, Levsen K, Radeck W (1994) Gas-chromatographic determination of phenols in aqueous samples after solid phase extraction. *Fresenius journal of analytical chemistry*, 348:654-659.

Nakamura S, Oda Y, Shimada T, Oki I, Sugimoto K (1987) SOS-inducing activity of chemical carcinogens and mutagens in *Salmonella typhimurium* TA1535/pSK1002: examination with 151 chemicals. *Mutation research*, 192:239-246.

Naniwa S (1979) Industrial contact dermatitis due to nitro and amino derivatives. 1st report: mass-examination of a factory. *Journal of dermatology*, 6:59-63.

Nasseredine-Sebaei SM, Crider AM, Carroll RT, Hinko CN (1993) Determination of *m*-nitrophenol and nipecotic acid in mouse tissues by high performance liquid chromatography after administration of the anticonvulsant *m*-nitrophenyl-3-piperidinecarboxylate hydrochloride. *Journal of pharmaceutical sciences*, 82:39-43.

Neuhauser EF, Loehr RC, Malecki MR, Milligan DL, Durkin PR (1985) The toxicity of selected organic chemicals to the earthworm *Eisenia fetida*. *Journal of environmental quality*, 14:383-388.

Neuhauser EF, Durkin PR, Malecki MR, Anatra M (1986) Comparative toxicity of ten organic chemicals to four earthworm species. *Comparative biochemistry and physiology*, C 83:197-200.

Nick K, Schoeler HF (1992) Gas-chromatographic determination of nitrophenols after derivatization with diazomethane. *Fresenius journal of analytical chemistry*, 343:304-307.

Nojima K, Kawaguchi A, Ohya T, Kanno S, Hirobe M (1983) Studies on photochemical reaction of air pollutants. X. Identification of nitrophenols in suspended particulates. *Chemical and pharmaceutical bulletin*, 31:1047-1051.

NTP (1993) *Toxicology and carcinogenesis studies of p-nitrophenol* (CAS No. 100-02-7) in Swiss Webster mice (dermal studies). Research Triangle Park, NC, US Department of Health and Human Services, National Toxicology Program (NTP Report No. TR-417).

Nyholm N, Lindgaard-Joergensen P, Hansen N (1984) Biodegradation of 4-nitrophenol in standardized aquatic degradation tests. *Ecotoxicology and environmental safety*, 8:451-470.

Oberly TJ, Bewsey BJ, Probst GS (1984) An evaluation of the L5178Y TK⁺ mouse lymphoma forward mutation assay using 42 chemicals. *Mutation research*, 125:291-306.

Ohkura K, Iwamoto K, Terada H (1990) Transcellular permeation of nitrophenols through newborn rat skin epidermal cells in monolayer culture. *Chemical and pharmaceutical bulletin*, 38:2788-2791.

Ou L-F (1985) Methyl parathion degradation and metabolism in soil: Influence of high soil-water contents. *Soil biology and biochemistry*, 17:241-243.

Pagga U, Haltrich WG, Guenther W (1982) Investigations of the effect of 4-nitrophenol on activated sludge. *Vom Wasser*, 59:51-65 (in German).

Paterson B, Cowie CE, Jackson PE (1996) Determination of phenols in environmental waters using liquid chromatography with electrochemical detection. *Journal of chromatography, A* 731:95-102.

Pitter P (1976) Determination of biological degradability of organic substances. *Water research*, 10:231-235.

Pocurull E, Marce RM, Borrull F (1996) Determination of phenolic compounds in natural waters by liquid chromatography with ultraviolet and electrochemical detection after on-line trace enrichment. *Journal of chromatography*, 738:1-9.

Poirier MC, De Cicco BT, Lieberman MW (1975) Nonspecific inhibition of DNA repair synthesis by tumor promoters in human diploid fibroblasts damaged with *N*-acetoxy-2-acetylaminofluorene. *Cancer research*, 35:1392-1397.

Probst GS, McMahon RE, Hill LE, Thompson CZ, Epp JK, Neal SB (1981) Chemically-induced unscheduled DNA synthesis in primary rat hepatocyte cultures: a comparison with bacterial mutagenicity using 218 compounds. *Environmental mutagenesis*, 3:11-32.

Pruett SB, Chambers JE (1988) Effects of paraoxon, *p*-nitrophenol, phenyl saligenin cyclic phosphate, and phenol on the rat interleukin 2 system. *Toxicology letters*, 40:11-20.

- Pruppacher HR, Klett JD (1978) Microphysics of clouds and precipitation. Dordrecht/Boston/London, D. Reidel Publishing Co.
- Puig D, Barcelo D (1996) Determination of phenolic compounds in water and waste water. *Trends in analytical chemistry*, 15:362-375.
- Rashid KA, Mumma RO (1986) Screening pesticides for their ability to damage bacterial DNA. *Journal of environmental science and health*, 21:319-334.
- Reinke LA, Moyer MJ (1985) *p*-Nitrophenol hydroxylation. A microsomal oxidation which is highly inducible by ethanol. *Drug metabolism and disposition*, 13:548-552.
- Richartz H, Reischl A, Trautner F, Hutzinger O (1990) Nitrated phenols in fog. *Atmospheric environment*, 24:3067-3072.
- Rippen G, Flothmann D, Witt W (1984) *Improvement of the OECD test guideline A 80/9 and comparative evaluation of other relevant methods for the measurement of volatility*. Frankfurt a. M., Batelle-Institut e.V. (Report No. 106 02 024/06) (in German).
- Roberts BL, Dorough HW (1984) Relative toxicities of chemicals to the earthworm *Eisenia fetida*. *Environmental toxicology and chemistry*, 3:67-78.
- Robinson D, Smith JN, Williams RT (1951) Studies in detoxication. 39. Nitro compounds. (a) The metabolism of *o*, *m*, and *p*-nitrophenols in the rabbit. (b) The glucuronides of the mononitrophenols and observations on the anomalous optical rotations

of triacetyl - σ -nitrophenylglucuronide and its methyl ester.

Biochemical journal, 50:221-227.

Rott B, Viswanathan R, Freitag D, Korte F (1982) Comparative investigation on the feasibility of different tests for the evaluation of the degradation of environmental chemicals. *Chemosphere*, 11:531-538 (in German).

Ruana J, Urbe I, Borrull F (1993) Determination of phenols at the ng/l level in drinking and river waters by liquid chromatography with UV and electrochemical detection. *Journal of chromatography, A* 655:217-226.

Rubin HE, Subba-Rao RV, Alexander M (1982) Rates of mineralization of trace concentrations of aromatic compounds in lake water and sewage samples. *Applied environmental microbiology*, 43:1133-1138.

Rush GF, Newton JF, Hook JB (1983) Sex differences in the excretion of glucuronide conjugates: The role of intrarenal glucuronidation. *Journal of pharmacology and experimental therapeutics*, 227:658-662.

Sax NI, Lewis RJ (1987) *Hawley's condensed chemical dictionary*, 11th ed. New York, NY, Van Nostrand Reinhold Co.

Scheer V, Luettke J, George C, Levsen K, Frenzel A, Behnke W, Zetzsch C (1996) Atmospheric nitration of phenol in clouds by N_2O_5 and $ClNO_2$. In: Borrell PM, Borrell P, Kelly K, Cvitas T, Seiler W, eds. *Transport and transformation of pollutants in the troposphere*.

Proceedings of EUROTRAC Symposium '96. Garmisch-Partenkirchen, 25-29 March 1996. Southampton, Computational Mechanics Publications.

Scheubel JB (1984) *Assessment of the feasibility and evidence of the test method of level 1 and 2 of the chemical act.* Marl, Chemische Werke Huels AG (Report No. 106 04 011/5 CWH) (in German).

Scheunert I (1984) *Examination and optimization of the "GSF-Cold-Finger-Method" and comparative calculations of the volatility.* Gesellschaft fuer Strahlen- und Umweltforschung (Report No. 10602024/08) (in German).

Schoene K, Steinhanses J (1984) *Comparative measurements of the volatility in open systems.* Schmalleberg, Fraunhofer Institute for Toxicology and Aerosol Research (Report No. 10602024/7 Part II) (in German).

Scholz N (1986) *Development of test guidelines on marine species for ecotoxicological studies according to the chemicals act - Bryozoa/Camptozoa.* Berlin, Umweltbundesamt (Report No. 10603042/02) (in German).

Schwarzenbach RP, Stierli R, Folsom BR, Zeyer J (1988) Compound properties relevant for assessing the environmental partitioning of nitrophenols. *Environmental science and technology*, 22:83-92.

Sewekow B (1983) *Feasibility of test guidelines and evidence of the base set testing according to the chemicals legislation.* Muenchen, Gesellschaft fuer Strahlen- und Umweltforschung (in German).

Shimizu M, Yano E (1986) Mutagenicity of mono-nitrobenzene derivatives in the Ames test and rec assay. *Mutation research*, 170:11-22.

- Smith LW, Hall GT, Kennedy GL (1988) Acute and repeated dose inhalation toxicity of para-nitrophenol sodium salt in rats. *Drug chemistry and toxicology*, 11:319-327.
- Snodgrass HL Jr (1983) *Phase I, dermal penetration and distribution of ¹⁴C-labeled paranitrophenol (PNP)*. Aberdeen Proving Ground, MD, US Army Environmental Hygiene Agency (Study No. 75-51-0047-84).
- Spain JC, van Veld PA, Monti CA, Pritchard PH, Cripe CR (1984) Comparison of *p*-nitrophenol biodegradation in field and laboratory test systems. *Applied environmental microbiology*, 48:944-950.
- Storer RD, McKelvey TW, Kraynak AR, Elia MC, Barnum JE, Harmon LS, Nichols WW, DeLuca JG (1996) Revalidation of the *in vitro* alkaline elution/rat hepatocyte assay for DNA damage: improved criteria for assessment of cytotoxicity and genotoxicity and results for 81 compounds. *Mutation research*, 368:59-101.
- Subba-Rao RV, Rubin HE, Alexander M (1982) Kinetics and extent of mineralization of organic chemicals at trace levels in freshwater and sewage. *Applied environmental microbiology*, 43:1139-1150.
- Suzuki J, Koyama T, Suzuki S (1983) Mutagenicities of mono-nitrobenzene derivatives in the presence of norharman. *Mutation research*, 120:105-110.
- Tabak HH, Quave SA, Mashni CI, Barth EF (1981) Biodegradability studies with organic priority pollutant compounds. *Journal of the Water Pollution Control Federation*, 52:1503-1518.

Tan GH, Chong CL (1993) Trace monitoring of water-borne phenolics in the Klang River basin. *Environmental monitoring and assessment*, 24:267-277.

Thompson MJ, Ballinger LN, Cross SE, Roberts MS (1996) High-performance liquid chromatographic determination of phenol, 4-nitrophenol, beta-naphthol and a number of their glucuronide and sulfate conjugates in organ perfusate. *Journal of chromatography, B* 677:117-122.

Tremaine LM, Diamond GL, Quebbemann AJ (1984) *In vivo* quantification of renal glucuronide and sulfate conjugation of 1-naphthol and *p*-nitrophenol in the rat. *Biochemical pharmacology*, 33:419-427.

Tremp J, Mattrel P, Fingler S, Giger W (1993) Phenols and nitrophenols as tropospheric pollutants: Emissions from automobile exhausts and phase transfer in the atmosphere. *Water, air, and soil pollution*, 68:113-123.

TRI (1998) *Toxics release inventory*. Washington, DC, US Environmental Protection Agency, Office of Toxic Substances (17 December 1998).

Tseng S, Lin M (1994) Treatment of organic wastewater by anaerobic biological fluidized bed reactor. *Water science and technology*, 29:157-166.

Urano K, Kato Z (1986) Evaluation of biodegradation ranks of priority organic compounds. *Journal of hazardous materials*, 13:147-159.

- Van Veld PA, Spain JC (1983) Degradation of selected xenobiotic compounds in three types of aquatic test systems. *Chemosphere*, 12:1291-1305.
- Vasilenko NM, Volodchenko VA, Baturina TS, Kolodub FA (1976) Toxicological peculiarities of mononitrophenols with regard for their isomeric form. *Farmakologiya i Toksikologiya*, 39:718-721.
- Vernot EH, MacEwen JD, Haun CC, Kinkead ER (1977) Acute toxicity and skin corrosion data for some organic and inorganic compounds and aqueous solutions. *Toxicology and applied pharmacology*, 42:417-423.
- Verschueren K, ed. (1983) *Handbook of environmental data on organic chemicals*, 2nd ed. New York, NY, Van Nostrand Reinhold Co.
- Vozňáková Z, Podehradská J, Kohlicková M (1996) Determination of nitrophenols in soil. *Chemosphere*, 33:285-291.
- Wagner R, Braeutigam H-J (1981) Development and testing of a method for studying the degradation of organic compounds under anaerobic conditions (report no. 03 7221). In: Biehl HM, Fuehr F, Seibert K, eds. *Methods for the ecotoxicological evaluation of chemicals, Part I, Aquatic systems*. Juelich, Forschungszentrum, pp. 20-41 (in German).
- Weast RC (1979) *CRC handbook of chemistry and physics*, 69th ed. Boca Raton, FL, CRC Press, Inc.
- Wiggins BA, Jones SH, Alexander M (1987) Explanations for the

acclimation period preceding the mineralization of organic chemicals in aquatic environments. *Applied environmental microbiology*, 43:791-796.

Yamada K, Murakami H, Yasumura K, Shirahata S, Shinohara K, Omura H (1987) Production of DNA-breaking substance after treatment of monophenols with sodium nitrite and then with dimethyl sulfoxide. *Agricultural and biological chemistry*, 51:247-248.

Yoshida K, Shigeoka T, Yamauchi F (1983) Non-steady-state equilibrium model for the preliminary prediction of the fate of chemicals in the environment. *Ecotoxicology and environmental safety*, 7:179-190.

Yoshioka Y, Ose Y, Sato T (1985) Testing for the toxicity of chemicals with *Tetrahymena pyriformis*. *The science of the total environment*, 43:149-157.

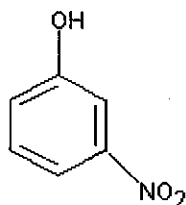
Zetzsch C, Rinke M, Scharpring H, Schueler P, Urbanik E, Wahner A, Wiedelmann A, Witte F (1984) *Upper limits of the persistence of chemicals in the atmosphere from their reactivity against OH radicals*. University of Bochum, Bochum, pp. 1-20 (BMFT Report No. PTU 037253).

Zimmering S, Mason JM, Valencia R, Woodruff RC (1985) Chemical mutagenesis testing in *Drosophila*. II. Results of 20 coded compounds tested for the National Toxicology Program. *Environmental mutagenesis*, 7:87-100.

付録1— 3-ニトロフェノール

物質の同定並びに物理的・化学的特性

3-ニトロフェノール (CAS番号 554-84-7 ; 3-ヒドロキシ-1-ニトロベンゼン、メタ-ニトロフェノール)は実験式 $C_6H_5NO_3$ を有する。その構造式は下記の通りである。



3-ニトロフェノールの物理化学的性状を表 A-1 に示している。

表 A-1 3-ニトロフェノールの物理化学的性状

パラメータ	値
分子量(g/mol)	139.11
融点(°C)	96-97 (1)(2)
沸点(°C)	194 (1)
蒸気圧(kPa; 20 °C)	0.10 (3)
水に対する溶解度(g/L; 25 °C)	13.5 (1)
n-オクタノール/水分配係数(log Kow)	2.00 (4)
解離定数(pKa) (18 °C)	8.34 (2)
換算係数	1 mg/m ³ = 0.173 ppmv 1 ppmv = 5.78 mg/m ³

出典 : (1) Verschueren (1983); (2) Budavari et al. (1996); (3) HSDB (1998);

(4) Hansch & Leo (1979)

環境中の移動・分布・変換

3-ニトロフェノールの非生物的分解に関するデータは入手されなかった。

表 A-2 に要約されている 3 件の生物的分解に関する研究が、本異性体は好氣的条件下の水域で本質的に生分解を受けることを示している。

表 A-2 好氣的条件下における 3-ニトロフェノールの生物的分解

試験	濃度 (mg/L)	追加炭素源	試験期間(日)	除去率(%)	出典
易生分解性に関する試験					
MITI I	100	なし	14	0	Gerike & Fischer (1979); Urano & Kato (1986)
本質性生分解性に関する試験					
バッチ試験、通気 200 COD ^a	200 COD ^a	なし	5	95	Pitter (1976)
呼吸測定試験	300	あり	10	44	Kayser et al. (1994)

^a COD = 化学的酸素要求量

好氣的条件下での下水汚泥および都市污水处理場の初期嫌氣性段階の汚泥を用いた生物的分解に関する試験において、初期濃度が 96.5~579 mg/L 範囲の 3-ニトロフェノールは 7~60 日以内では全く分解されなかった (Wagner & Braeutigam, 1981; Battersby & Wilson, 1989)。しかし、Boyd ら(1983)は培養 1 週間以内に 50 mg/L の完全な嫌氣的除去を認めた。この試験で、無機化は培養期間を 10 週間まで延長した場合にだけ証明された。高い初期濃度のニトロフェノールであったが、その嫌氣的分解が Tseng および Lin (1994)により見出された。すなわち、彼等は 3 種の異なる種類の廃水による生物学的流動層反応器中で 3-ニトロフェノール (350~650 mg/L)の 90%の除去を認めた。入手できる報告結果から、適応微生物による嫌氣的条件下での 3-ニトロフェノールの緩慢な分解を予想できる。

Boyd (1982)によって測定された土壌吸着係数(K_{oc})の 52.83 と、HanschおよびLeo (1979)により報告されたn-オクタノール/水分配係数 ($\log K_{ow}$) の 2.0 が、生物濃縮ばかりでなく土壌吸着性に対しても低~中等度であることを示している。

環境中濃度

1994年に、3-ニトロフェノールは日本の大気27試料で検出（検出限界8 ng/m³）されなかった（Japan Environment Agency, 1995）。3-ニトロフェノールは、1978、1979および1994年に、日本の表層水の177試料で検出されず（検出限界0.04~10 µg/L）、また177の底質でも検出されなかった（検出限界0.002~0.8 µg/kg）（Japan Environment Agency, 1979, 1980, 1995）。1979および1994年に3-ニトロフェノールは129の魚試料で検出されなかった（検出限界0.005~0.2 µg/kg）（Japan Environment Agency, 1980, 1995）。

実験動物およびヒトでの体内動態並びに代謝の比較

3-ニトロフェノールのヒトにおける吸収、代謝または排泄に関する定量的情報を提供している試験は確認されなかった。さらに、実験動物での情報は極めて限られている。胃管強制によって150~200 mg/kg体重を単回投与されたウサギで、適用量の大部分（80%を超える）が24時間以内に尿に排泄された。約68~86%がグルクロン酸とスルホン酸に抱合したのに対して、約7~13%はアミノフェノールに還元された（Robinson et al., 1951）。皮膚浸透もいくつかのin vitro 実験で明らかにされた（Huq et al., 1986; Jetzer et al., 1986; Ohkura et al., 1990）。情報は限られているが、生物体内での3-ニトロフェノールの生物濃縮はその迅速な代謝と排泄により予期されない。

実験哺乳類動物およびin vitro（試験管内）試験系への影響

3-ニトロフェノールの経口LD₅₀はラットでは ≥ 930 mg/kg体重（Vasilenko et al., 1976; Vernot et al., 1977）およびマウスで $\geq 1,070$ mg/kg体重（Vasilenko et al., 1976; Vernot et al., 1977）であると見積もられている。

3-ニトロフェノールの入手できるin vitro とin vivo の遺伝毒性試験を表A-3に要約している。3-ニトロフェノールは変異原性試験（rec-assay）で変異原性が示され、サルモネラ菌・マイクロソーム試験では一貫性のない結果を出していた。1件の試験がネズミチフス菌のTA98とTA100

株で非変異原性であることを示したのに対し、別の 1 試験はこれらの両株で代謝活性化の存在・非存在のいずれの場合も変異原性を示した。サルモネラ菌・マイクロソーム試験の矛盾した結果と染色体異常に関するデータがないことを考慮すると、3-ニトロフェノールの変異原性に関する結論は出せない。

表 A-3 3-ニトロフェノールの in vitro および in vivo での遺伝毒性

種族 (試験系)	エンドポイント	濃度範囲	結果 ^a		注釈	出典
			代謝活性化なし	代謝活性化あり		
In vitro 試験						
枯草菌 H17, M45	組換え試験	0.01-5 mg/プレート	+	0	≥0.5 mg/プレートで陽性	Shimizu & Yano (1986)
ネズミチフス菌 TA1535、 TA1537、 TA1538	復帰突然変異	0.01-5 mg/プレート	-	-		Shimizu & Yano (1986)
ネズミチフス菌 TA98、TA100	復帰突然変異	0.1-5 mg/プレート	+	+	日本での試験 (表より得たデータ)	Kawai et al. (1987)
ネズミチフス菌 TA98、TA100	復帰突然変異	0.01-5 mg/プレート	-	-	また、Suzuki ら (1983) はノルハルマン存在下で両菌株を試験して、やはり陰性結果を出していた。	Suzuki et al. (1983); Shimizu & Yano (1986)
In vivo 試験						
キイロシヨウジ ヨウバエ	SLRL 試験	混餌 (5,000 ppm) または注射 (1,200 ppm)				Foureman et al. (1994)

^a -, 陰性; +, 陽性; 0, 試験されなかった。

3-ニトロフェノールの場合、刺激作用または感作作用、反復暴露、生殖発生毒性、ヒトへの影響に関して入手できる試験はない。

水生生物種への影響

各種の水生生物に対する3-ニトロフェノールの毒性について行われた試験（表 A-4 を参照）で、3-ニトロフェノールは中等度ないし高度な毒性を示した。

表 A-4 3-ニトロフェノールの水生生物毒性

種族（試験法・エンドポイント）	影響濃度（mg/L）	出典
細菌		
シュードモナス・プチダ <i>Pseudomonas putida</i> (細胞増殖阻害試験)	16-時間 MIC*: 7.0	Bringmann & Kuehn (1977)
原生動物		
鞭毛原虫 <i>Entosiphon sulcatum</i> (細胞増殖阻害試験)	72-時間 MIC: 0.97	Bringmann (1978); Bringmann et al. (1980)
藻類		
イカダモ緑藻 <i>Scenedesmus subspicatus</i> クロレラ・ブルガリス <i>Chlorella vulgaris</i> (細胞増殖阻害試験)	6-時間 EC ₅₀ : 6.21	Kramer et al. (1986)
無脊椎動物		
タマミジンコ <i>Moina macrocopa</i> (急性) (遊泳阻害)	3-時間 LC ₅₀ : 1.7	Yoshioka et al. (1985)
魚類		
コイ <i>Cyprinus carpio</i> (止水)	96-時間 LC ₅₀ : 17.5	Lang et al. (1996)

* MIC = 最小発育阻止濃度

付録2 — 出典

BUA (1992): *BUA-Stoffbericht 2- und 4-Nitrophenol.*

Beratergremium fuer Umweltrelevante Altstoffe. Weinheim, VCH VerlagsGmbH (Report No. 75; February 1992)

BUA の検討プロセスのために、報告書の作成を担当する会社（通常、ドイツにおける最大生産者）が広範な資料検索文献の他、自社試験結果を用いて素案を用意する。本草案は、政府機関、学会および業界からの代表者よりなる作業委員会の数度のピアレビューが読み込み期間に委ねられている。

BUA 報告 No. 75 (BUA 報告 2-ニトロフェノールおよび 4-ニトロフェノール。環境関連既存化学物質に関する GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance. Stuttgart, Hirzel Verlag [1992年2月]) の英訳は 1993 年に公開された。

ATSDR (1992): ニトロフェノール類の毒性学的全容 : 2-ニトロフェノールおよび 4-ニトロフェノール。Atlanta, GA, US Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (報告番号 TP-91/23)

ATSDR ニトロフェノール類の毒性学的全容 : 2-ニトロフェノールおよび 4-ニトロフェノール(ATSDR, 1992)の写しは下記の機関から入手できる。

Agency for Toxic Substances and Disease Registry
Division of Toxicology
1600 Clifton Road, E-29
Atlanta, Georgia 30333
USA

ニトロフェノール類の毒性学的全容 : 2-ニトロフェノールおよび 4-ニトロフェノールの初期の草案は Agency for Toxic Substances and Disease Registry、US Centers for Disease Control、US National Toxicology Program およびその他の連邦政府機関からの科学者達によって審査された。また、草案は次の委員より構成される非政府組織審査員の専門委員会により再検討された。

Dr Martin Alexander、コーネル大学
Dr Gary Booth、ブリガムヤング大学
Dr Samuel Cohen、ネブラスカ大学医療センター
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Dr Frederick Oehme、カンザス州立大学

付録3 — CICAD のピアレビュー

モノシロフェノール類に関する CICAD 草案を、IPCS の各国コンタクト・ポイントおよび参加機関と予め連絡を取って、国際化学物質安全性計画 IPCS により認定されている専門家ばかりでなく、機関および組織にも審査のために送付した。コメントを下記の機関から受け取った。

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Institute of Terrestrial Ecology, Huntingdon, United Kingdom

Joint Food Safety and Standards Group, Department of Health, London, United Kingdom

National Institute of Health Sciences, Tokyo, Japan

National Institute of Public Health, Prague, Czech Republic

United States Department of Health and Human Services [National Institute of Environmental Health Sciences, Research Triangle Park], USA

United States Environmental Protection Agency [National Center for Environmental Assessment, Washington, DC; Region VIII], USA

World Health Organization/International Programme on Chemical Safety, Montreal, Canada

付録3 CICAD の最終検討委員会

1998年12月8～11日

米国、ワシントンDC

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