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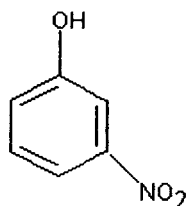
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付録1 — 3-ニトロフェノール

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≥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・ミクロゾ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		
タマジシコ <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

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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。

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付録3 — CICAD のピアレビュー

モノク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

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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

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