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ABOGADOS
Calle 94 A No. 7 A - 09
Bogotá, D.C., COLOMBIA

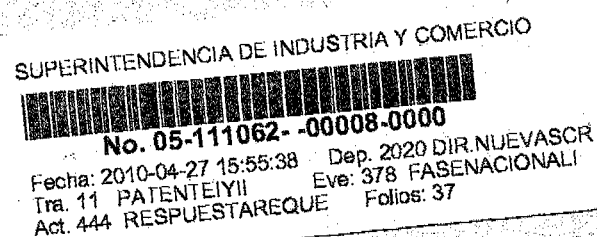
Señora

Jefe de la División de Nuevas Creaciones

Superintendencia de Industria y Comercio

Ministerio de Desarrollo Económico

E. S. D.



Ref.: Expediente No. 05.111.062

Solicitud de Patente de Invención para: **COMPOSICION AGROQUIMICA EN
SUSPENSION ACUOSA**

Solicitante: **KUMIAI CHEMICAL INDUSTRY CO., LTD.**

RESPUESTA AL EXAMEN DE FONDO

MARGARITA CASTELLANOS ABONDANO, mayor de edad, identificada y domiciliada como aparece al pie de mi firma, atentamente me permito presentar respuesta al oficio No. 864 notificado por fijación en lista el 29 de enero de 2010 correspondiente al examen de fondo, estando dentro del término legal en los siguientes términos:

Reivindicaciones

Con el fin de superar la objeción sobre las reivindicaciones, presento a consideración del señor examinador un nuevo pliego reivindicatorio donde se ha restringido el alcance de la invención a los ejemplos de la descripción. En efecto, los ingredientes agroquímicamente activos han sido restringidos a bispiribac-sodio y flucarbazona-sodio. Adicionalmente, el compuesto B ha sido restringido en relación al pliego reivindicatorio anterior.

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Nivel inventivo

En cuanto al nivel inventivo, presento a consideración del señor examinador las razones por las cuales la invención reivindicada no era obvia ni evidente para una persona versada en la materia en vista de las enseñanzas de los documentos D2-D4.

En primer lugar, ninguno de los documentos citados por el señor examinador revela el uso de los ingredientes activos reivindicados bispiribac-sodio y flucarbazona-sodio (ver Pág. 97, 427 y 428 del Manual de Pesticidas adjunto). En efecto, el documento D2 apenas revela suspensiones líquidas concentradas dispersables de ingredientes activos tipo sulfonilurea o sus sales. Sin embargo, el documento D2 no revela ni sugiere como formular otro tipo de ingredientes agroquímicamente activos teniendo en cuenta que tanto el compuesto bispiribac-sodio como el compuesto flucarbazona-sodio no corresponden a compuestos del tipo sulfonilurea.

Ahora bien, el objeto de la presente invención era el de formular suspensiones acuosas con ingredientes agroquímicamente activos que presentan elevada solubilidad en agua. Tal como se observa en los ejemplos de la descripción, la separación y formación de capas se podía eliminar durante el almacenamiento permitiendo así el almacenamiento a largo plazo de este tipo de formulaciones debido a la poca ocurrencia de crecimiento de partículas con el paso del tiempo. Este efecto inesperado se consiguió al combinar el ingrediente activo altamente soluble en agua (A) seleccionado de bispiribac-sodio y flucarbazona-sodio con el compuesto soluble en agua (B) seleccionado del grupo compuesto por bicarbonato de sodio, carbonato de sodio, cloruro de sodio, acetato de sodio y bicarbonato de amonio.

En este orden de ideas, el efecto inesperado de la presente invención obtenido mediante la combinación de los compuestos (A) y (B) reivindicados no era obvio para una persona versada en la materia en vista de los documentos citados por el examinador.

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Por su parte, el documento D3 revela formulaciones agroquímicas del tipo suspensión obtenidas mediante la dispersión de finas partículas de un químico sólido hidrofóbico en agua o en medio acuoso (página 2, líneas 27-29 y líneas 46-47) mientras que el documento D4 proporciona medios para suspender sustancias biocidas o agroquímicamente activas relativamente insolubles en agua en medio acuoso (Pág 2, líneas 3-4).

En este orden de ideas, es claro que en los documentos D3 y D4 no existe ninguna enseñanza ni sugerencia sobre la utilización de ingredientes agroquímicamente activos solubles en agua como los acá reivindicados, bispiribac-sodio y flucarbazona- sodio.

Tal como puede observar el señor examinador en el Manual de Pesticidas adjunto, los compuestos agroquímicos sólidos revelados en D3 presentan una solubilidad en agua menor a 0.1 g/100g mientras que los valores para el bispiribac sodio y flucarbazona sodio reivindicados son 7.33 y 4.4 g/100 ml respectivamente.

Adicionalmente, el documento D3 revela el uso de sales inorgánicas y bases (Pág. 3, líneas 53-57) pero de ninguna manera revela ejemplos de ácidos inorgánicos. Por lo tanto, una persona versada en la materia no habría llegado a la presente invención en vista de D3 toda vez que en dicho documento se revelan técnicas de formulación de agroquímicos débilmente solubles en agua.

Por otra parte, las sustancias biocidas o agroquímicamente activas reveladas en D4 son casi insolubles en agua tal como se observa en el Manual de Pesticidas adjunto. Tal como se enseña en D4 (Pág.2, líneas 26-31), la formulación sustancias insolubles requiere del uso de solventes orgánicos inmiscibles en agua los cuales son indeseables tanto ecológicamente como desde el punto de vista de la seguridad personal. Por lo tanto, un objeto de D4 es el de proporcionar una suspensión que contenga un agroquímico menos soluble en agua sin la necesidad de utilizar un solvente orgánico inmiscible en agua.

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Ahora bien, en D4 es posible obtener una formulación acuosa mediante la suspensión en un medio suspensor acuoso de partículas o droplets de una sustancia biocida o agroquímicamente activa la cual ha sido encapsulada o coacervada con un encapsulante soluble en agua el cual es a su vez insoluble en el medio suspensor acuoso.

Adicionalmente, es preferible que el medio suspensor acuoso comprenda un tensoactivo y suficiente electrolito con el fin de proporcionar una estructura capaz de soportar las partículas sólidas suspendidas y prevenir la disolución del encapsulante (Pág 6, líneas 1-6). Así mismo, se requiere que el electrolito interactúe con el tensoactivo (Pág 5, línea 53).

De acuerdo a lo anterior, el objetivo de D4 se puede lograr previniendo la interacción entre la sustancia biocida o agroquímicamente activa con el medio suspensor acuoso y los aditivos. Se pueden adicionar ácidos o bases con el fin de ajustar el pH y así mejorar la estabilidad del sólido suspendido o el líquido dispersado o disminuir la fitotoxicidad.

En este orden de ideas, los ácidos o bases en el electrolito contribuyen a dar una mayor interacción entre el electrolito y el tensoactivo con el fin de mantener suspendido la sustancia biocida agroquímicamente activa en el medio suspensor acuoso sin la interacción entre las sustancias activas y el medio acuoso.

En vista de lo anterior, los ácidos o las bases no se encuentran directamente relacionados con la estabilidad de la sustancia biocida o agroquímicamente activa. De esta forma, el sistema de interacción arriba mencionado es causado entre la sustancia activa insoluble en agua y el medio suspensor acuoso. Por lo tanto, una persona versada en la materia no estaría motivada por las enseñanzas de D4 para llegar a la formulación reivindicada que contiene bispiribac sodio y flucarbazona sodio los cuales son relativamente solubles en agua.

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En conclusión, una persona versada en la materia no estaría motivada por los documentos D2-D4 para llegar a la formulación reivindicada donde los ingredientes agroquímicos altamente solubles en agua son formulados en suspensión acuosa y mas aún teniendo en cuenta que los ingredientes activos revelados en D3 y D4 son insolubles en agua. Adicionalmente, pongo de presente al señor examinador que la formulación de ingredientes activos altamente solubles en agua no podían formularse en suspensión acuosa por lo cual, la presente invención es inventiva ya que se ha superado un prejuicio técnico del estado de la técnica.

Finalmente, solicito al señor examinador conceder el privilegio de patente a la presente invención toda vez que la misma es inventiva en vista de los documentos D2-D4. Sin embargo, si el señor examinador considera que los argumentos presentados no son suficientes para superar el nivel inventivo, solicito respetuosamente que se expida una tercera acción oficial con el fin de que el solicitante pueda presentar datos comparativos de ser necesario ya que los mismos toman varios meses en llevarse a cabo.

Anexos

- Nuevo pliego reivindicatorio
- Formulario de modificaciones
- Recibo de pago

De la Señora Jefe,


Margarita Castellanos Abondano

C.C. No. 39.779.654 de Usaquén

T.P.A. No. 70819 del C. Sup. de la Judicatura

Calle 94 A No. 7 A - 09

Teléfonos: 610 74 20

Bogotá, D.C.,

27 ABR. 2010



Espacio reservado para el adhesivo de radicación

FORMULARIO ÚNICO DE CORRECCIONES Y MODIFICACIONES

1

SOLICITUD DE:

☐ Corrección de Error Material

☒ Modificación a una solicitud

2	Nombre: KUMIAI CHEMICAL INDUSTRY CO., LTD.	IDENTIFICACIÓN	
	Dirección: 4-26, Ikenohata 1-chome, Taïto-ku, Tokyo, JAPON	C.C. ☐	NIT ☐
	Domicilio: Tokyo - JAPON	C.E. ☐	Otro ☐
	Lugar de Constitución: JAPON		Cual _____
	Teléfono: _____ Fax: _____	Número _____	
	E-mail: _____		
3 REPRESENTANTE O APODERADO	Nombre: MARGARITA CASTELLANOS A.	IDENTIFICACIÓN	
	Dirección: Calle 94 A No. 7 A-09	C.C. ☒	NIT ☐
	Teléfono: 610 7420 Fax: 610 0706	C.E. ☐	Otro ☐
	E-mail: info@castellanosyco.com		Cual _____
		Número 39'779.654	TPA 70.819

4

Número de Expediente:

05.111.062

5

Descripción de la corrección o modificación solicitada:

Presento nuevo capítulo reivindicatorio sobre el cual solicito que se realice el examen de patentabilidad.

6

Comprobante de pago No. 10-30.647

Fecha 21 de abril de 2010

7

Anexos:

☒ Comprobante de pago de la tasa.

☐ Poderes si fuere el caso, junto con la sustitución de los mismos a mi favor.

☐ Documento que acredita la existencia y representación legal de las partes, cuando sean personas jurídicas

☒ Nuevo capítulo reivindicatorio

8

NOMBRE MARGARITA CASTELLANOS A.

FIRMA

CC 39'779.654 Usaquén - TPA 70.819 CSJ

Instrucciones para el diligenciamiento del presente formulario, ver reverso de esta página - P1259

27 ABR 2010

SUPERINTENDENCIA DE INDUSTRIA Y COMERCIO

NIT : 800176089-2

RECIBO OFICIAL DE CAJA : 10 - 30,647
FECHA : ABRIL 21 DE 2010

***** CONSIGNACION *****

DEPOSITANTE	TIPO PAGO	BANCO	CUENTA	No. PAGO	FECHA PGO	Vr. PAGO
ALVARO CASTELLANOS	CONSIGNACION	BANCO DE BOGOTA	062754387	21968800	21/04/2010	7,505,000.00

***** CONCEPTO *****

CANT.	RENTISTICO	CONCEPTO	TOTAL CONCEPTO
1	50005-01-03	CAMBIO DE MODALIDAD Y MODIFICA	
12		MARCAS Y LEMAS COMERCIALES	114,000.00
		TOTAL :	\$ 114,000.00

SON: CIENTO CATORCE MIL PESOS

RESPONSABLE :



RECIBO DE CAJA APLICADO AL EXPEDIENTE No. _____

REIVINDICACIONES

1. Una composición agroquímica en suspensión acuosa que contiene:

(A) Al menos una clase de un ingrediente agroquímicamente activo seleccionado del grupo de (2,6-bis(4,6-dimetoxipirimidin-2-iloxi) benzoato de sodio y sal de sodio de 4,5-dihidro-3-metoxi-4-metil-5-oxo-N-[(2-(trifluorometoxi) fenilsulfonil]-1H-1,2,4-triazol-1-carboxamida;

(B) al menos una clase de un compuesto soluble en agua seleccionado del grupo que consiste de: bicarbonato de sodio, carbonato de sodio, cloruro de sodio, acetato de sodio y bicarbonato de amonio; y

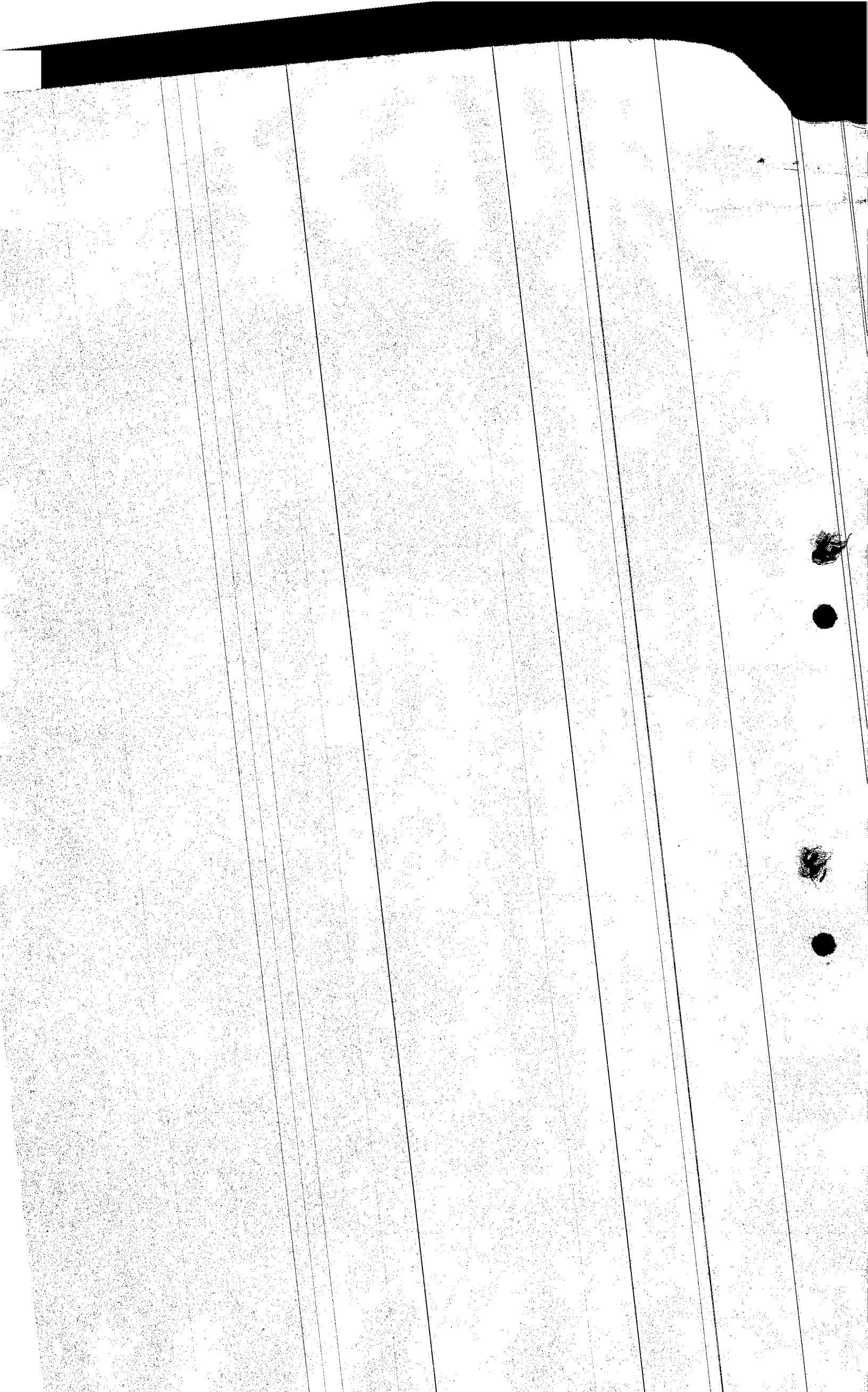
(C) agua,

la cantidad de los componentes (A) y (B) en la composición está en el rango de 5 a 60 partes en peso y en un rango de 0.1 a 10 partes en peso por 100 partes en peso de la cantidad total de la composición agroquímica respectivamente, teniendo el componente (A) una solubilidad a 20°C de 0.4-2 g/100 ml en una solución acuosa del componente (B) de la cual la proporción de composición del componente (B) y agua es la misma que en la composición.

2. La composición agroquímica en suspensión acuosa de acuerdo a la reivindicación 1 en la cual el componente (A) es sal de sodio de 4,5-dihidro-3-metoxi-4-metil-5-oxo-N-[(2-trifluorometoxifenilsulfonil]-1H-1,2,4-triazol-1-carboxamida.

3. La composición agroquímica en suspensión acuosa de acuerdo a la reivindicación 1 en la cual el componente (A) es 2,6-bis(4,6-dimetoxipirimidin-2-iloxi)benzoato de sodio.

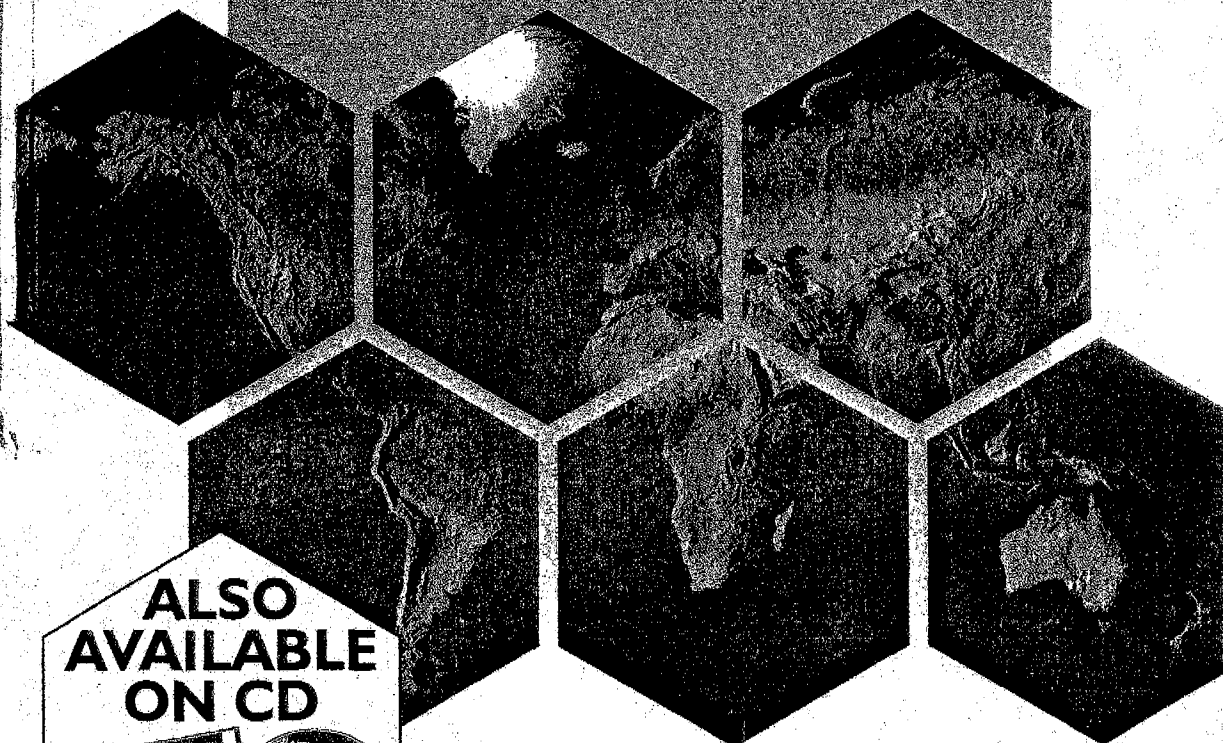
	Claim	Example	General Name	Page	Chemical Name
Present invention	1	1.2.3.4	bispyribac-sodium	97	sodium 2,6-bis(4,6-dimethoxypyrimidin-2-yloxy)benzoate
	1	5	flucarbazone-sodium	427	4,5-dihydro-3-methoxy-4-methyl-5-oxo-N-[(2-trifluoromethoxy)phenylsulfonyl]-1H-1,2,4-triazole-1-carboxamide sodium salt
D2	16.22	1.2	chlorsulfuron	175	2-chloro-N-[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)aminocarbonyl]benzenesulfonamide
	17	3	chlormuron-ethyl	161	2-[[[(4-chloro-6-methoxypyrimidin-2-yl)aminocarbonyl]aminosulfonyl]benzoic acid,ethyl ester
	18	4	metsulfuron-methyl	644	2-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)aminocarbonyl]aminosulfonyl]benzoic acid,methyl ester
	21	5	sulfometuron-methyl	851	2-[[[(4,6-dimethylpyrimidin-2-yl)aminocarbonyl]aminosulfonyl]benzoic acid,methyl ester
	23	6	bensulfuron-methyl	76	2-[[[(4,6-dimethoxypyrimidin-2-yl)aminocarbonyl]aminosulfonylmethyl]benzoic acid,methyl ester
	19	7	(unknown)	-	N-[[[(4,6-dimethylpyrimidine-2-yl)aminocarbonyl]-2-hydroxybenzenesulfonamide,ethanesulfonate
	20	8	thifensulfuron-methyl	899	3-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)aminocarbonyl]aminosulfonyl]-2-thiophenecarboxylic acid,methyl ester
D3	3	1.2.3.4	loxynyl-octanoate	648	3,5-diiodo-4-octanoyloxybenzonitrile
	3	5	trifluralin	942	a,a,a-trifluoro-2,6-dinitro-N,N-dipropyl-p-toluidine
	3	6	benfluralin	69	N-butyl-N-ethyl-a,a,a-trifluoro-2,6-dinitro-p-toluidine
	3	7.8	phosalone	731	3-diethoxyphosphorylthiomethyl-6-chlorobenzoxazolone
	3	10.11.12	methyl isothiocyanate	630	methylisothiocyanate
D4	12	1.2.3.4.7	ethofumesate	364	(RS)-2-ethoxy-2,3-dihydro-3,3-dimethylbenzofuran-5-yl methanesulfonate
	(none)	5	atrazine	42	6-chloro-N ² -ethyl-N ⁴ -isopropyl-1,3,5-triazine-2,4-diamine
	12	6	amitraz	31	N-methylbis(2,4-xylyliminomethyl)amine
	12	8	triforine	945	N,N'-[piperazine-1,4-diylbis[(trichloromethyl)methylene]]diformamide
	12	9.10.11	phenmedipham	722	methyl 3-(3-methylcarbaniloyloxy)carbanilate
	12	12	mancozeb	578	manganese ethylenebis(dithiocarbamate) (polymeric) complex with zinc salt
	12	13	methylene bithiocyanate	(none)	methylene bis(thiocyanate)
	12	14	dazomet	250	3,5-dimethyl-1,3,5-thiadiazinane-2-thione



The Pesticide Manual

Twelfth Edition

Editor: C D S Tomlin



BRITISH
CROP
PROTECTION
COUNCIL

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Before handling, storing or using any approved crop protection product, it is essential to follow the instructions on the label.

Foreword

The Publisher

Editorial Advisory Board

Preface

INTRODUCTION

Guide to using the Main Entries

Stereochemistry Nomenclature

Resistance to Pesticides

MAIN ENTRIES

SUPERSEDED ENTRIES

REFERENCE

Glossary of Species

Directory of Companies

Abbreviations and Codes

1. Common names - r
2. GCPF (formerly GIL)
3. WIPO country codes
4. WHO and EPA tox
5. IOBC codes for be
6. EC risk symbols and
7. IARC carcinogenicit
8. General abbreviatio

Bibliography

INDEXES

1. CAS Registry Num
2. Molecular Formulae
3. Code Numbers
4. General Names
5. Classes

ig/kg. Fish LC₅₀ (96 h) for sunfish 0.0024 mg/l; (48 h) for sh in laboratory tests. ant environmental hazard, due) 0.0008 mg/l. Bees Very toxic

polism in rats was principally by ge and conjugation reactions. ation products) penetrated the r on the skin of cucumbers is ightly adsorbed on soil.

Fungicide

Accepted in lieu of common

Colourless crystals. M.p. 69-71°C. Soluble in water. Readily soluble in water. Stable in acidic and alkaline media.

trus-rotting fungi described by

ulation. **Uses** Used to impregnate impregnated material.

Gunther et al., *Analyst* (London), 1960, 85, 100. Man et al., *J. Assoc. Off. Anal. Chem.*, 1979, 62, 100. Alo et al., *J. Chromatogr.*, 1979, 187, 1, 6) or by hplc

(see p. 2 of the Bibliography) 0 mg/kg. Depression of the central nervous system in experimental animals. Concentrations >0.005 mg/l air is considered hazardous. ADI (JMPR) 0.125 mg/kg.

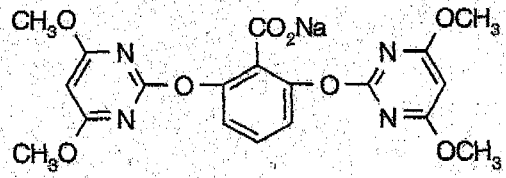
[1967]. **Toxicity class** WHO (a.i.) III (Table 5); EPA (formulation) III **EC hazard** Xi; R36/37/38; N, R50, R53

ENVIRONMENTAL FATE: **Animals** In mammals, following oral administration, metabolites identified include 4-hydroxybiphenyl and other phenolic compounds (H. D. West et al., *Arch. Biochem. Biophys.*, 1956, 60, 14-20). **Plants** Residues in fruit have been reviewed (A. Rajzman, *Residue Rev.*, 1964, 8, 1; S. W. Souci & G. Maier-Haerländer, *ibid.*, 1966, 16, 103).

82 bispyribac-sodium

Herbicide

HRAC B: WSSA 2; pyrimidinyl-oxybenzoic



NOMENCLATURE: **Common name** bispyribac-sodium (BSI, pa ISO) **IUPAC name** sodium 2,6-bis(4,6-dimethoxypyrimidin-2-yloxy)benzoate **Chemical Abstracts name** sodium 2,6-bis[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoate **CAS RN** [125401-75-4] for acid; [125401-92-5] for sodium salt **Development codes** KIH-2023; KUH-911-V-10029

PHYSICAL CHEMISTRY: **Composition** Tech. is >93%. **Mol. wt.** 452.4 **M.f.** C₁₉H₁₇N₄NaO₈; C₁₉H₁₇N₄O₈ for the acid **Form** White powder. **M.p.** 223-224°C **V.p.** 5.05 × 10⁻⁶ mPa (25°C) **K_{ow}** log P = 1.03 (23°C) **Henry** 3.12 × 10⁻¹¹ Pa m³ mol⁻¹ (calc.) **S.g./density** Bulk density 0.733 (20°C, CIPAC MT-3) **Solubility** In water 73.3 g/l (25°C). In methanol 26.3, acetone 0.043 g/l (25°C). **Stability** Stable in water; DT₅₀ >1 y (pH 7 & 9), 448 h (pH 4). Stable to light. Not decomposed after 14 d at 55°C. **pKa** 3.05

COMMERCIALISATION: **History** Discovered in 1988. Reported by Kumiai Chemical Industry Co., Ltd (M. Yokoyama et al., *Proc. Br. Crop Prot. Conf. - Weeds*, 1993, 1, 61). Developed jointly by Kumiai and Iihara Chemical Industry Co., Ltd and introduced in 1997. **Patents** US 4906285; EP 321846 **Manufacturers** Iihara/Kumiai.

APPLICATIONS: **Biochemistry** Branched chain amino acid synthesis (ALS or AHAS) inhibitor. **Mechanism of action** Selective, systemic post-emergence herbicide, absorbed by foliage and roots. **Use** Control of grasses, sedges and broad-leaved weeds, especially *Echinochloa* spp., in direct-seeded rice, at rates of 15-45 g/ha. Also used to stunt growth of weeds in non-crop situations. **Formulation types** SC, water-soluble liquid. **Selected tradenames** 'Grass-short' (non-crop land) (Riken); 'Nominet' (Kumiai); 'Short-keep' (non-crop land) (Riken Green)

ANALYSIS: By hplc. Details available from Kumiai.

ENVIRONMENTAL TOXICOLOGY: **Oral** Acute oral LD₅₀ for male rats 4111, female rats 2635, and female mice 3524 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >2000 mg/kg. Irritating to skin; slightly irritating to eyes (rabbits). **Inhalation** LC₅₀ (4 h) for rats

bispyribac-sodium 97

Main Entries

-5-(trifluoromethyl)-1H-pyrazol-

JV 485

4N₂O₂ Form Fluffy, white, crystalline
w logP = 5.44 Henry 7.89 × 10⁻³ Pa
ty Stable at pH 4 and pH 5;

et al. (Proc. Br. Crop Prot. Conf.
under development by Twinagro, 11
485, WO 9206962

se inhibitor. Mode of action Causes
der development for use as pre-
ecurus myosuroides, Lolium spp. Aben-
ved weeds such as Galium aparine, A.

rats >5000 mg/kg. Skin and eye Acute
g to eyes; not irritating to skin (rabbits)
is >1.7 mg/l. Other Negative in Ames

il and mallard ducks >2130 mg/kg. Doses
Fish LC₅₀ (96 h) for rainbow trout and
19.7 g/l. Worms LC₅₀ (14 d) for

y DT₅₀ (3 field and 1 standard soil)
(pH 5.1, o.c. 1.94%) 2.5 × 10⁴ and
0.7 × 10⁴, in silt loam (pH 6.3
3.0, o.c. 1.30%) 2.0 × 10⁴ and 1.6 × 10⁴
<0.01 µg/l.

Chemical Abstracts name N-[[[4-chloro-3-[[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenyl]=
amino]carbonyl]-2,6-difluorobenzamide
CAS RN 186811-58-7] Development codes CGA 157 419

PHYSICAL CHEMISTRY: Mol. wt. 506.2 M.f. C₂₀H₁₀Cl₂F₅N₃O₃ Form White to pink, odourless,
fine crystalline powder. M.p. 219°C (decomp.) V.p. 1.2 × 10⁻⁷ mPa (20°C) K_{ow} logP = 5.1
(calc. method). Henry <3.04 × 10⁻⁶ Pa m³ mol⁻¹ (calc.) S.g./density 1.59 (20°C) Solubility In
water <0.02 ppm (20°C). In methanol 2.4, isopropanol 0.9 (both in g/l, 20°C). Stability Stable up
to 219°C Hydrolysis DT₅₀ (25°C) 14 d (pH 3), 7 d (pH 5), 20 h (pH 7), 0.5 h (pH 9).

COMMERCIALISATION: Manufacturers Novartis.

APPLICATIONS: Biochemistry Interaction with chitin formation. Mode of action Systemic acarine
growth regulator with contact and stomach action. Uses Strategic control of the cattle tick
Rhipicephalus microplus (including all known resistant strains) on beef cattle. Formulation types PO.
Trade names 'Acatak' (Novartis)

ANALYSIS: By hplc.

ENVIRONMENTAL TOXICOLOGY: Reviews JECFA 48 (see part 2 of Bibliography). Oral Acute oral
LD₅₀ for rats >5000 mg/kg (OECD 401). Skin and eye Acute percutaneous LD₅₀ for rats
>5000 mg/kg (OECD 402). Inhalation LC₅₀ (4 h) for rats >5994 mg/m³ (OECD 403).
LD₅₀ (1 y) for dogs 7.5 mg/kg b.w. daily; (life-time) for rats 400, mice (males and females)
100 mg b.w. daily. In 2-generation reproduction tests (rats), NOEL 100 ppm. No carcinogenic,
mutagenic, teratogenic or reprotoxicity potential. ADI (JMPR) 0.04 mg/kg b.w. [1997] (JECFA
1997). Toxicity class WHO (a.i.) III

ENVIRONMENTAL TOXICOLOGY: Birds Acute oral LD₅₀ for bobwhite quail, mallard ducks >2000 mg/kg.
LD₅₀ for bobwhite quail, mallard ducks >5200 ppm. Fish LC₅₀ for rainbow trout >15, carp
>1500 ppm (OECD class "harmful"). Daphnia LC₅₀ 0.0006 mg/l (OECD class "very toxic").
Algae EC for freshwater green algae 27.9 mg/l (virtually non-toxic). Bees OECD class "not
harmful". Worms LC₅₀ (14 d) for earthworms >1000 mg/kg (not toxic) (OECD 207).

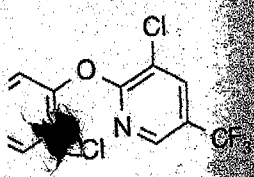
ENVIRONMENTAL FATE: Animals Virtually no metabolism. Plants Not relevant.
Environment Not investigated; environmental contamination is unlikely because of pour-on

Index

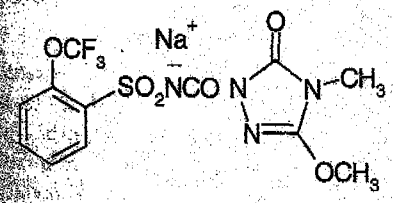
flucarbazone-sodium

Herbicide

CAS 2, sulfonaminocarbonyltriazolinone



pa E-ISO, INN)
yl-2-pyridyloxy]phenyl]] =



Common name flucarbazone-sodium (BSI, pa ISO)

flucarbazone-sodium 427

Main Entries

IUPAC name 4,5-dihydro-3-methoxy-4-methyl-5-oxo-*N*-(2-trifluoromethoxyphenyl)-1*H*-1,2,4-triazole-1-carboxamide sodium salt

Chemical Abstracts name 4,5-dihydro-3-methoxy-4-methyl-5-oxo-*N*-[[2-(trifluoromethylsulfonyl)-1*H*-1,2,4-triazole-1-carboxamide, sodium salt

CAS RN [181274-17-9]; (acid [145026-88-6]) **Development codes** MKH 6562, SGL

PHYSICAL CHEMISTRY: Mol. wt. 418.3 M.f. $C_{12}H_{10}F_3N_4NaO_6S$ Form Colourless crystalline powder. M.p. 200°C (decomp.) V.p. $<1 \times 10^{-6}$ mPa (20°C, calc.) K_{ow} 1.0 (pH 4), -1.85 (pH 7), -1.89 (pH 9), -2.80 (unbuffered) (all 20°C) Henry $<1 \times 10^{-11}$ m³ mol⁻¹ (20°C, calc.) S.g./density 1.59 g/ml. Solubility In water 44 g/l (pH 4-9, 20°C) pKa 1.9

COMMERCIALISATION: **History** Reported by H. J. Santel et al., (Proc. Br. Crop Prot. Weeds, 1999, 1, 23). Under development by Bayer AG. **Manufacturers** Bayer

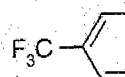
APPLICATIONS: **Biochemistry** Branched chain amino acid synthesis (ALS or AHAS) inhibited by inhibiting biosynthesis of the essential amino acids valine and isoleucine, hence stops cell division and plant growth. **Mode of action** Absorbed through foliage and roots and translocated acropetally and basipetally. **Uses** For post-emergence control of grass weeds, especially *fatusa* and *Setaria viridis*, and some broad-leaved weeds, in wheat; applied at 21 g/ha. **Formulation types** WG.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats >5000 mg/kg. Skin and subcutaneous LD₅₀ for rats >5000 mg/kg. Non-irritating to skin; slightly/moderately irritating to eyes (rabbits). Not a skin sensitiser (guinea pigs). **Inhalation** (acute) for rats >5.43 mg/kg. **NOEL** (2 y) for rats 125, mice 1000 mg/kg diet; (1 y) for female dogs 200, male dogs 100 mg/kg diet. **ADI** 0.04 mg/kg b.w. (Bayer, proposed). **Other** No evidence for any neurotoxic, teratogenic or carcinogenic potential.

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail >2000 mg/kg. Subacute oral LC₅₀ for bobwhite quail >5000 ppm. **Fish** LC₅₀ (96 h) for bluegill sunfish >99.3 mg/l. **Daphnia** EC₅₀ (48 h) >109 mg/l. **Algae** EC₅₀ for *Selenastrum capricornutum* 6.4 mg/l. **Other aquatic spp.** EC₅₀ for *Lemna gibba* 0.0126 mg/l. **Bees** Non-toxic to bees. **Worms** LC₅₀ for earthworms >1000 mg/kg.

ENVIRONMENTAL FATE: **Animals** Almost completely excreted via faeces and urine after oral administration to rats. **Plants** Extensively metabolised in wheat plants. The relevant metabolites for enforcement purposes are the parent compound and the *N*-desmethyl metabolite. **Soil/Environment** Average soil DT₅₀ 17 d. Photolytic DT₅₀ in soil and water >500 d. No product in soil; in dissipation studies, no product residues detected below 30 cm.

fluchloralin



SYNOPSIS: **Common name** fluchloralin **Chemical Abstracts name** *N*-(2-chloroethyl)-2,6-dinitro-*N*-(2-chloroethyl)- α,α,α -trifluoro-2,6-dinitrophenyl **Chemical Abstracts name** *N*-(2-chloroethyl)-2,6-dinitro-*N*-(2-chloroethyl)- α,α,α -trifluoro-2,6-dinitrophenyl **Development codes** 13245-39-5

PHYSICAL CHEMISTRY: **Composition** Tech. 95% $C_{12}H_{10}Cl_2F_3N_4O_6$ **Form** Orange-yellow crystals. M.p. 40°C. V.p. 53 mPa at 50°C. Sol. in benzene, diethyl ether, ethyl acetate >100 g/100 ml. **Stability** Decomposed by u.v. light. Stable in container at normal room temperature.

COMMERCIALISATION: **History** Herbicide introduced by BASF (1972, 5, 189). Introduced in 1972 to BASF. **Manufacturers** BASF

APPLICATIONS: **Biochemistry** Cell division inhibited in shoots and roots, with acropetal and other physiological growth processes. **Uses** For post-emergence control of grass weeds and some broad-leaved weeds, in wheat, maize, beans, okra, jute, sunflowers. **Formulation types** EC. **Selected t**

ANALYSIS: **Product and residue analysis by**

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats >5000 mg/kg. Skin and eye Acute percutaneous LD₅₀ for rats >5000 mg/kg. **Inhalation** LC₅₀ (4 h) for rats 8.4 mg/kg. **ADI** 0.04 mg/kg b.w. (WHO, a.i.) III; EPA (formulation)

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail >2000 mg/kg. **Fish** LC₅₀ (96 h) for bluegill sunfish >99.3 mg/l.

ENVIRONMENTAL FATE: **Plants** In plants, 100% converted into plant structures. **Soil/Environment** Average soil DT₅₀ 17 d. Photolytic DT₅₀ in soil and water >500 d. No product in soil; in dissipation studies, no product residues detected below 30 cm. **Chemical Abstracts name** *N*-(2-chloroethyl)-2,6-dinitro-*N*-(2-chloroethyl)- α,α,α -trifluoro-2,6-dinitrophenyl **Chemical Abstracts name** *N*-(2-chloroethyl)-2,6-dinitro-*N*-(2-chloroethyl)- α,α,α -trifluoro-2,6-dinitrophenyl **Development codes** 13245-39-5

Insecticide, acaricide

E-ISO, ANSI, ESA):

othioate
idiny) phosphorothioate
ial codes OMS 1155; ENT 27 520

22.5 M.f. C₇H₇Cl₃NO₃PS
-46.5°C V.p. 3 mPa (25°C)
density 1.64 (23°C) Solubility in
e 120 (all in g/kg, 20°C).
) Aqueous photolysis DT₅₀ 1.8 d

H. Rigterink & E. E. Kenaga (J. Agric.
(now Dow AgroSciences).
es.

ode of action Non-systemic insecticide
Uses Control of Coleoptera, Diptera
is), and various foliar crop pests in
berries, vegetables, tomatoes.
uses include control of Muscidae and
grams (e.g. *Anopheles* spp., vectors of
Compatibility Incompatible with aldrin
(Dow AgroSciences)

by glc (Man. Pestic. Residue Anal., 1990
5; Analyst (London), 1979, 104, 425
, 85). Details available from Dow

67 (see part 2 of the Bibliography)
nea pigs 2250, rabbits 2000 mg/kg
rats >3700 mg/kg. Non-irritating to skin
IEL In 2 y feeding trials, NOEL based on
rats ADI (JMPR) 0.01 mg/kg bw
rule III

ducks >1590, bobwhite quail 922 mg/kg
Fish LC₅₀ (96 h) for rainbow trout 0.4
025 ppm. Algae EC₅₀ (72 h) for
. Toxic to crustaceans. LC₅₀ (36 h) for

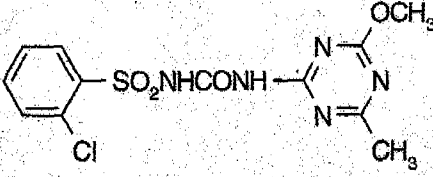
grayish 0.004 mg/l. Bees Very toxic to bees. LD₅₀ (contact) 0.38 µg/bee. Worms LC₅₀ (15 d)
for *Isenia foetida* 182 mg/kg soil.

ENVIRONMENTAL FATE: EHC 63 (WHO, 1986; a general review of organophosphorus
insecticides). Animals In rats and other mammals, following oral administration, rapid metabolism
occurs, the principal metabolite being 3,5,6-trichloropyridin-2-ol. Excretion is principally in the
urine. Soil/Environment In soil, undergoes microbial degradation to 3,5,6-trichloropyridin-2-ol,
which is subsequently degraded to organochlorine compounds and CO₂; DT₅₀ 1.5-33 d,
DT₉₀ 14-47 d, depending upon soil type and microbial activity. K_d 3.5-407 ml/g, depending on soil
type. K_{oc} is more constant: 1190-8100 ml/g.

146 chlorsulfuron

Herbicide

WSSA 2; sulfonylurea



NOMENCLATURE: Common name chlorsulfuron (BSI, draft E-ISO, (m) draft F-ISO, ANSI, WSSA)
UPAC name 1-[(2-chlorophenyl)sulfonyl]-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)urea
Chemical Abstracts name 2-chloro-N-[[[4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]=
sulfonamide
CAS RN 76490-72-3 EEC no. 265-268-5 Development codes DPX 4189; W4189

PHYSICAL CHEMISTRY: Mol. wt. 357.8 M.f. C₁₂H₁₂ClN₅O₄S Form White crystalline solid.
mp 174-178°C V.p. 3 x 10⁻⁶ mPa (25°C) K_{ow} log P = -0.99 (pH 7) Henry 3.0 x 10⁻⁹ Pa
at 25°C Sg/density 1.48 Solubility In water 587 ppm (pH 5), 3.18 g/100g (pH 7) (both 25°C).
In chloroform 1.4, acetone 4, methanol 15, toluene 3, hexane <0.01 (all in g/l, 20°C).
Stable to light when dry. Decomposes at 192°C. In aqueous solutions, DT₅₀ 4-8 w
(pH 5.7-7.0, 20°C); significant degradation in 24-48 h (pH <5). Hydrolysis is also promoted by
organic solvents such as methanol and acetone. pKa 3.6

COMMERCIALISATION: History Herbicide reported by P. G. Jensen (Weed Control, 1980, 21st,
1981) produced by E. I. du Pont de Nemours and Co. Patents US 4127405 Manufacturers Du
Pont

INDICATIONS: Biochemistry Branched chain amino acid synthesis (ALS or AHAS) inhibitor. Acts
by blocking biosynthesis of the essential amino acids valine and isoleucine, hence stopping cell
division and plant growth. Selectivity derives from rapid metabolism in the crop. Metabolic basis of
selectivity in sulfonylureas reviewed (M. K. Koeppel & H. M. Brown, Agro-Food-Industry, 6,
1995). Mode of action Selective systemic herbicide, absorbed by the foliage and roots, with
translocation acropetally and basipetally. Uses Control of most broad-leaved weeds and
annual grasses in wheat, barley, oats, rye, triticale, flax, and on non-crop land. Applied pre-
emergence, early post-emergence, pre-plant, or early post-plant incorporated, at 9-25 g/ha.
Phytotoxic to many broad-leaved crops, particularly sugar beet and brassicas.

chlorsulfuron 175

Main Entries

ethyl acetate 3.7, dichloromethane 1.5, hexane 0.5. **Stability** Stable up to 50°C in sunlight (xenon lamp).

Fischer (Weed Res., 1962, 2, 177).
DE 1105232 **Manufacturers** BASF

port inhibitor at the photosystem II level. Rapidly absorbed by the roots, with annual broad-leaved weeds in sugar beets, pre-emergence, or post-emergence with other herbicides.

lima beans and tomatoes.
Irt' (BASF); 'Pyramin' (BASF); 'Tol' (Caffaro); 'Gladiator' (Tripan); 'Inmerac' (sugar beet) (BASF); 'Rebel'

CIPAC Handbook, 1988, D, 31).
von Pflanzenschutzmitteln, 1987

ale rats 3830, female rats 2140, male rats cutaneous LD₅₀ for rats
lethal LC₅₀ (4 h) for rats >5.4 mg/l (0.5 mg/kg). **Other** Non-mutagenic (Table 5); EPA (formulation III)

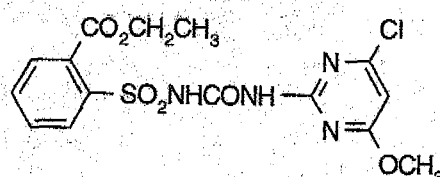
ail >2000 mg/kg b.w. Dietary effect. **Fish** LC₅₀ (96 h) for trout 32-40 mg/kg. LC₅₀ (120 h) for *Chlorella fusca* (act) >200 µg/bee.

oral application, 85% is excreted in urine. In oral applications, excretion proceeds in beet, conjugation to form the glucuronide, which is not herbicidally active. c. 6-8 weeks under sufficiently moist

135 chlorimuron-ethyl

Herbicide

HRAC B. WSSA 2: sulfonylurea



NOMENCLATURE: *chlorimuron-ethyl*

Common name chlorimuron-ethyl

UPAC name ethyl 2-(4-chloro-6-methoxypyrimidin-2-ylcarbamoylsulfamoyl)benzoate

Chemical Abstracts name ethyl 2-[[[(4-chloro-6-methoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonylbenzoate

CAS RN 90982-32-4 **Development codes** DPX-F6025

chlorimuron

Common name chlorimuron (BSI, ANSI, WSSA, draft E-ISO, draft F-ISO)

UPAC name 2-(4-chloro-6-methoxypyrimidin-2-ylcarbamoylsulfamoyl)benzoic acid

Chemical Abstracts name 2-[[[(4-chloro-6-methoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonylbenzoic acid

CAS RN 90983-00-8

PHYSICAL CHEMISTRY: *chlorimuron-ethyl*

Composition Tech. is >95%. **Mol. wt.** 414.8 **M.f.** C₁₅H₁₅ClN₄O₆S **Form** Colourless crystals.

Mp. 181°C **V.p.** 4.9 × 10⁻⁷ mPa **K_{ow} logP** = 0.11 (pH 7) **Henry** 1.7 × 10⁻¹⁰ Pa m³ mol⁻¹

Density 1.51 (25°C) **Solubility** In water 9 (pH 5), 1200 (pH 7) (both in mg/l, 25°C). Low solubility in organic solvents. **Stability** In water DT₅₀ 17-25 d (pH 5, 25°C). **pKa** 4.2

chlorimuron

Mol. wt. 386.8 **M.f.** C₁₃H₁₁ClN₄O₆S

COMMERCIALISATION: **History** Chlorimuron-ethyl introduced as herbicide by E. I. du Pont de Nemours and Co. First US registration in 1986. **Patents** US 4394506; US 4547215

Manufacturers Du Pont; IPESA; JIE.

APPLICATIONS: *chlorimuron-ethyl*

Mode of action Branched chain amino acid synthesis (ALS or AHAS) inhibitor. Acts by inhibiting the synthesis of the essential amino acids valine and isoleucine, hence stopping cell division and plant growth. Crop selectivity derives from plant metabolism both by homogluthathione conjugation and by glucuronidation (M. K. Koeppe & H. M. Brown, *Agro-Food-Industry*, 6, 9-14 (1995)). **Uses** Used for emergence for control of important broad-leaved weeds, such as cocklebur, pigweed, morning glory and annual morning glory, in soya beans and peanuts. Active at 9-13 g/ha.

Formulation types WG. **Selected tradenames** 'Classic' (Du Pont); 'Darban' (IPESA); 'Sponsor' (Du Pont).

ANALYSIS: Product analysis by hplc (R. A. Guinivan et al., *Anal. Methods Pestic. Plant Growth Regul.*, 1988, 16, 17). Residues determined by hplc (J. L. Prince & R. A. Guinivan, *J. Agric. Food Chem.*, 1988, 36, 1). Methods for sulfonylurea residues in crops, soil and water reviewed (A. C. Barefoot et al., *Proc. 1st Crop Prot. Conf. - Weeds*, 1995, 2, 707).

chlorimuron-ethyl 161

Main Entries

ENVIRONMENTAL FATE: Animal occurs within 96 hours, about equal undergoes oxidative deamination at

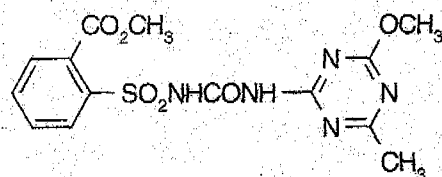
Soil/Environment Metribuzin is rapidly degraded in soil; microbial breakdown is the major mechanism of loss. Degradation involves deamination, followed by further degradation to soluble conjugates. Photodecomposition on soil surfaces and in aqueous solution is an important process for the degradation of metribuzin in the environment.

als, following oral administration, 98% in urine and the faeces. **Plants** In plants, metribuzin is rapidly degraded to water-soluble conjugates.

ed in soil; microbial breakdown is the major mechanism of loss. Degradation involves deamination, followed by further degradation to soluble conjugates. Photodecomposition on soil surfaces and in aqueous solution is an important process for the degradation of metribuzin in the environment.

536 metsulfuron-methyl

HRAC B WSSA 2; sulfonylurea



NOMENCLATURE: *metsulfuron-methyl*

Chemical Abstracts name methyl 2-[[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]-amino]sulfonyl]benzoate

CAS RN [74223-64-6] Development codes DPX-T6376

metsulfuron

Common name metsulfuron (BSI, WSSA, ANSI, draft E-ISO, (m) draft F-ISO)

IUPAC name 2-(4-methoxy-6-methyl-1,3,5-triazin-2-ylcarbamoylsulfamoyl)benzoic acid

Chemical Abstracts name 2-[[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]-amino]sulfonyl]benzoic acid

CAS RN [79510-48-8]

PHYSICAL CHEMISTRY: *metsulfuron-methyl*

Mol. wt. 381.4 M.f. $C_{14}H_{15}N_5O_6S$ Form Colourless crystals; (tech., off-white solid, with a faint ester-like odour). M.p. 158°C V.p. 3.3×10^{-7} mPa (25°C) K_{ow} logP = -1.74 (pH 7)

Henry 2.3×10^{-10} Pa m³ mol⁻¹ (calc.) S.g./density 1.47 Solubility In water 0.55 (pH 5),

2.79 (pH 7), 213 (pH 9) (all in g/l, 25°C). In hexane 0.00079, xylene 0.58, ethanol 2.3, methanol

7.3, acetone 36, dichloromethane 121 (all in g/l, 20°C). Stability Stable in air up to c. 140°C.

Hydrolysis DT₅₀ (25°C) 22 d (pH 5), stable (pH 7 and 9). pKa 3.3

metsulfuron

Mol. wt. 367.3 M.f. $C_{13}H_{13}N_5O_6S$ Form Solid.

COMMERCIALISATION: History Herbicidal properties of metsulfuron-methyl reported by R. I. Doig et al. (Proc. Int. Congr. Plant Prot., 10th, 1983, 1, 324). Introduced by E. I. du Pont de Nemours and Co. Patents US 4370480 Manufacturers Du Pont; IPESA; JIE; Reposo.

APPLICATIONS: *metsulfuron-methyl*

Biochemistry Branched chain amino acid synthesis (ALS or AHAS) inhibitor. Acts by inhibiting biosynthesis of the essential amino acids valine and isoleucine, hence stopping cell division and plant

growth. Activity derives from rapid metabolic breakdown (M. K. Koeppel & H. M. ... Selective systemic herbicide a ... both atropetally and basipetally ... emergence treatment, and are killed ... on certain broad-leaved ... and perennial broad-leaved v ... application, at 4-7.5 g/ha pre ... 'Ally' (Du Pont); 'Maiba ... Product analysis by hplc (L. W. ... 1988, 16, 83). Residues ... in crops, soil and water ... (1995, 2, 707).

TOXICOLOGY: *metsulfuron-methyl* Acute oral LD₅₀ for male and female rats for rabbits >2000 mg/kg. Mild skin irritant. Inhalation LC₅₀ for rats 500, male dogs 500, female dogs 500. Non-mutagenic in the Ames test. No (formulation) IV

metsulfuron Hazard N; R50, R53

ECOTOXICOLOGY: *metsulfuron-methyl* Acute oral LD₅₀ for mallard ducks >5100 mg/kg diet. Fish LC₅₀ >150 mg/l. Daphnia EC₅₀ (48 h) >150 mg/l. aquatic spp. NOEC for Lemna gibba >1000 mg/kg.

ENVIRONMENTAL FATE: *metsulfuron-methyl* In mammals, following oral administration, the methoxycarbonyl and sulfonyl groups are metabolised. The methoxycarbonyl and sulfonyl groups are metabolised by hydrolysis and conjugation. In addition, metabolites include methyl 2-(aminosulfonyl)benzoate. Soil/Env breakdown being more rapid at lower soil moisture. K_{oc} 35 (pH 7).

dro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl)-
nethyl)-4,5-dihydro-3-methyl-5-oxo-

1C 97285

$\text{H}_2\text{F}_2\text{N}_4\text{O}_3\text{S}$ Form Tan solid.
= 1.48 S.g./density 1.21 g/ml (20°C)
(all in mg/g, 25°C): Soluble, to some
ility Stable to hydrolysis. Readily

in Saun et al. (Proc. Br. Crop Prot. Conf.
turers FMC.

dase inhibitor (chlorophyll biosynthesis,
ots and foliage, with translocation pro-
Jses Control of annual broad-leaved
r cane and tobacco. Applied pro-
s SC; WG.
azil) (FMC): 'Capaz' (Latin America)

or rats 2855 mg/kg. Skin and eye Acute
ng to skin; mild eye irritant (rabbits).
/rats >4.14 mg/l. NOEL 10 mg/kg diet
mouse lymphoma and in vivo
only ill

ducks >2250 mg/kg. Dietary LC_{50} (8 d)
luégill sunfish 93.8, rainbow trout

administered sulfentrazone is excreted
the parent sulfentrazone is metabolized
irs. This analogue is also rapidly converted
o of which are glycosidic derivatives. It
in soil (DT_{50} 18 mo). In water, DT_{50}
 DT_{50} <0.5 d). Low affinity for organic matter.
t. Low potential to bioaccumulate.

Insecticides

H_2CH_3

NSI, draft E-ISO)

Chemical Abstracts name N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptafluoro-1-octane-
onamide
CASRN [4151-50-2] Development codes GX 071

PHYSICAL CHEMISTRY: Composition Tech. is 98.0%. Mol. wt. 527.2 M.f. $\text{C}_{10}\text{H}_6\text{F}_{17}\text{NO}_2\text{S}$
Form Colourless crystals. M.p. 96°C; (tech., 87-93°C) B.p. 196°C V.p. 0.057 mPa (25°C)
 $\log P$ >6.8 (unionised) Solubility Insoluble in water (25°C). In dichloromethane 18.6, hexane
1.4, methanol 833 (all in g/l). Stability Stable >90 d at 50°C; to light >90 d in closed jar. pKa 9.5.
Weak acid F.p. >93°C (Seta flash)

COMMERCIALISATION: History Insecticide introduced in USA (1989) by Griffin Corp.
Patents US 4921696 Manufacturers Griffin.

APPLICATIONS: Biochemistry Uncouples oxidative phosphorylation. Uses For household control
of Formicidae and Blattellidae. Formulation types RB.

ANALYSIS: Product analysis by glc.

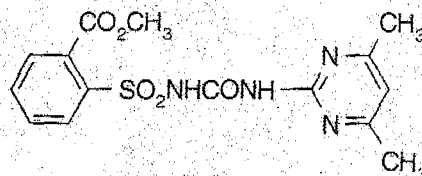
ENVIRONMENTAL TOXICOLOGY: Oral Acute oral LD_{50} for rats >5000 mg/kg. Skin and eye Acute
irritation LD_{50} for rabbits >2000 mg/kg. Mild skin irritant; practically non-irritating to eyes
(rabbits). Inhalation LC_{50} (4 h) for rats >4.4 mg/l. NOEL (90 d) for male dogs 33, female dogs
10, rats 10 ppm. Toxicity class WHO (a.i.) III

ECOTOXICOLOGY: Birds Acute oral LD_{50} for bobwhite quail 45 mg/kg. LC_{50} (8 d) for bobwhite
quail 100, mallard ducks 165 ppm diet. Fish LC_{50} (96 h) for fathead minnow >9.9, rainbow trout
>700 mg/l. Daphnia LC_{50} (48 h) 0.39 mg/l.

713 sulfometuron-methyl

Herbicide

WSSA 2; sulfonyleurea



NOMENCLATURE: sulfometuron-methyl

CASRN [74223-97-2] Development codes DPX T5648

Chemical name

Common name sulfometuron (BSI, E-ISO, (m) F-ISO, ANSI, WSSA)

WSSA name 2-[[[(4,6-dimethylpyrimidin-2-yl)ureido]sulfonyl]benzoic acid;

2-[[[(4,6-dimethylpyrimidin-2-yl)ureido]sulfonyl]benzoic acid

Chemical Abstracts name 2-[[[(4,6-dimethyl-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]benzoic

CASRN [74223-56-6] Development codes DPX 5648

sulfometuron-methyl 851

PHYSICAL CHEMISTRY: *sulfometuron-methyl*

Composition Tech. is >93%. Mol. wt. 364.4 M.f. $C_{15}H_{16}N_4O_5S$ Form Colourless solid (lith.) M.p. 203-205°C V.p. 7.3×10^{-11} mPa (25°C) K_{ow} logP = 1.18 (pH 5), -0.51 (pH 7) Henry 1.2×10^{-13} Pa m³ mol⁻¹ (25°C) S.g./density 1.48 Solubility in water 244 mg/l (pH 7, 25°C). In acetone 3300, acetonitrile 1800, ethyl acetate 650, diethyl ether 60, hexane <1, methanol 550, methylene chloride 15000, dimethyl sulfoxide 32000, octanol 140, toluene 240 (all in mg/l, 25°C). Stability Aqueous suspensions are stable to hydrolysis at pH 7 to pH 9, DT₅₀ < 10 d (pH 5), pKa 5.2

sulfometuron

Mol. wt. 350.3 M.f. $C_{14}H_{14}N_4O_5S$

COMMERCIALISATION: History The methyl ester introduced as a herbicide by E. I. du Pont or Nemours and Co. Manufacturers Du Pont.

APPLICATIONS: *sulfometuron-methyl*

Biochemistry Branched chain amino acid synthesis (ALS or AHAS) inhibitor. Acts by inhibiting biosynthesis of the essential amino acids valine and isoleucine, hence stopping cell division and plant growth. **Mode of action** Broad-spectrum herbicide, absorbed rapidly by the leaves and roots, with translocation throughout the plant. **Uses** Control of annual and perennial grasses (especially *Sorghum halepense*) and broad-leaved weeds in non-crop land. Also used for selective weed control in Bermuda grass and certain other turf grasses; and in forestry to control woody tree species in pine trees. Applied either pre- or post-emergence. **Phytotoxicity** Not to be applied near desirable trees and plants. **Formulation types** WG. **Compatibility** Incompatible with alkaline materials. **Selected tradenames** 'Oust' (Du Pont)

ANALYSIS: Product and residue analysis by hplc (E. W. Zahnow & T. J. Waeghe, *Anal. Methods Pestic. Plant Growth Regul.*, 1988, 16, 105). Details available from Du Pont.

MAMMALIAN TOXICOLOGY: *sulfometuron-methyl*

Oral Acute oral LD₅₀ for male rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >2000 mg/kg; slight skin and eye irritant (rabbits). No skin sensitisation (guinea pigs). **Inhalation** LC₅₀ (4 h) for rats >11 mg/l air. **NOEL** (2 y) for rats 50 mg/kg diet. In 2-generation reproduction studies. NOEL for rats 500 mg/kg diet. Teratogenicity effects in rats at 1000 mg/kg diet, and in rabbits at 300 mg/kg diet. **Toxicity class** WHO (a.i.) III (Table 5); EPA (formulation) IV

ECOTOXICOLOGY: *sulfometuron-methyl*

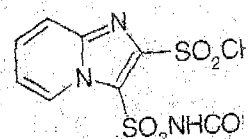
Birds Acute oral LD₅₀ for mallard ducks >5000, bobwhite quail >5620 mg/kg. **Fish** LC₅₀ (96 h) for rainbow trout and bluegill sunfish >12.5 mg/l. **Daphnia** LC₅₀ >12.5 ppm. **Bees** Contact LD₅₀ >100 µg/bee

ENVIRONMENTAL FATE: *sulfometuron-methyl*

Animals Metabolised to hydroxylated sulfometuron-methyl. **Soil/Environment** Degraded by microbial action and by hydrolysis. DT₅₀ in soil c. 4 w. K_{oc} 85.

714 sulfosulfuron

CLASS: WSSA 2: sulfonyleurea



SYNONYMS: Common name sulfosulfuron
CAAC name 1-[(4,6-dimethoxypyrimidin-2-yl)-3-(2-

Chemical Abstracts name N-[[[4,6-dimethoxy-2-pyridinyl-3-yl]pyridine-3-sulfonamide
CAS No. [141776-32-1] **Development codes** M-

PHYSICAL CHEMISTRY: Mol. wt. 470.48 M.f. $C_{14}H_{14}N_4O_5S_2$ M.p. 201.7°C V.p. $<1 \times 10^{-3}$ mPa K_{ow} logP = 3.83 (pH 7), 2.97 (pH 9) (all in mg/l, 25°C). 1627 (pH 7), 482 (pH 9) (all in mg/l, 25°C)

COMMERCIALISATION: History Discovered by J. K. Parrish et al. (*Proc. Br. Crop Prot. Conf.* - Weeds, 1995, 2, 105). Introduced by Takeda and introduced in 1997. Manufacturer Takeda

APPLICATIONS: **Biochemistry** Branched chain amino acid synthesis (ALS or AHAS) inhibitor. Acts by inhibiting biosynthesis of the essential amino acids valine and isoleucine, hence stopping cell division and plant growth. Selectivity derives from its mode of action in sulfonyleureas reviewed (M. K. Koe, *Proc. Br. Crop Prot. Conf.* - Weeds, 1995, 2, 105). **Mode of action** Systemic herbicide, absorbed by leaves and roots, with translocation to symplast and apoplast. **Uses** Broad-spectrum herbicide, absorbed rapidly by the leaves and roots, with translocation throughout the plant. **Phytotoxicity** Not to be applied near desirable trees and plants. **Formulation types** WG. **Compatibility** Incompatible with alkaline materials. **Selected tradenames** 'Oust' (Du Pont)

ANALYSIS: Methods for sulfonyleurea residues in crops. *Proc. Br. Crop Prot. Conf.* - Weeds, 1995, 2, 105.

MAMMALIAN TOXICOLOGY: Oral Acute percutaneous LD₅₀ for rats >5000 mg/kg. No skin sensitiser (guinea pigs). **Inhalation** Practical LD₅₀ >100 µg/bee. **Toxicity class** EPA (formulation) III

0.82; mysid shrimp 2.0 mg/l. IC_{50} (14 d) >1000 mg/kg soil. **Worms** LC_{50} (14 d) >1000 mg/kg soil. **Bees** slightly harmful to predatory mites.

ly metabolised and eliminated. Oxidised d via oxidative de-esterification. DT_{50} 64 d (8–150 d). Vertical mobility es. The monoacid metabolite also has photolysed in soil, but DT_{50} 15 d in er contamination.

Plant growth regulator



(m) F-ISO, ANSI)

orm Colourless, odourless crystals. ngmuir method) K_{ow} $\log P = 1.77$ water 31 mg/l (pH 7, 25°C). In 0.400, acetone 6.67, ethyl acetate 1.400, 1-phenyl-3-(1,2,5-thiadiazol-5-yl)urea at room temperature from pH 5–9. 4°C). pK_a 8.86

ted by F. Arndt et al. (Plant Physiol., Aventis CropScience).

ion Plant growth regulator. ion layer between the plant stem. Used for defoliation of NP; Only flowable.

ic or by glc with ECD of a

MAMMALIAN TOXICOLOGY: Oral Acute oral LD_{50} for mice >5000 , rats >4000 mg/kg. **Skin and eye** Acute percutaneous LD_{50} for rats >1000 , rabbits >4000 mg/kg. Mild eye irritant; non-irritating to skin (rabbits). No skin sensitisation (guinea pigs). **Inhalation** LC_{50} (4 h) for rats 3 mg/l air. **NOEL** (90 d) for rats 200 mg/kg diet; (1 y) for dogs 100 mg/kg diet. No significant effects observed in a 2 y carcinogenicity study in mice and a 3-generation reproduction study in rats. **Other** Acute i.p. LD_{50} for rats 4200 mg/kg. Non-mutagenic. **Toxicity class** WHO (a.i.) III (Table 5); EPA (formulation) III.

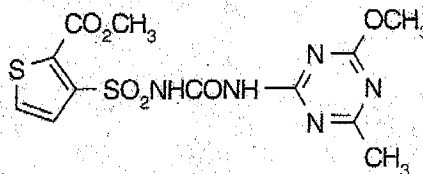
ECOTOXICOLOGY: **Birds** Acute oral LD_{50} for Japanese quail >3160 mg/kg. Dietary LC_{50} (8 d) for bobwhite quail and mallard ducks >5000 mg/kg diet. **Fish** LC_{50} (96 h) for rainbow trout, bluegill sunfish, and catfish >1000 mg/l. **Daphnia** LC_{50} (48 h) >10 mg/l. **Bees** Non-toxic to honeybees. **Worms** LC_{50} (14 d) for earthworms >1400 mg/kg.

ENVIRONMENTAL FATE: **Animals** In rats and goats, metabolism involves hydroxylation of the phenyl group, followed by formation of water-soluble conjugates. Following oral administration, the compound is excreted in the urine and faeces within 96 hours. **Plants** Only small amounts of residue (normally <0.1 mg/kg) are likely in cottonseed. **Soil/Environment** Strongly adsorbed by soil. DT_{50} in soil c. 26–144 d (aerobic), 28 d (anaerobic). Essential soil microbial processes are only temporarily influenced, if at all.

754 thifensulfuron-methyl

Herbicide

HRAC B WSSA 2; sulfonyleurea



NOMENCLATURE: thifensulfuron-methyl

Chemical Abstracts name methyl 3-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]amino]sulfonyl]-2-thiophenecarboxylate

CAS RN [79277–27–3] **Development codes** DPX- M6316

thifensulfuron

Common name thifensulfuron (BSI, ANSI, draft E-ISO); thiameturon* (WSSA former name)

IUPAC name 3-(4-methoxy-6-methyl-1,3,5-triazin-2-ylcarbamoylsulfamoyl)thiophen-2-carboxylic acid

Chemical Abstracts name 3-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]amino]sulfonyl]-2-thiophenecarboxylic acid

CAS RN [79277–67–1]

PHYSICAL CHEMISTRY: thifensulfuron-methyl

Mol. wt. 387.4 **M.f.** $C_{12}H_{13}N_5O_6S_2$ **Form** Colourless, odourless crystals. **M.p.** 176°C

V.p. 1.7×10^{-5} mPa (25°C, Knudsen method) K_{ow} $\log P = 0.20$ (pH 5), 0.02 (pH 7)

Henry 4.4×10^{-10} Pa m^3 mol^{-1} **S.g./density** 1.49 **Solubility** In water 230 (pH 5), 6270 (pH 7) (both in mg/l, 25°C). In hexane <0.1 , xylene 0.2, ethanol 0.9, methanol, ethyl acetate 2.6.

thifensulfuron-methyl 899

that in grass weeds, which is enhanced by addition of the safener mefenpyr-diethyl (6.7 g/ha).
post-emergence control of grass and broad-leaved weeds in winter, spring and durum wheat,
triticale and rye, applied at 10 g/ha, in mixture with the safener mefenpyr-diethyl (6.7 g/ha).
Formulation types WG; Oil formulation.

MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats 2678 mg/kg. Skin and percutaneous LD₅₀ for rats >2000 mg/kg. Non-irritating to skin and eyes (rabbits); not a skin sensitiser (guinea pigs). Other Non-mutagenic *in vitro* and *in vivo*.

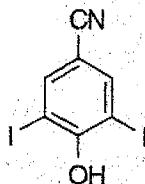
ECOTOXICOLOGY: Fish LC₅₀ for fish 100 mg/l. Algae EC₅₀ for green algae 0.02 mg/l. Other aquatic spp. EC₅₀ for *Lemna gibba* 0.8 µg/l.

ENVIRONMENTAL FATE: Soil/Environment Photodegradation DT₅₀ c. 50 d. Abiotic hydrolysis DT₅₀ 31 d (pH 5), >365 d (pH 7), 362 d (pH 9) (20°C). Soil DT₅₀ 1–5 d (7–10 d with low soil moisture); degradation is mainly microbial. Iodosulfuron-methyl and its metabolites have almost no vertical movement in soil; lysimeter and computer simulation studies indicate that neither iodosulfuron-methyl nor its metabolites would be transported to soil layers deeper than 1 m.

455 ioxynil

Herbicide

HRAC C₃, also M WSSA 6; hydroxybenzonitrile



NOMENCLATURE: ioxynil

Common name ioxynil (BSI, E-ISO, (m) F-ISO, WSSA)

IUPAC name 4-hydroxy-3,5-di-iodobenzonitrile

Chemical Abstracts name 4-hydroxy-3,5-diiodobenzonitrile

CAS RN [1689-83-4] EEC no. 216-881-1 Development codes ACP 63-303 (Amchem); M&B 8873 (May & Baker)

→ ioxynil octanoate

Common name ioxynil octanoate (BSI, E-ISO, (m) F-ISO, WSSA); ioxynil (JMAF)

IUPAC name 4-cyano-2,6-di-iodophenyl octanoate

Chemical Abstracts name 4-cyano-2,6-diiodophenyl octanoate

CAS RN [3861-47-0] EEC no. 223-375-4 Development codes 15830.RP; M&B 11 641

ioxynil-sodium

CAS RN [2961-62-8]

PHYSICAL CHEMISTRY: ioxynil

Composition Tech. grade is c. 95% pure. Mol. wt. 370.9 M.f. C₇H₃I₂NO Form Colourless solid; (tech., cream-coloured, with faint phenolic odour). M.p. 212–213°C (sublimes at c. 140°C/0.1 mm

Hg <1 mPa (20 °) K_{ow} logP = 0.89. (u.v. absorption max. 265 nm, ε 10⁴ l./mol. cm). Solubility: water 0.01 g/l (20°C), methanol 20, cyclohexanone 140, acetone 10, carbon tetrachloride <1 (all in g/l, 20°C). In acetone 60, 20% aqueous acetone 770 (all in g/l, 20–25°C). Stability: stable to u.v. light. Acidic in reaction, decomposed by u.v. light.

Octanoate
M.p. 59°C. Solubility: water 0.01 g/l (20–25°C). In acetone 100, dichloromethane 700, ethanol 150 (all in g/l, 20°C). Stability: stable to u.v. light.

Sodium
M.p. c. 392.9°C. Solubility: water 120, 20% m/V aqueous acetone 67 (all in g/l).

COMMERCIALISATION: History Herbicide. L. Wain (Nature (London), 1963, 200, 28). D. Hart et al. (Proc. Br. Weed Control Conf., 1966). Heywood (Chem. Ind. (London), 1966, 1967, 1968). Products Inc. (both now Aventis CropScience). US 3397054 to Union Carbide. Manufacture

APPLICATIONS: Biochemistry Photosynthesis: ioxynil inhibits the photosynthetic electron acceptor site; also uncouples oxidative phosphorylation with some systemic activity. Absorbed by roots and leaves. Its salts and esters are used for post-emergence control of weeds, especially young seedlings of the P. species. Iodosulfuron-methyl, flax, sugar beet, onions, leeks, garlic, shallots. Used in combination with other herbicides. Formulation types EC; SL. Compatibility: ioxynil is compatible with formulations of 2,4-D. Selected trade names: (Makhteshim-Agan); 'Sanoxynil' (octanoate) (Agriphar).

ANALYSIS: ioxynil

Product analysis by rp hplc with u.v. detection. Estimation of iodine (H. S. Segal & M. Food Addit., 1967, 5, 423; Anal. Methods). Residues determined by glc of derivative alkylation (E. G. Cotterill, Analyst, 1982).

ioxynil octanoate

Product determined by gc (GIPAC Handb.

MAMMALIAN TOXICOLOGY: ioxynil
Oral Acute oral LD₅₀ for rats 110, mice rats >2000 mg a.i./kg. Inhalation LC₅₀ for bacterial systems. Toxicity class WHC R21

enpyr-diethyl (q.v.) **Uses** For
pring and durum wheat,
npyr-diethyl (q.v.).

mg/kg. **Skin and eye** Acute
eyes (rabbits); not a skin

green algae 0.02 mg/l.

50 c. 50 d. Abiotic hydrolysis
-5 d (7-10 d with low soil
its metabolites have almost no
; indicate that neither
il layers deeper than 1 m.

Herbicide

lg) V.p. <1 mPa (20 °) $K_{ow} \log P = 0.89$ (unstated pH); 3.43 (25 °C, unionised,
Chamberlain et al., *Pestic. Sci.*, **47**, 265 (1996)) **Solubility** In water 50 mg/l (20 °C). In acetone
0, ethanol, methanol 20, cyclohexanone 140, tetrahydrofuran 340, dimethylformamide 740,
chloroform 10, carbon tetrachloride <1 (all in g/l, 25 °C). Potassium salt: In water 107 g/l
20-25 °C). In acetone 60, 20% aqueous acetone 560, tetrahydrofurfuryl alcohol 750, methyl
cellosolve 770 (all in g/l, 20-25 °C). **Stability** Stable in storage, but readily hydrolysed by alkali.
Decomposed by u.v. light. Acidic in reaction, and forms salts. **pKa** 3.96

ioxynil octanoate

Mol. wt. 497.1 M.f. $C_{15}H_{17}NO_2$ M.p. 59-60 °C V.p. 3.7 mPa (105 °C) **Solubility** Practically
insoluble in water (20-25 °C). In acetone 100, benzene, chloroform 650, cyclohexanone, xylene
500, dichloromethane 700, ethanol 150 (all in g/l). **Stability** Stable to storage, but readily
hydrolysed by alkali.

ioxynil-sodium

Mol. wt. 392.9 M.f. $C_7H_{12}NNaO$ M.p. c. 360 °C **Solubility** In water 140 g a.e./l (20-25 °C). In
acetone 120, 20% m/v aqueous acetone 670, 2-methoxyethanol 640, tetrahydrofurfuryl alcohol
650 (all in g/l).

COMMERCIALISATION: **History** Herbicidal properties of ioxynil reported independently by
R. L. Vain (*Nature (London)*, 1963, **200**, 28), by K. Carpenter & B. J. Heywood (*ibid.*, p. 28) and by
R. D. Hart et al. (*Proc. Br. Weed Control Conf.*, 7th, 1964, p. 3). Development reviewed by
B. J. Heywood (*Chem. Ind. (London)*, 1966, p. 1946). Introduced by May & Baker Ltd and by Amchem
Products Inc. (both now Aventis CropScience). **Patents** GB 1067033 to May & Baker;
US 3397054 to Union Carbide **Manufacturers** Aventis; CFPI Nufarm; Makhteshim-Agan; Sanachem.

APPLICATIONS: **Biochemistry** Photosynthetic electron transport inhibitor at the photosystem II
receptor site; also uncouples oxidative phosphorylation. **Mode of action** Selective contact herbicide
with some systemic activity. Absorbed by the foliage, with limited translocation. **Uses** Ioxynil and
its salts and esters are used for post-emergence control of a wide range of annual broad-leaved
weeds, especially young seedlings of the Polygonaceae, Compositae, and Boraginaceae, in cereals,
moss, leeks, garlic, shallots, flax, sugar cane, forage grasses, lawns, and newly-sown turf. Often
used in combination with other herbicides, in order to extend the spectrum of control.

Formulation types EC; SL. **Compatibility** Incompatible with liquid fertilisers and water-soluble
formulations of 2,4-D. **Selected tradenames** 'Actril' (Aventis); 'Totril' (Aventis); 'Iotril'
(Makhteshim-Agan); 'Sanoxynil' (octanoate) (Sanachem); mixtures 'Trionyl' (+ bromoxynil)
(Agropha).

ANALYSIS: ioxynil

Product analysis by rp hplc with u.v. detection (*CIPAC Handbook*, 1992, E, 101-4), or by titration or
estimation of iodine (H. S. Segal & M. L. Sutherland, *Anal. Methods Pestic., Plant Growth Regul.*
Ann. Rept., 1967, **5**, 423; *Anal. Methods Pestic. Plant Growth Regul.*, 1972, **6**, 654).

Residues determined by glc of derivatives (*loc. cit.*), by i.r. spectrometry as ioxynil, or by hplc after
derivatization (E. G. Cotterill, *Analyst*, 1982, **107**, 76).

ioxynil octanoate

Residues determined by gc (*CIPAC Handbook*, 1995, G, 94-97).

ITALIAN TOXICOLOGY: ioxynil

Acute oral LD₅₀ for rats 110, mice 230 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for
rats 2000 mg a.i./kg. **Inhalation** LC₅₀ (6 h) for rats >3 mg/l air. **Other** Non-mutagenic in
bacterial systems. **Toxicity class** WHO (a.i.) II; EPA (formulation) II **EC hazard** R63| T; R25| Xn;

ioxynil 549

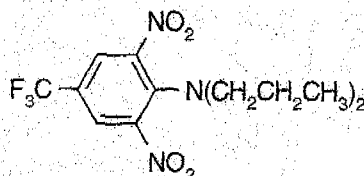
Main Entries

ENVIRONMENTAL FATE: **Animals** Trifluralin labelled in the 2-chlorobenzoyl moiety was metabolised in rats by hydrolytic cleavage, forming metabolites which contained only the phenyl ring and were partly hydroxylated and conjugated. Correspondingly, in experiments with labelling in the 4-trifluoromethoxyphenyl group, metabolites were found which contained the 4-trifluoromethoxyphenyl ring, partly in hydroxylated form. **Plants** Following spray application to apples, soya beans and potatoes, trifluralin is only slightly metabolised; metabolites were similar to those formed in animals. For residue analyses, it is sufficient to determine the parent compound in the harvested crops. **Soil/Environment Degradation:** In laboratory tests, trifluralin was moderately quickly degraded in the soil; degradation in the field was more rapid by a factor of 2. Repeated applications over 3 years to soil without vegetation did not result in any accumulation in the soil. In practice-relevant applications in forests, the concentrations of residues found in the soil were very low at all times, and declined below the limit of detection after a few months. **Metabolism:** In soil, 50% of applied trifluralin labelled in the 2-chlorobenzoyl moiety was degraded to CO₂ within 112 days and c. 20% of the radioactivity was bound to the soil. When using trifluralin labelled in the 4-trifluoromethoxyphenyl moiety, the compound was mineralised more slowly, while the percentage of bound residues was markedly increased. Metabolism was mainly induced by microbes, and resulted in metabolites which contained just one of the two rings in each case.

791 trifluralin

Herbicide

HRAC K₁ WSSA 3; dinitroaniline



NOMENCLATURE: Common name trifluralin (BSI, E-ISO, ANSI, WSSA, JMAF); trifluraline ((f) F-ISO)

IUPAC name α,α,α -trifluoro-2,6-dinitro-*N,N*-dipropyl-*p*-toluidine

Chemical Abstracts name 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)benzenamine

CAS RN [1582-09-8] EEC no. 216-428-8 Development codes L-36 352 (DowElanco); EL-152

PHYSICAL CHEMISTRY: Mol. wt. 335.3 M.f. C₁₃H₁₆F₃N₃O₄ Form Yellow-orange crystals. M.p. 48.5–49°C; (tech., 43–47.5°C) B.p. 96–97°C/24 Pa V.p. 6.1 mPa (25°C) (EEC A4) K_{ow} logP = 4.83 (20°C) (EEC A8) Henry 15 Pa m³ mol⁻¹ (calc.) S.g./density 1.36 (22°C) (EEC A3) Solubility In water 0.184 (pH 5), 0.221 (pH 7), 0.189 (pH 9) (all in mg/l) (EEC A6); tech. 0.343 (pH 5), 0.395 (pH 7), 0.383 (pH 9) (all in mg/l) (EEC A6). In acetone, chloroform, acetonitrile, toluene, ethyl acetate >1000, methanol 33–40, hexane 50–67 (all in g/l, 25°C). Stability Stable at 52°C (highest storage temperature tested). Stable to hydrolysis at pH values of 3, 6 and 9 (52°C). Decomposed by u.v. irradiation (E. Leitis & D. G. Crosby, *J. Agric. Food Chem.*, 1974, 22, 842). F.p. 151°C (closed cup); tech. 153°C (open cup) (both Pensky-Martens)

COMMERCIALISATION: History Herbicide reported by E. F. Alder *et al.* (*Proc. North Cent. Weed Control Conf.*, 1960, p. 23). Introduced in USA (1961) by Eli Lilly & Co. (agrochemical interests now Dow AgroSciences). Patents US 3257190 Manufacturers Budapest Chemical; Defensa; Dintec; Makhteshim-Agan; Nortox; Nufarm Ltd; Oxon; Q.E.A.C.A.; Westrade.

942 trifluralin

APPLICATIONS: Biochemistry Microtubule inhibitor which acts by entering the seedling meristem. Uses Pre-emergence control of weeds in beans, peas, carrots, parsnips, lettuce, strawberries, raspberries, citrus fruit, ornamentals, cotton, sugar beet, etc. Trifluralin for control of annual grasses and weeds pre-planting with soil incorporation, or possible for some crops. Formulation (Defensa); 'Eflurin' (Eftymiadis); 'Iperis' (Defensa); 'Sinfluran' (Westrade); 'Makhteshim-Agan'; 'Trifsan' (S. Zene); 'Tristar' (PBI); 'Zeltoxone' (Zene); 'Zeltone' (+ clomazone) (FMC)

ANALYSIS: Product analysis by glc with FID (15, 173-14) or by u.v. spectrometry (ibid. 15, 173-14) or by u.v. spectrometry (ibid. 15, 173-14). J. E. Scroggs, *Anal. Methods for Pestic. Plant Growth Regul.*, 1972, 1, 173-174. Details from Dow AgroScience

MAMMALIAN TOXICOLOGY: IARC reprotoxic. Skin and eye Acute percutaneous slightly irritating to eyes (rabbits). In acute trials in rats, the only effect at the oral LD₅₀ has been shown to be reversible. This has been shown to be reversible. NOEL in mice was 73 mg/kg daily. Toxicity class WHO (a) Hazardous Material containing <0.5 ppm

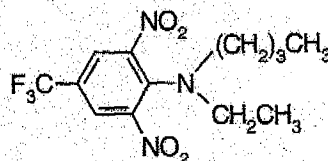
ECOTOXICOLOGY: Birds Acute oral LD₅₀ bobwhite quail and mallard ducks >5000 mg/kg, young bluegill sunfish 0.089 mg/l. 1051 mg/l. Algae EC₅₀ (7 d) for *Selenastrum* spp. LD₅₀ (96 h) for grasshopper >100 µg/bee. Worms LC₅₀ (>1000 mg/kg).

ENVIRONMENTAL FATE: Animals De C. Anderson, *Toxicol. Appl. Pharmacol.* 1988, 95, 1-10. Eliminated in the urine and 15% in the feces. Soil/Environment Absorbed by the soil, movement in the soil. Metabolism involves conversion to an amino group, partial oxidation, subsequent degradation to smaller fragments. DT₅₀ 57–126 d. Duration of residual activity was more rapid under anaerobic conditions (aerobic) 116–201 d. Soil photolysis DT₅₀ ranges from 3.75 (0.01% a.m., pH 6) to 44 (1995).

61 benfluralin

Herbicide

HRAC K₁ WSSA 3; dinitroaniline



NOMENCLATURE: Common name benfluralin (BSI, E-ISO); benfluraline ((f) F-ISO); benefin (WSSA); bethrodine (JMAF)
IUPAC name *N*-butyl-*N*-ethyl- α,α,α -trifluoro-2,6-dinitro-*p*-toluidine
Chemical Abstracts name *N*-butyl-*N*-ethyl-2,6-dinitro-4-(trifluoromethyl)benzenamine
CAS RN [1861-40-1] **EEC no.** 217-465-2 **Development codes** EL-110

PHYSICAL CHEMISTRY: Mol. wt. 335.3 M.f. C₁₃H₁₆F₃N₃O₄ Form Yellow-orange crystals.
 M.p. 65–66.5°C B.p. 121–122°C/0.5 mmHg; 148–149°C/7 mmHg V.p. 8.76 mPa (25°C)
 K_{ow} logP = 5.29 (20°C, pH 7) Henry 29.4 Pa m³ mol⁻¹ (25°C, calc.) S.g./density 1.28 (20°C) (tech.)
Solubility In water 0.1 mg/l (25°C). In acetone, ethyl acetate, dichloromethane, chloroform >1000; toluene 330–500, acetonitrile 170–200, hexane 18–20, methanol 17–18 (all in g/l, 25°C).
Stability Decomposed by u.v. light. Stable for up to 30 days at pH 5–9 (26°C). F.p. 151°C (Setafish closed cup; ASTM D-3278)

COMMERCIALISATION: **History** Herbicide reported by J. F. Schwer (*Proc. North Cent. Weed Control Conf.*, 1965). Introduced in USA (1963) by Eli Lilly & Co (agrochemical interests now Dow AgroSciences). **Patents** US 3257190 **Manufacturers** Budapest Chemical; Dintec; Makhteshim-Agan.

APPLICATIONS: **Biochemistry** Microtubule assembly inhibition. **Mode of action** Selective soil herbicide, absorbed by the roots. Affects seed germination and prevents weed growth by inhibition of root and shoot development. **Uses** Control of annual grasses and some annual broad-leaved weeds in peanuts, lettuce, cucumbers, chicory, endive, field beans, french beans, lentils, alfalfa, clovers, trefoil, tobacco and established turf. Applied pre-emergence with soil incorporation, at 1.0–1.5 kg a.i./ha. **Formulation types** EC; GR; WG. **Selected tradenames** 'Balan' (Dow AgroSciences); 'Plante'; 'Benefex' (Makhteshim-Agan); **mixtures** 'Team' (+ trifluralin) (Dow AgroSciences); 'XL-2G' (+ oryzalin) (Dow AgroSciences)

ANALYSIS: Product analysis by u.v. spectrometry (AOAC Methods, 1995, 973.13) or by glc with FID (ibid., 973.14; CIPAC Handbook, 1983, 1B, 1726). **Residues** by glc with ECD (W. S. Johnson & R. Frank, *Anal. Methods Pestic. Plant Growth Regul.*, 1976, 8, 335). Details available from Dow AgroSciences.

MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats >10000, mice >5000, dogs and rabbits >2000 mg/kg. Skin and eye Acute percutaneous LD₅₀ for rabbits >5000 mg/kg. Moderately irritating to skin and eyes (rabbits). **Inhalation** LC₅₀ (4 h) >2.16 mg/l air. NOEL (2 y) for rats 0.5 mg/kg b.w. daily, for mice 6.5 mg/kg b.w. daily. **ADI** 0.005 mg/kg. **Toxicity class** WHO (a.i.) III (Table 5); EPA (formulation) II

ECOTOXICOLOGY: Birds Acute oral LD₅₀ for mallard ducks, bobwhite quail, and chickens >2000 mg/kg. Fish LC₅₀ for bluegill sunfish 0.065, rainbow trout 0.081, sheepshead minnow

benfluralin 69

Main Entries

being 2,3-isopropyl=
 pKa 8.8, v. weak acid

oc. Br. Insectic. Fungic.
 produced by Fisons Ltd.,
 rop protection and by
 ie, now marketed for
 ventis; Kuo Ching.

Systemic insecticide with
 l activity. **Uses** Active
 , Blattodea, Culicidae,
 odour and lack of
 onrol of a broad
 ular formulations for the
 a linearis, *Oscinella frit*,
 crops to control
 i as directed. Not to be
 patibility Incompatible with
 ntis); 'Garvox' (crop
 in use) (Aventis)

AC Methods, 1995, 986.09).

2. of the Bibliography).
 35 mg/kg.
 ritating to skin and eyes.
 rats 10 mg/kg diet. In 90 d
 versible inhibition of
 NO (a.i.) II;

obwhite quail 19, domestic
 sunfish 1.65, rainbow trout
 Toxic to bees. Oral LD₅₀ for

amate insecticides in general).
 owing oral administration or
 inated almost completely
 ipal metabolite 2,2-dimethyl-
 1. **Soil/Environment** Bendiocarb
 and heterocyclic rings, followed by
 ble mineralisation of the phenyl
 nt, with slower breakdown
 liocarb in agricultural soils and
 pe, nature and temperature
 dimethyl-1,3-benzodioxol-4-ol
 3–40); however, because it is

ivity derives from metabolic conversion to systemic insecticide and acaricide with Aleoerodidae, Aphididae, and nematodes (*Meloidogyne* spp.) in beans, broad beans, celery, maize, lowers, sugar cane, alfalfa, cotton, -3.5 lb/a. **Phytotoxicity** Phytotoxic to beans, maize, and tomatoes if granules.

Preparation types GR. **Water-containing preparations** (a); 'Dhan' (Dhanuka); 'Kurunai' (n)

Handbook, 1983, 1B, 1890; AOAC Methods determined by glc (*Pestic. Anal. Man. al.*, 1987, 1, 3, 6, S8, S13, S16, S17, S19 (London), 1980, 105, 515; A. Ambrus et al. from BASF.

9 (see part 2 of the Bibliography); c. 6 mg/kg. **Skin and eye** Acute pigs 20-30, male rabbits 5.6, female rier, test method and animal species; male rabbits 93-245 mg a.i. (as ts 0.011 mg/l). **NOEL** In 90 d feeding than depression of cholinesterase; mutagenic, not teratogenic, not (n) I **EC hazard** T+; R27/28

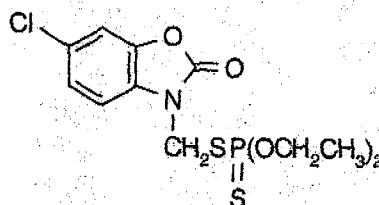
cks 0.62, ring-necked pheasants; el catfish 0.28 mg/l. **Bees** Toxic to

il review of organophosphorus oxidised to the sulfoxide and sulfone, and dithio-, thio-, and orthophosphoric /Environment In soil, metabolic rothioate analogues, and these then ertain conditions (D. L. Suett, *Pestic. Sci.*

613 phosalone

Insecticide, acaricide

organophosphorus



NOMENCLATURE: Common name phosalone (BSI, E-ISO, (f) F-ISO, ANSI, ESA, JMAF); benzofos* (former exception, USSR)

CIPAC name S-6-chloro-2,3-dihydro-2-oxobenzoxazol-3-ylmethyl O,O-diethyl phosphorodithioate **Chemical Abstracts name** S-[(6-chloro-2-oxo-3(2H)-benzoxazolyl)methyl] O,O-diethyl phosphorodithioate

Other names benzphos **CAS RN** [2310-17-0] **EEC no.** 218-996-2

Development codes 11 974 RP; NPH 1090 **Official codes** ENT 27 163

PHYSICAL CHEMISTRY: Mol. wt. 367.8 M.f. $C_{12}H_{15}ClNO_4PS_2$ Form Colourless crystals, with odour of garlic. M.p. 42-48°C (tech.) V.p. <0.06 mPa (25°C) K_{ow} logP = 4.01 (20°C) $\text{Henry} / 4 \times 10^{-3} \text{ Pa m}^3 \text{ mol}^{-1}$ (calc.) S.g./density 1.338 g/ml (20°C) Solubility In water 105 mg/l (25°C). In ethyl acetate, acetone, acetonitrile, benzene, chloroform, dichloromethane, toluene, methyl ethyl ketone, toluene, xylene c. 1000, hexane 11 (all in g/l, 20°C). Stability Hydrolysed by strong alkalis and acids; DT₅₀ 9 d (pH 9).

COMMERCIALISATION: History Insecticide reported by J. Desmoras et al. (*Phytiatr. Phytopharm.*, 1963, 12, 199). Introduced by Rhône-Poulenc Agrochimie (now Aventis CropScience). **Patents** GB 1005372; BE 609209; FR 1482025 **Manufacturers** Aventis; Jiangsu.

APPLICATIONS: Biochemistry Cholinesterase inhibitor. Mode of action Non-systemic insecticide and acaricide showing localised penetration of plant cuticle; with contact and stomach action.

Use A non-systemic acaricide and insecticide used primarily in pome and stone fruit trees. Effective against Coleoptera, Homoptera (Aphididae), Lepidoptera (*Cydia pomonella*) and Thysanoptera on fruit trees. It is selective of most beneficial insects and widely used in integrated pest management programmes. Also used in grapes, oilseed rape, ornamentals, potatoes and vegetables.

Toxicity Non-phytotoxic when used at the recommended application rates. At higher application rates Golden Delicious and other yellow apple varieties have been injured.

Formulation types EC; SC; WP. **Selected tradenames** 'Zolone' (Aventis)

ANALYSIS: Product analysis by glc or hplc (*CIPAC Handbook*, 1988, D, 141). Residues determined by (A. Ambrus et al., *J. Assoc. Off. Anal. Chem.*, 1981, 64, 733; *Man. Pestic. Residue Anal.*, 1987, 1, 3, 6, S8, S19; *Anal. Methods Residues Pestic.*, 1988, Part I, M2, M5, M12).

TOXICOLOGY: Reviews FAO/WHO 80, 82 (see part 2 of the Bibliography).

Acute oral LD₅₀ for rats 120 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats 120 mg/kg. Inhalation LC₅₀ (4 h) for female rats 0.7 mg/l. **NOEL** (2 y) for rats 2.5 mg/kg b.w. (a.i.) 0.02 mg/kg b.w. [1997]. **Toxicity class** WHO (a.i.) II **EC hazard** T; R25| Xn; R21| N; R33

TOXICOLOGY: Birds Acute oral LD₅₀ for mallard ducks >2150 mg/kg. Dietary LC₅₀ (8 d) for white quail 2033, mallard ducks 1659 ppm diet. Fish LC₅₀ (96 h) for rainbow trout 0.63, mg/l. Daphnia EC₅₀ (48 h) 0.74 µg/l. **Algae** Low toxicity. **Worms** Moderately toxic.

phosalone 731

Main Entries

PHYSICAL CHEMISTRY: **Composition** A mixture of enantiomers of the (E)- isomer. Tech. is $\geq 95\%$. **Mol. wt.** 128.2 **M.f.** $C_8H_{16}O$ **Form** Clear liquid, with a characteristic odour. **B.p.** $90-92^\circ C/10$ mmHg **Solubility** Low miscibility with water. Miscible with *n*-heptane, benzene and methanol.

COMMERCIALISATION: **History** First reported by INRA group, France. Report of field use by A. C. Oehlschlager et al., *Naturwissen.*, **79**, 134 (1992). Introduced into Costa Rica in 1991. Report of field use to control *R. palmarum*, C. M. Chinchilla et al., "Management of Red Ring Disease". **Manufacturers** ChemTica.

APPLICATIONS: **Mode of action** Attracts both males and females when presented in combination with food, such as sugar cane or palm tissue. **Uses** For control of *Rhynchophorus palmarum*. Food is necessary in combination with the pheromone to attract the insects. The food is treated with a non-repellent insecticide such as carbofuran, to kill attracted weevils. **Formulation types** Plastic sachets from which the pheromone slowly evaporates. **Selected tradenames** 'Rhyncopherol' (ChemTica), 'Rhynkolure' (ChemTica).

524 methyl isothiocyanate

Nematicide, fungicide, insecticide, herbicide



NOMENCLATURE: **Common name** methyl isothiocyanate (BSI, E-ISO, JMAF, accepted in lieu of a common name); isothiocyanate de méthyle (F-ISO, accepted in lieu of a common name) **IUPAC name** methyl isothiocyanate

Chemical Abstracts name isothiocyanatomethane

Other names MIT; MITC **CAS RN** [556-61-6] **EEC no.** 209-132-5

PHYSICAL CHEMISTRY: **Composition** Tech. is $\geq 94.5\%$ pure. **Mol. wt.** 73.1 **M.f.** C_2H_3NS **Form** Colourless crystals, with a horseradish-like odour. **M.p.** $35-36^\circ C$; (tech., $25.3-27.6^\circ C$) **B.p.** $118-119^\circ C$ **V.p.** 2.13 kPa ($25^\circ C$) **K_{ow} logP** = 1.37 (calc.) **S.g./density** 1.069 ($37^\circ C$); (tech., 1.0537 ($40^\circ C$)) **Solubility** In water 8.2 g/l ($20^\circ C$). Readily soluble in common organic solvents, such as ethanol, methanol, acetone, cyclohexanone, dichloromethane, chloroform, carbon tetrachloride, benzene, xylene, petroleum ether, and mineral oils. **Stability** Unstable and reactive. Rapidly hydrolysed by alkalis, more slowly in acidic and neutral solutions, DT₅₀ 85 h (pH 5), 490 h (pH 7), 110 h (pH 9) ($25^\circ C$). Sensitive to oxygen and to light. Stable up to $200^\circ C$. **pKa** 12.3 **F.p.** $26.9^\circ C$

COMMERCIALISATION: **History** Nematicidal activity reported by E. A. Pieroh et al. (*Anz. Schaedlingsskd.*, 1959, **32**, 183). Introduced by Schering AG (now Aventis CropScience). **Patents** US 3113908 **Manufacturers** Aventis.

APPLICATIONS: **Uses** Multi-purpose soil fumigant for control of nematodes, soil fungi, soil insects, and weed seeds. **Phytotoxicity** Phytotoxic to all green plants. **Formulation types** EC. **Selected tradenames** 'Trapex' (Aventis)

ANALYSIS: **Product analysis** by glc or by hplc. **Residues** determined by glc with FPD (M. Ottstad et al., *Anal. Methods Pestic. Plant Growth Regul.*, 1978, **10**, 563). Details available from Aventis.

630 methyl isothiocyanate

159
ENVIRONMENTAL TOXICOLOGY: **Oral Acute** LD₅₀ for rats 1000 mg/kg. **Acute percutaneous** LD₅₀ for rabbits 1000 mg/kg. **Inhalation** LD₅₀ for rats 1000 mg/kg. **Inhalation** LD₅₀ for dogs 0.4 mg/kg b.w. daily; (1 y) for dogs 0.4 mg/kg b.w. daily. **EC hazard** T

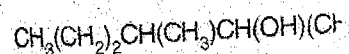
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for mallards 10936, pheasants >5000 mg/kg. **Fish** Acute oral LD₅₀ for rainbow trout 0.09, mirror carp 0.37-0.5 mg/kg. **Algae** EC₅₀ (96 h) 0.248 mg/l; NOEC (96 h) not directed.

ENVIRONMENTAL FATE: **Soil/Environment** Half-life of the substance occurs within 3 weeks at $0-6^\circ C$. At the lower temperature, the potential for groundwater degradation.

525 4-methylnonane 4-methylnonane

See also The BioPesticide Manual

pheromone



4-methylnonane-5-ol

These two substances constitute the pheromone of the *ferrugineus*.

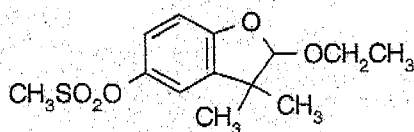
NOMENCLATURE: **IUPAC name** 4-methylnonane-5-ol. **Chemical Abstracts name** 4-methylnonane-5-ol. **Other names** ferrugineol. **CAS RN** 1000-90-0

PHYSICAL CHEMISTRY: **Composition** and both enantiomers of 4-methylnonane isomers, in the ratio 9:1. **M.f.** $C_{10}H_{22}O$ (nonanol); $C_{10}H_{20}O$ (nonanal). **B.p.** $87^\circ C/7$ mmHg (nonanol). **Odour** almost insoluble. Miscible with *n*-hexane. **Other properties** Viscosity 35 cP (20°C).

304 ethofumesate

Herbicide

HRAC N WSSA 8; benzofuran



NOMENCLATURE: Common name ethofumesate (BSI, E-ISO, (m) F-ISO, ANSI, WSSA)

IUPAC name (±)-2-ethoxy-2,3-dihydro-3,3-dimethylbenzofuran-5-yl methanesulfonate

Chemical Abstracts name (±)-2-ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate

CAS RN [26225-79-6] EEC no. 247-525-3 Development codes AE BO49913; NC 8438;

SN 49913; ZK 49913

PHYSICAL CHEMISTRY: Mol. wt. 286.3 M.f. $C_{13}H_{18}O_5S$ Form White, crystalline solid; (tech. is a light brown, crystalline solid; mild aromatic odour). M.p. 70–72°C; (tech., 69–71°C) V.p. 0.12 to 0.65 mPa (25°C) K_{ow} logP = 2.7 (pH 6.5–7.6, 25°C) Henry 3.7×10^{-3} to 6.8×10^{-3} Pa $m^3 mol^{-1}$ S.g./density 1.29 (20°C, tech.) Solubility In water 50 mg/l (25°C). In acetone, dichloromethane, dimethyl sulfoxide, ethyl acetate >600; toluene, p-xylene 300–600; methanol 120–150, ethanol 60–75, isopropanol 25–30, hexane 4.67 (all in g/l; 25°C). Stability Stable to hydrolysis in water at pH 7 and 9. At pH 5.0, DT₅₀ 940 d, forming the hydroxy analogue. Phototransformed in water, DT₅₀ 31 h. Degraded in air, DT₅₀ 4.1 h.

COMMERCIALISATION: History Herbicide reported by R. K. Pfeiffer (*Symp. New Herbic.*, 3rd, 1969, p. 1). Introduced by Fisons Ltd, Agrochemical Division (now Aventis CropScience) in 1974. Patents GB 1271659 Manufacturers Aventis; Feinchemie Schwebda; Griffin; Punjab; United Phosphorus.

APPLICATIONS: Biochemistry Inhibits lipid synthesis (not ACCase inhibition).

Mode of action Selective systemic herbicide, absorbed by the emerging shoots (grasses) and roots (broad-leaved plants), with translocation to the foliage. Not readily absorbed by leaves after the plant has generated a mature cuticle. Inhibits the growth of meristems, retards cellular division, and limits formation of waxy cuticle. **Uses** Used pre- and/or post-emergence in sugar and other beet crops, turf, ryegrass and the other pasture grasses, at 0.3–2.0 kg a.i./ha. It is effective in controlling a wide range of important grasses and broad-leaved weeds, with a good persistence of activity in the soil. In beet crops, 1.0–2.0 kg/ha can be used, but ethofumesate is normally recommended at 0.2–2.0 kg/ha in tank-mixtures or co-formulations with other residual or contact herbicides for use in beet. A high degree of tolerance is also shown by strawberries, sunflowers, Phaseolus beans and tobacco, depending on the time of application. **Phytotoxicity** Onions, peas, beans, carrots, and cotton are tolerant to some extent. **Formulation types** EC; SC. **Selected tradenames** 'Betanal Progress' (Aventis); 'Betanal Tandem' (Aventis); 'Nortron' (Aventis); 'Prograss' (Aventis); 'Tramat' (Aventis); 'Ethosat' (Feinchemie Schwebda); 'Ethosin' (Agriphar); 'Keeper' (Barclay); 'Kubist' (Griffin); 'Primasan' (Mirfield).

ANALYSIS: Product and residue analysis by glc with FPD (R. J. Whiteoak et al., *Anal. Methods Pestic. Plant Growth Regul.*, 1978, 10, 353). Details available from Aventis.

MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats and mice >5000 mg/kg.

Skin and eye Acute percutaneous LD₅₀ for rats >2000 mg/kg. Not a skin or eye irritant. Not a skin sensitiser. Inhalation LC₅₀ (4 h) for rats >3.97 mg/l air. NOEL (2 y) for rats >1000 mg/kg diet

364 ethofumesate

(37.6 mg/kg b.w. daily). ADI 0.4 mg/kg (formulation) IV

ECOTOXICOLOGY: Birds Acute LD₅₀ >8743 mg/kg. Dietary LC₅₀ (8 d) for fish LC₅₀ (96 h) for rainbow trout 1 mg/l. Daphnia EC₅₀ (48 h) 13.52–22.0 mg/l (96 h) for *Grossostrea virginica* (Eastern oyster) 5.4 mg/l. Bees LC₅₀ (contact) >2000 g/ha.

ENVIRONMENTAL FATE: Animals Acute LD₅₀ >8743 mg/kg. Dietary LC₅₀ (8 d) for fish LC₅₀ (96 h) for rainbow trout 1 mg/l. Daphnia EC₅₀ (48 h) 13.52–22.0 mg/l (96 h) for *Grossostrea virginica* (Eastern oyster) 5.4 mg/l. Bees LC₅₀ (contact) >2000 g/ha. **Plants** 2-oxo derivatives, methanesulfonic acid degraded in soil to transient degradation products, mineralised to CO₂. Photodegradation (field). It has been demonstrated uptake by soil and that uptake by succeeding crops (mean K_{oc} 203), but field lysimeter studies being located in the top 30 cm. It de

305 ethoprop

organophosphorus

NOMENCLATURE: Common name ethoprop (Society of Nematologists (USA))

IUPAC name O-ethyl S,S-dipropyl phosphorothioate

Chemical Abstracts name O-ethyl S,S-dipropyl phosphorothioate

CAS RN [13194-48-4] EEC no. 23 Co.)

PHYSICAL CHEMISTRY: Mol. wt. 266. B.p. 86–91°C/0.2 mmHg V.p. 46.5 S.g./density 1.094 (20°C) Solubility 1,2-dichloroethane, diethyl ether, ethyl acetate. Stability Very stable in neutral and weakly acidic water up to 100°C at pH 7. F.p.

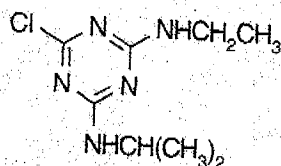
COMMERCIALISATION: History Introduced by Rhône-Poulenc Agrochimie (US 3268393 to Mobil Manufacturer

ENVIRONMENTAL FATE: **Animals** In rats, following oral administration, 85–96% of the dose is eliminated, predominantly in the urine, within 3 days. **Soil/Environment** Has a short persistence in soil, DT₅₀ c. 6–14 d. Soil metabolism is by loss of amino group, cleavage of carbamate group, or acetylation of amino group.

39 atrazine

HRAC C₁ WSSA 5; 1,3,5-triazine

Herbicide



NOMENCLATURE: Common name atrazine (BSI, E-ISO, (f) F-ISO, ANSI, WSSA, JMAF)
IUPAC name 6-chloro-N²-ethyl-N⁴-isopropyl-1,3,5-triazine-2,4-diamine
Chemical Abstracts name 6-chloro-N-ethyl-N⁴-(1-methylethyl)-1,3,5-triazine-2,4-diamine
CAS RN [1912-24-9] EEC no. 217-617-8 Development codes G 30 027

PHYSICAL CHEMISTRY: Composition Tech. is ≥96% pure. Mol. wt. 215.7 M.f. C₈H₁₄ClN₅
Form Colourless powder. M.p. 175.8°C B.p. 205.0°C/101 kPa V.p. 3.85 × 10⁻² mPa (25°C)
(OECD 104) K_{ow} logP = 2.5 (25°C) Henry 1.5 × 10⁻⁴ Pa m³ mol⁻¹ (calc.)
S.g./density 1.23 (22°C) Solubility In water 33 mg/l (pH 7, 22°C). In ethyl acetate 24, acetone 31, dichloromethane 28, ethanol 15, toluene 4.0, n-hexane 0.11, n-octanol 8.7 (all in g/l, 25°C).
Stability Relatively stable in neutral, weakly acidic and weakly alkaline media. Rapidly hydrolysed to the hydroxy derivative in strong acids and alkalis, and at 70°C in neutral media; DT₅₀ (pH 1) 9.5, (pH 5) 86, (pH 13) 5.0 d. pK_a 1.7, v. weak base

COMMERCIALISATION: History Herbicide reported by H. Gysin & E. Knüsli (Proc. Int. Congr. Crop Prot., 4th, Hamburg, 1957). Introduced by J. R. Geigy S.A. (now Novartis Crop Protection AG).
Patents BE 540590; GB 814947 Manufacturers Crystal; Du Pont; Makhteshim-Agan; Meghmani; Nagarjuna Agrichem; Novartis; Oxon; Rallis; Sanachem.

APPLICATIONS: Biochemistry Photosynthetic electron transport inhibitor at the photosystem II receptor site. Maize tolerance is attributed to rapid detoxification by glutathione transferases.
Mode of action Selective systemic herbicide, absorbed principally through the roots, but also through the foliage, with translocation acropetally in the xylem and accumulation in the apical meristems and leaves. Uses Pre- and post-emergence control of annual broad-leaved weeds and annual grasses in maize, sorghum, sugar cane, pineapples, chemical fallow, grassland, macadamia nuts, conifers, industrial weed control. In Europe, use is concentrated in maize and sorghum. Used also in combinations with many other herbicides. Phytotoxicity Phytotoxic to many crops, including most vegetables, potatoes, soya beans, and peanuts. Formulation types FW; GR; SC; WG; WP.
Selected tradenames 'AAtrex' (USA) (Novartis); 'Aktikon' (Nitrokémia); 'Atranex' (Makhteshim-Agan); 'Atrataf' (Rallis); 'Atratlone' (Agriphar); 'Atrazina' (Cequisa); 'Atrazol' (Sipcam); 'Coyote' (Defensa); 'Dhanuzine' (Dhanuka); 'Fogard' (Caffaro); 'Mebazine' (Aventis); 'Sanazine' (Sanachem); 'Surya' (Nagarjuna Agrichem); 'Triaflow' (Inquiport); 'Vectal' (Aventis); 'Zeazin S 40' (Istrochem);

mixtures 'Bicep II Magnum' + metolachlor) (Novartis); (dicamba as potassium salt)

ANALYSIS: Product analysis (CP/61); AOAC Methods, 15 (K. Ramsteiner et al., J. Ass. Growth Regul., 1972, 6, 600) go with FID (AOAC Methods detection (AOAC Methods, 15)

MAMMALIAN TOXICOLOGY: 1869–3090 mg tech./kg. m >3100 mg/kg. Mild skin irritation in humans. Inhalation LC₅₀ (0.5 mg/kg daily), for dogs daily). ADI 0.005 mg/kg b.w. (Table 5); EPA (formulation)

ECOTOXICOLOGY: Birds >2000 mg/kg for mallard & Japanese quail (chicks) >50 bluegill sunfish 16, carp 76. Algae EC₅₀ (72 h) for Scenedesmus 0.13 mg/l. Bees LD₅₀ (oral) foetida 78 mg/kg soil.

ENVIRONMENTAL FATE: and completely metabolise al., Toxicol. Lett., 1988, 44, Food Chem., 1990, 38, 141. Diaminochlorotriazine is transformed. More than 50% of the dose in tolerant plants, at conjugates, with further degradation. hydrolysis of the resulting plants, unaltered atrazine & metabolites under all conditions (median 41 d), the longer DT₅₀ 10–105 d (mean 55 system (M.J. Wood et al., Monograph 1991, 47, 175 values similar to those of

the leaves and roots and
l by the development of
as Post-emergence control of a
:at, durum wheat, barley, rye,
ation types WG.

as in crops, soil and water
95, 2, 707). Details available

nice ≥5000 mg/kg.
ation LC₅₀ (4 h) for rats
b.w. daily). ADI 0.2 mg/kg

ail >2000 mg/kg.
36 mg/l. **Algae** E_bC₅₀ (72 h)
g/bee. **Worms** LC₅₀ (14 d)

the rat is O-demethylation.
3–29 d. Degradation is
in the soil.

COMMERCIALISATION: **Production** Produced by a *Streptomyces* spp. and subsequently purified. **History** The hydrochloride salt introduced in 1997 by Abbott Laboratories (now Valent BioSciences Corporation). **Manufacturers** Abbott.

APPLICATIONS: *aminoethoxyvinylglycine hydrochloride*
Biochemistry Inhibits the production of endogenous ethylene in plant tissues by competitively inhibiting 1-aminocyclopropane-1-carboxylic acid synthase (ACC Synthase), an enzyme of the ethylene biosynthesis pathway. **Uses** Plant growth regulator for use in apple trees. Possible benefits achieved are dependent on the cultivar, orchard conditions, and grower objectives, and include: reduction in fruit drop, delay of fruit maturity, delayed or extended harvest, improved harvest management, maintenance of fruit quality (e.g. fruit firmness), natural enhancement of size and colour as a result of delayed harvest under favourable sizing and colouring conditions, reduction in incidence and/or severity of watercore and superficial scald, enhanced storage potential. **Formulation types** SP. **Selected tradenames** 'ReTain' (hydrochloride) (Valent BioSciences)

MAMMALIAN TOXICOLOGY: *aminoethoxyvinylglycine hydrochloride*
Oral Acute oral LD₅₀ for rats >5000 mg/kg. **Skin and eye** Acute dermal LD₅₀ for rabbits >2000 mg/kg. **Inhalation** (4 h) for rats 1.13 mg/l. **NOEL** (90 d) for rats 2.2 mg/kg b.w. daily. **ADI** RfD 0.002 mg/kg b.w. [1997] **Toxicity class** EPA III, IV (formulation and tech. a.i.)

ECOTOXICOLOGY: *aminoethoxyvinylglycine*
Birds Moderately toxic to birds. **Bees** Unlikely to be exposed following planned use.

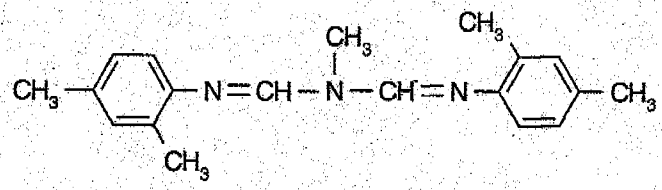
aminoethoxyvinylglycine hydrochloride
Birds Acute oral LD₅₀ for northern bobwhite quail 121 mg/kg. Dietary LC₅₀ (5 d) for northern bobwhite quail 230 ppm. **Fish** LC₅₀ (96 h) for trout >139 mg/l. **NOEL** (96 h) for trout 139 mg/l. **Daphnia** EC₅₀ (48 h) >135 mg/l. **NOEL** 135 mg/l. **Bees** Unlikely to be exposed, given use pattern.

t growth regulator

26 amitraz

Acaricide, insecticide

amidine



NOMENCLATURE: **Common name** amitraz (BSI, E-ISO, ANSI, ESA, BAN, JMAF); amitraxe ((m) F-ISO)
IUPAC name N-methylbis(2,4-xylyliminomethyl)amine
Chemical Abstracts name N'-(2,4-dimethylphenyl)-N-[[[(2,4-dimethylphenyl)imino]methyl]-=N-methylmethanimidamide
Other names N,N-bis(2,4-xylyliminomethyl)methylamine; N-methyl-N'-2,4-xylyl-N-(N-2,4-xylylformimidoylethyl)formamidine; 1,5-di-(2,4-dimethylphenyl)-3-methyl-1,3,5-triazapenta-1,4-diene
CAS RN [33089-61-1] **EEC no.** 251-375-4 **Development codes** BTS 27 419
Official codes OMS 1820; ENT 27 967

n white to tan powder
2 (in temperature)
on [α]_D²⁵ +89.2° (c 1, 0.1 M)

amitraz 31

PHYSICAL CHEMISTRY: Mol. wt. 293.4 M.f. $C_{19}H_{23}N_3$ Form White/pale yellow crystalline solid. M.p. 86–88°C V.p. 0.34 mPa (25°C) using clapeyron-clausius analysis K_{ow} logP = 5.5 (25°C, pH 5.8) Henry 1.0 Pa m³ mol⁻¹ (measured) S.g./density 1.128 (20°C) Solubility In water <0.1 mg/l (20°C). Soluble in most organic solvents; in acetone, toluene, xylene >300 g/l. Stability Hydrolysis DT₅₀ (25°C) 2.1 h (pH 5), 22.1 h (pH 7), 25.5 h (pH 9). U.V. light appears to have little effect on stability. pKa 4.2, weak base

COMMERCIALISATION: History Acaricide reported by B. H. Palmer et al. (*Proc. Int. Congr. Acarol.* 3rd, 1971, p. 687) for veterinary use and by D. M. Weighton et al. (*Médec. Fac. Landbouwwet. Rijksuniv. Gent*, 1972, 37, 765) for crop use. Introduced by The Boots Co. Ltd.; (now marketed by Aventis CropScience for crop protection and by Hoechst AG for veterinary use). Patents GB 1327935 (Boots) Manufacturers Aventis; Defensa; Rotam; Wujiu.

APPLICATIONS: Biochemistry Mode of action probably involves an interaction with octopamine receptors in the tick nervous system, causing an increase in nervous activity. Mode of action Non-systemic, with contact and respiratory action. Expellent action causes ticks to withdraw mouthparts rapidly and fall off the host animal. Uses Control of all stages of tetranychid and eriophyid mites, pear suckers, scale insects, mealybugs, whitefly, aphids, and eggs and first instar larvae of Lepidoptera on pome fruit, citrus fruit, cotton, stone fruit, bush fruit, strawberries, hops, cucurbits, aubergines, capsicums, tomatoes, ornamentals, and some other crops. Also used as an animal ectoparasiticide to control ticks, mites and lice on cattle, dogs, goats, pigs and sheep.

Phytotoxicity At high temperatures, young capsicums and pears may be injured.

Formulation types EC, PO, WP. **Compatibility** Incompatible with alkaline materials, parathion, and others. **Selected tradenames** 'Mitac' (for crop protection) (Aventis); 'Ovasyn' (Aventis); 'Taktic' (for veterinary) (Intervet); 'Byebye' (Agriphar); 'Edrizar' (Caffaro); 'Parsec' (Makhteshim-Agan); 'Racer' (Rotam); 'Sender' (Sanonda)

ANALYSIS: Product analysis by glc (*CIPAC Handbook*, 1995, G, 5–10). Residue analysis also by glc. Details available from Aventis.

MAMMALIAN TOXICOLOGY: Reviews FAO/WHO 83, 85 (see part 2 of the Bibliography). Oral Acute oral LD₅₀ for rats 650, mice >1600 mg/kg. Skin and eye Acute percutaneous LD₅₀ for rabbits >200, rats >1600 mg/kg. Inhalation LC₅₀ (6 h) for rats 65 mg/l air. NOEL In 2 y feeding trials, no adverse effect observed in rats receiving 50–200 ppm diet, or in dogs dosed 0.25 mg/kg daily. Human NOEL >0.125 mg/kg daily. ADI (JMPR) 0.01 mg/kg b.w. [1998]. Toxicity class WHO (a.i.) III; EPA (formulation) III EC hazard Xn; R22

ECOTOXICOLOGY: Birds LD₅₀ for bobwhite quail 788 mg/kg, LC₅₀ (8 d) for mallard ducks 7000, Japanese quail 1800 mg/kg. Fish LC₅₀ (96 h) for rainbow trout 0.74, bluegill sunfish 0.45 mg/l. Due to rapid hydrolysis, it is unlikely that this toxicity will be expressed in natural aquatic systems. Daphnia LC₅₀ (48 h) 0.035 mg/l. Due to rapid hydrolysis, it is unlikely that this toxicity will be expressed in natural aquatic systems. Algae EC₅₀ for *Selenastrum capricornutum* >12 mg/l. Bees Low toxicity to bees and predatory insects. LD₅₀ (contact) 50 µg/bee (formulation). Worms LC₅₀ (14 d) for earthworms >1000 mg tech./kg.

ENVIRONMENTAL FATE: Animals Rapid breakdown leading to excretion as a conjugate of 4-amino-3-methylbenzoic acid and, to a lesser extent, to N-(2,4-dimethylphenyl)-N'-methylformamidine. Plants Rapidly degraded, mainly to N-(2,4-dimethylphenyl)-N'-methylformamidine and, to a smaller extent, to 2,4-dimethylformanilide. Soil/Environment Rapidly broken down in soil under aerobic conditions (*J. Appl. Bacteriol.*, 1977, 42, 187; *ibid.* 1978, 44, 383); DT₅₀ in soil <1 d. Degradation occurs more rapidly in acid than in neutral or alkaline soils. Very strongly adsorbed to soil; K_{oc} c. 1000–2000.

NOMENCLATURE: C ATA (JMAF); aminotriaz IUPAC name 1H-1,2,4-triazole Chemical Abstracts name CAS RN [61-82-5] EI

PHYSICAL CHEMISTRY: M.p. 157–159°C; (tech. S.g./density 1.138 (20°C) 26 g/100 g (75°C). Mo Sparingly soluble in ethy solvents. Stability Stab. pKa pKa₁ 4.2. pKa₂ 10.7

COMMERCIALISATION: Weed Control Conf., 199 CropScience). Patents

APPLICATIONS: Biocyclase. Mode of action translocation in both th and broad-leaved weed vineyards and olive gro and on fallow land and for total herbicidal control of aquatic weeds in marsh Residue Rev., 1966, 12, 1975, 1, p. 377). Form Nufarm); 'Azolan' (Mal 'Rapir Neu' (+ diuron)

ANALYSIS: Product a 1984, 13, 191). by acid complex during titration mixtures being determined colorimetry (R. A. Her R. W. Storherr, *J. Assoc. Plant Growth Regul.* Foo 1980, 200, 234).

MAMMALIAN TOXICITY: IARC ref. 7, 41; class 2 percutaneous LD₅₀ for

Herbicide

J₂

CF₃

OPX-66037; IN 66037

1-(2-ylcarbamoylsulfamoyl)-
hoxy)-1,3,5-triazin-4-

Form White, crystalline solid
K_{ow} logP = 0.96 (pH 7)
1 (pH 3), 3 (pH 5),
80, acetone 120, methanol 7
olysed in water, DT₅₀ 3.7 d

Proc. Br. Crop Prot. Conf. -
Manufacturers Du Pont.

inhibitor. Acts by inhibiting
stopping cell division and plant
growth. *Proc. Br. Crop Prot.*
is reviewed (M. K. Koeppe &
emergence selective herbicide.
rol of many annual and
types WG.
identifies 'Debut' (W. Europe)
(Du Pont)

cutaneous LD₅₀ for rabbits
ing to skin (guinea pigs).

Inhalation LC₅₀ (4 h) for rats >5.1 mg/l. NOEL (1 y) for dogs 875 ppm; (18 mo) for mice
150 ppm; (2 y) for male rats 100, female rats 750 ppm. ADI (UK) 0.05 mg/kg.
Other: Non-mutagenic in the Ames test. Toxicity class WHO (a.i.) III (Table 5)

ECOTOXICOLOGY: triflurosulfuron-methyl

Birds LD₅₀ for mallard ducks and bobwhite quail 2250 mg/kg. Dietary LC₅₀ for mallard ducks and
bobwhite quail >5620 ppm. Fish LC₅₀ (96 h) for bluegill sunfish 760, trout 730 mg/l.
Daphnia LC₅₀ (48 h) >960 mg/l. Algae EC₅₀ (120 h) for green algae 0.62 mg/l.
Other aquatic spp. LC₅₀ (14 d) for *Lemna gibba* 9.0 µg/l. Bees Oral LD₅₀ (48 h) >1000 ppm.
Worms LD₅₀ for earthworms >1000 mg/kg.

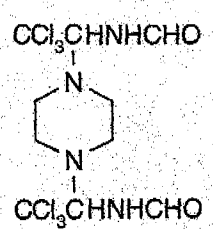
ENVIRONMENTAL FATE: triflurosulfuron-methyl

The compound rapidly degrades in water, soil, plants, and animals. The primary metabolic pathways
in all the systems are the cleavage of the sulfonylurea bridge, yielding methyl saccharin and triazine
amine, followed by N-demethylation to N-desmethyl triazine amine, and N,N-bis-desmethyl triazine
amine. The metabolic pathway is consistent in aquatic, soil, and biological systems.
Soil/Environment Degrades rapidly in soil by chemical and microbial mechanisms. Microbial
degradation is important in alkaline conditions, but plays only a minor role in neutral and acidic
conditions because chemical hydrolysis is very rapid. Half-life in soil 3 d. Bioaccumulation is unlikely
to occur.

793 triforine

Fungicide

FRAC 3; DMI: piperazine



NOMENCLATURE: Common name triforine (BSI, E-ISO, (f) F-ISO, ANSI, JMAP)
IUPAC name N,N'-[piperazine-1,4-diylbis[(trichloromethyl)methylene]]diformamide;
[1,4-piperazine-1,4-diylbis-[[N-(2,2,2-trichloroethyl)formamide]]
Chemical Abstracts name N,N'-[1,4-piperazinediylbis(2,2,2-trichloroethylidene)]bisformamide
CAS RN [26644-46-2] Development codes Cela W524

PHYSICAL CHEMISTRY: Mol. wt. 435.0 M.f. C₁₀H₁₄Cl₆N₄O₂ Form White to light brown
crystals. M.p. 155°C (decomp.) V.p. 8 x 10⁻¹ mPa (25°C) K_{ow} logP = 2.2 (20°C, unstated pH)
Henry 2.5 Pa m³ mol⁻¹ S.g./density 1554 kg/m³ (20°C). Solubility In water 9 mg/l (20°C). In
dimethylformamide 330, dimethyl sulfoxide 476, N-methylpyrrolidone 476, acetone 11,
dichloromethane 1, methanol 10 (all in g/l). Also soluble in tetrahydrofuran; slightly soluble in
dioxane and cyclohexanone; insoluble in benzene, petroleum ether and cyclohexane.
Stability Stable ≤180°C. Decomposed in aqueous solution exposed to u.v. or daylight. Decomposed
in strongly acidic media (to trichloroacetaldehyde and piperazine salts) and in strongly alkaline media
(to chloroform and piperazine); DT₅₀ (pH 5-7, 25°C) 3.5 d. pKa 10.6, strong base

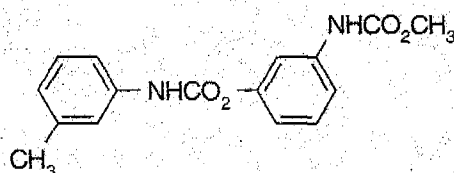
triforine 945

Main Entries

605 phenmedipham

Herbicide

HRAC C₁ WSSA 5; bis-carbamate



NOMENCLATURE: Common name phenmedipham (BSI, E-ISO, ANSI, WSSA, JMAF); phenmedipham ((m) F-ISO)

IUPAC name methyl 3-[(3-methylcarbaniloyloxy)carbanilate]; 3-methoxycarbonylamino phenyl 3'-methylcarbanilate

Chemical Abstracts name 3-[(methoxycarbonyl)amino]phenyl (3-methylphenyl)carbamate

Other names PMP **CAS RN** [13684-63-4] **Development codes** SN 38 584; ZK 15320; EP-452

PHYSICAL CHEMISTRY: **Composition** Tech. grade is >97% pure. **Mol. wt.** 300.3 **M.f.** C₁₆H₁₆N₂O₄ **Form** Colourless crystals. **M.p.** 143–144°C; (tech.) 140–144°C **V.p.** 1.33 × 10⁻⁶ mPa (25°C) **K_{ow} log P** = 3.59 (pH 3.9) **Henry** 5 × 10⁻⁸ Pa m³ mol⁻¹ (calc.) **S.g./density** 0.34–0.54 (20°C) **Solubility** in water 4.7 mg/l (room temperature). Soluble in polar organic solvents. In acetone, cyclohexanone c. 200, methanol c. 50, chloroform 20, benzene 2.5; hexane c. 0.5, dichloromethane 16.7, ethyl acetate 56.3, toluene c. 0.97, 2,2,4-trimethylpentane 1.16 (all in g/l, 20°C). **Stability** Stable up to 200°C. Very stable in acidic media, but hydrolysed in neutral and alkaline media; DT₅₀ (22°C) 50 d (pH 5), 14.5 h (pH 7), 10 min (pH 9). In solution (pH 3.8) irradiated at 280 nm, DT₅₀ 9.7 d. **pKa** <0.1

COMMERCIALISATION: **History** Herbicide reported by F. Arndt & C. Kötter (*Abstr. Int. Congr. Plant Prot.*, 6th, Vienna, 1967, p. 433). Introduced by Schering AG (now Aventis CropScience). **Patents** GB 1127050 **Manufacturers** Aventis; Griffin; Synthesia; United Phosphorus Ltd.

APPLICATIONS: **Biochemistry** Photosynthetic electron transport inhibitor at the photosystem II receptor site. **Mode of action** Selective systemic herbicide, absorbed through the leaves, with translocation primarily in the apoplast. **Uses** Used post-emergence, at 1 kg a.i./ha, in beet crops, especially sugar beet, after the emergence of most broad-leaved weeds and before they develop more than 2–4 true leaves; also used on strawberries, spinach, peas, mangold and red beet.

Phytotoxicity Non-phytotoxic to beet crops. **Formulation types** EC; SC; oil-SC; SL; WG.

Compatibility Incompatible with alkaline substances. **Selected tradenames** 'Alegro' (Aventis); 'Betanal' (Aventis); 'Kemifam' (Aventis); 'Spin-aid' (Aventis); 'Beetup' (United Phosphorus Ltd); 'Beta' (Stefes); 'Betapost' (Agriphar); 'Dephend' (Headland); 'Fender' (ISK Biosciences); 'Herbasan' (Mirfield, Stefes); 'Kontakt' (Feinchemie Schwebda); 'Mandolin' (Griffin); 'Protrum K' (Atlas Crop Protection); 'Punter' (Barclay); 'Vanguard' (FCC)

ANALYSIS: **Product analysis** by titration (*CIPAC Proc.*, 1980, 2, 215; *CIPAC Handbook* 1985, 1C, 2181) or by hplc (*ibid.*); method available from Aventis. **Residues** by glc (K. Kossmann & N. A. Jenny, *Anal. Methods Pestic. Plant Growth Regul.*, 1973, 7, 611); in soil by hplc or by hydrolysis to m-toluidine, derivatives of which are determined by glc with ECD or by colorimetry (K. Kossmann, *Weed Res.*, 1970, 10, 340). Details available from Aventis.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats and mice >8000, guinea pigs and dogs >4000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits 1000, rats 2500 mg/kg.

722 phenmedipham

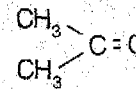
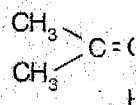
Not a skin sensitiser. **Inhalation** LD₅₀ 1000 mg/kg; (90 d) for rats and dogs >5000 mg/kg. **Toxicity class** II

ECOTOXICOLOGY: **Birds** Acute Dietary LC₅₀ (8 d) for mallard duck rainbow trout 1.4–3.0, bluegill sunfish (formulation). **Daphnia** LC₅₀ (72 h) >23 µg/bee; (co

ENVIRONMENTAL FATE: **Animals** within 72 hours, mainly in the urine conjugation to glucuronides and excretion of N-(3-hydroxyphenyl)carbamate is 1 c. 25 d, DT₉₀ c. 108 d. **Metabolites:** m-aminophenol, and subsequently *Contam. Toxicol.*, 1971, 6, 322–327 relevant uptake by following crops groundwater contamination is to b

606 phenoth

pyrethroid



NOMENCLATURE: Common name (1R)-cis-trans- isomers; phenothrin **IUPAC name** (for phenothrin): 3-(1-phenyl)cyclopropanecarboxylate (1R)-3-phenoxybenzyl (±)-cis-trans- isomers; 3-phenoxybenzyl (1R)-cis-trans- isomers **Chemical Abstracts name** (3-phenoxy)cyclopropanecarboxylate

480 *Mamestra brassicae* NPV

Biological insecticide

Nuclear polyhedrosis virus used for control of Lepidoptera. For full details, see *The BioPesticide Manual*.

481 mancooper

Fungicide

multi-site: alkylenebis(dithiocarbamate)

NOMENCLATURE: Common name mancooper (BSI, E-ISO, F-ISO)

IUPAC name ethylenebis(dithiocarbamate) mixed metal complex containing c. 13.7% manganese and c. 4% copper

Chemical Abstracts name [[1,2-ethanediybis[carbamodithioato]](2-)]manganese mixture with [[1,2-ethanediybis[carbamodithioato]](2-)]copper

CAS RN [53988-93-5]

COMMERCIALISATION: History Fungicide introduced by Rohm & Haas Co. Manufacturers Rohm & Haas.

APPLICATIONS: Biochemistry Non-specific thiol reactant, inhibiting respiration.

Mode of action Fungicide with protective action. **Uses** Control of downy mildew on vines. Also used as a seed treatment for control of *Septoria* and *Fusarium* spp. on cereals.

Formulation types WP; Seed treatment. **Selected tradenames** 'Dithane C-90' (Rohm & Haas)

ANALYSIS: Details from Rohm & Haas.

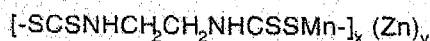
MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats 9600 mg/kg.

ENVIRONMENTAL FATE: EHC 78 (WHO, 1988; general review of dithiocarbamates).

482 mancozeb

Fungicide

FRAC Y: multi-site: alkylenebis(dithiocarbamate)



NOMENCLATURE: Common name mancozeb (BSI, E-ISO); mancozèbe ((m) F-ISO); manzeb (JMAF)

IUPAC name manganese ethylenebis(dithiocarbamate) (polymeric) complex with zinc salt

Chemical Abstracts name [[1,2-ethanediybis[carbamodithioato]](2-)]manganese mixture with [[1,2-ethanediybis[carbamodithioato]](2-)]zinc

578 mancozeb

CAS RN [8018-01-7] (formerly [8018-01-7] manganese and zinc ethylenebis(dithiocarbamate))

PHYSICAL CHEMISTRY: Composition containing 20% of manganese and 2% of mancozeb chloride. Form Greyish white. V.p. Negligible at 20°C. S.g./density 1.8. Solubility: Soluble in most organic solvents; dissolves in water from them. Stability Stable under normal conditions. On hydrolysis (25°C), DT is unstable and the tech. not isolated; F.p. 137.8°C (Tag open cup)

COMMERCIALISATION: History 17. Introduced by Rohm & Haas Co. (manufacture or market it). Patents Manufacturers Aimco; CAC; Crystal Sanachem; Sinon; United Phosphorus

APPLICATIONS: Biochemistry No Mode of action Fungicide with protective action. Particular uses include control of early blight (a.i./ha); *Rhizoctonia solani* and *Strep. cucurbitis*, beet, berries and currants; beans, apples and plums (at 1.6 kg/ha); cucurbits, ornamentals and tobacco; *Phytophthora blight* on apples; scab (*Cercospora musae*) in bananas; shot-hole diseases of vegetables; diseases of cereals. Used for foliar application. SC; WG; WP. Selected tradenames 'Manex II' (Griffin); 'Manzate' (Griffin); 'Indofil M-45' (Indofil); 'Sancozeb' (Sanachem); 'Saver' (Sanachem); 'Zeb' (Nagarjuna Agrichem); 'Zebr' (Syngenta PM) (+ cymoxanil + folpet) (+ folpet) (Griffin); 'Micexanil' (+ cymoxanil + oxadixyl) (Novartis); 'Tairel' (+ oxadixyl) (Aventis); 'Trecatol' (+ benalaxyl) (Aventis)

ANALYSIS: Product analysis by distillation, either by glc or by a titrimetric method (CIPAC Handbook). Residues determined by reaction with 2,4-dinitrophenylhydrazine (Analyst (London), 1981, 1987, I, S21; Anal. Methods Residue)

MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats >5000 mg/kg, rabbits >5000 mg/kg, Mice Inhalation LC₅₀ (4 h) for rats >5.1

CAS RN [8018-01-7] (formerly [8065-67-6]); [8018-01-7] is also applied to other mixed manganese and zinc ethylenebis(dithiocarbamate) complexes

PHYSICAL CHEMISTRY: Composition The ISO definition is 'a complex of zinc and maneb containing 20% of manganese and 2.55% of zinc, the salt present being stated (for instance mancozeb chloride)'. **Form** Greyish-yellow powder. **M.p.** Decomposes at 192–204°C. **V.p.** Negligible at 20°C. **S.g./density** 1.92. **Solubility** In water 6.2 ppm (pH 7.5, 25°C). Insoluble in most organic solvents; dissolves in solutions of powerful chelating agents but cannot be recovered from them. **Stability** Stable under normal, dry storage conditions. Slowly decomposed by heat and moisture. On hydrolysis (25°C), DT₅₀ 20 d (pH 5), 17 h (pH 7), 34 h (pH 9). Mancozeb a.i. is unstable and the tech. not isolated; the formulated product is produced in continuous process. **F.p.** 137.8°C (Tag open cup)

COMMERCIALISATION: History Fungicide reported in *Fungic. Nematic. Tests*, 1961, 17. Introduced by Rohm & Haas Co. and by E. I. du Pont de Nemours and Co. (who no longer manufacture or market it). **Patents** GB 996264; US 3379610; US 2974156 all to Rohm & Haas. **Manufacturers** Aimco; CAC; Crystal; Elf Atochem; Griffin; Hindustan; Indofil; Rohm & Haas; Sanachem; Sinon; United Phosphorus.

APPLICATIONS: Biochemistry Non-specific thiol reactant, inhibiting respiration. **Mode of action** Fungicide with protective action. **Uses** Control of many fungal diseases (e.g. blight, leaf spot, rust, downy mildew, scab, etc.) in field crops, fruit, nuts, vegetables, ornamentals, etc. Particular uses include control of early and late blights of potatoes and tomatoes (at 1.36 kg a.i./ha); *Rhizoctonia solani* and *Streptomyces scabies* on seed potatoes; leaf spot diseases on celery, cucurbits, beet, berries and currants; rusts on cereals, vegetables, roses, carnations, asparagus, beans, apples and plums (at 1.6 kg/ha); downy mildews on hops, vines, onions, leeks, lettuce, cucurbits, ornamentals and tobacco; *Gloeodes pomigena*, *Glomerella cingulata*, *Microthyriella rubi* and *Phytophthora obtusa* on apples; scab on apples and pears (at 2.4–3.6 kg/ha); sigatoka disease (*Cercospora musae*) in bananas; shot-hole of stone fruit; anthracnose of beans and cucurbits; damping-off diseases of vegetables; black leg of beet; needle cast in forestry; and many seed-borne diseases of cereals. Used for foliar application or as a seed treatment. **Formulation types** DP; DS; SC; WG; WP. **Selected tradenames** 'Dithane M-45' (Rohm & Haas); 'Manconex' (Griffin); 'Manex II' (Griffin); 'Manzate' (Griffin); 'Aimcozeb' (Aimco); 'Critttox' (Caffaro); 'Hilthane' (Hindustan); 'Indofil M-45' (Indofil); 'Kifung' (Inquiport); 'Lucazebl' (Lucava); 'Micene' (Sipcam); 'Sancozeb' (Sanachem); 'Saver' (Sanonda); 'Uthane' (United Phosphorus); 'Vondozeb' (Elf Atochem); 'Zeb' (Nagarjuna Agrichem); 'Zebra' (Headland); **mixtures** 'Manex C-8' (+ cymoxanil) (Griffin); 'Sygan PM' (+ cymoxanil + folpet) (Griffin); 'Syphal PM' (+ copper oxychloride + cymoxanil + folpet) (Griffin); 'Micexanil' (+ cymoxanil) (Sipcam); 'Patafol' (+ ofurace) (Aventis); 'Sandofan' (+ oxadixyl) (Novartis); 'Tairel' (+ benalaxyl) (Isagro); 'Tattoo' (+ propamocarb hydrochloride) (Aventis); 'Trecatol' (+ benalaxyl) (Isagro); 'Pulsan' (+ cymoxanil + oxadixyl) (Novartis)

ANALYSIS: Product analysis by decomposition with acid and measurement of the carbon disulfide liberated, either by glc or by a titrimetric method (CIPAC Handbook, 1980, 1A, 1288). Identified colorimetrically (CIPAC Handbook, 1994, F, 320) or by u.v. absorbance (*ibid.*, 411).

Residues determined by reaction with acid to form carbon disulfide which is measured by standard methods (*Analyst (London)*, 1981, 106, 782; *Pestic. Anal. Man.*, 1979, II; *Manu. Pestic. Residue Anal.*, 1987, I, S21; *Anal. Methods Residues Pestic.*, 1988, Part II).

MAMMALIAN TOXICOLOGY: Reviews FAO/WHO 68, 70 (see part 2 of the Bibliography).

Oral Acute oral LD₅₀ for rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >10000, rabbits >5000 mg/kg. Mild to moderate skin irritant; moderate eye irritant.

Inhalation LC₅₀ (4 h) for rats >5.14 mg/l. **ADI** (JMPR) 0.03 mg/kg b.w. (group ADI with maneb,

mancozeb 579

ogical insecticide

tails, see *The BioPesticide*

Fungicide

ing c. 13.7% manganese and
ganese mixture with

s Co.

piration.
Y mildew on vines. Also
eals.
C-90' (Rohm & Haas)

biocarbamates).

Fungicide

: (F-ISO); manzeb

ex with zinc salt
ganese mixture with

with wetting agents, alkaline materials, oils, and copper-containing compounds.

Selected tradenames 'Alar' (Uniroyal); 'B-Nine' (Uniroyal)

ANALYSIS: Product analysis by hplc. Details available from Uniroyal. **Residues** determined by glc of a derivative (J. R. Lane, *Anal. Methods Pestic., Plant Growth Regul. Food Addit.*, 1967, 5, 499) or by alkaline hydrolysis to liberate 1,1-dimethylhydrazine which is determined colorimetrically (*Anal. Methods Pestic. Plant Growth Regul.*, 1972, 6, 697; V. P. Lynch, *ibid.*, 1976, 8, 491).

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 62, 64 (see part 2 of the Bibliography). **Oral** Acute oral LD₅₀ for rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >5000 mg/kg. **Inhalation** LC₅₀ (4 h) for rats >2.1 mg/l air. **NOEL** (1 y) for dogs 188 mg/kg b.w. daily, for rats 5 mg/kg b.w. daily. Non-oncogenic in 2 y feeding trials in rats and mice at 10000 mg/kg diet. NOEL for teratogenicity and embryotoxicity in rabbits was 300 mg/kg diet. In 3-generation reproductive study, NOEL for rats was 50 mg/kg b.w. daily. Non-mutagenic in *in vivo* test. **ADI** (JMPR) 0.5 mg/kg b.w., for daminozide containing <30 mg 1,1-dimethylhydrazine/kg [1991]. **Toxicity class** WHO (a.i.) III (Table 5); EPA (formulation) IV **EC hazard** R40

ECOTOXICOLOGY: **Birds** Dietary LC₅₀ (8 d) for mallard ducks and bobwhite quail >10000 mg/kg diet. **Fish** LC₅₀ (96 h) for rainbow trout 149, bluegill sunfish 423 mg/l. **Daphnia** LC₅₀ (96 h) 76 mg/l. **Algae** EC₅₀ for *Chlorella* 180 ppm. **Bees** Not toxic to bees; LD₅₀ >100 µg/bee (85% formulation). **Worms** LC₅₀ for earthworms >632 ppm.

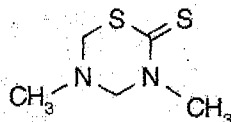
ENVIRONMENTAL FATE: **Plants** Metabolites include 1,1-dimethylhydrazine.

Soil/Environment Daminozide quickly dissipates in soil with most residues becoming bound, with some CO₂ formation. In aerobic soil, half of the daminozide is no longer recoverable after 17 h. No 1,1-dimethylhydrazine (UDMH) or *N*-nitrosodimethylamine were detected. In soil under anaerobic conditions, half of the daminozide had dissipated in 7.5 days. The major products were bound residues and CO₂. In a field study on bare ground, about 90% of the daminozide had disappeared after 7 days. Neither hydrolysis nor photolysis are significant pathways for the degradation of daminozide.

210 dazomet

Nematicide, fungicide, herbicide, insecticide

HRAC Z WSSA 27



NOMENCLATURE: **Common name** dazomet (BSI, E-ISO, (m) F-ISO, WSSA, JMAF); tiazon (USSR); DMTT* (former WSSA name)

IUPAC name 3,5-dimethyl-1,3,5-thiadiazinane-2-thione; tetrahydro-3,5-dimethyl-1,3,5-thiadiazine-2-thione

Chemical Abstracts name tetrahydro-3,5-dimethyl-2H-1,3,5-thiadiazine-2-thione

250 dazomet

CAS RN [533-74-4] EEC no. 208
Crag Fungicide 974 (Rhône-Poulenc)

PHYSICAL CHEMISTRY: **Compos**
Form Colourless crystals. M.p. 10.
K_{ow} logP = 0.15 (pH 7) **Henry** 2.0
Solubility In water 3 g/kg (20°C). In
ethanol 15, diethyl ether 6 (all in g/
Sensitive to temperatures >50°C. In
formaldehyde, and methylamine.

COMMERCIALISATION: **History**
15, 891), later introduced as a soil

APPLICATIONS: **Biochemistry** N
Mode of action A pre-planting soil
Uses Soil sterilant, applied prior to
(*Fusarium*, *Pythium*, *Rhizoctonia*, *Scie*
(*atramentarium*)), nematodes, germ
pulp and paper manufacture, and a
phytotoxic to all green plants. Tree
and its degradation products. For
(BASF)

ANALYSIS: **Product** analysis by a
iodometric titration (CIPAC *Handb*
Growth Regul. Food Addit., 1964, 3,
Isothiocyanate in crops by glc. Det

MAMMALIAN TOXICOLOGY:
710, rabbits 320-620 mg/kg. **SKI**
formulation is a skin and eye irrita
NOEL in rats 20 mg/kg diet. **OTI**
EPA (formulation) III **EC hazard**

ECOTOXICOLOGY: **Birds** LD₅₀
mallard ducks >5000 mg/kg diet.
Algae EC₅₀ (96 h) for *Scenedesmu*
Pseudomonas putida 1.8 mg/l. **Be**

ENVIRONMENTAL FATE: **Plant**
of its degradation products meth
at >0.01 ppm in the fruit. **Soil/E**
degradation to methyl(methylami
degradation to methyl isothiocyar
See N. Drescher & S. Otto, *Resia*

g compounds.

royal. Residues determined by glc at Food Addit., 1967, 5, 499) or by ermined colorimetrically (Anal. l., 1976, 8, 491).

ee part 2 of the Bibliography) e percutaneous LD₅₀ for rabbits DEL (1 y) for dogs 188 mg/kg b.w. rials in rats and mice at in rabbits was 300 mg/kg diet. In b.w. daily. Non-mutagenic in vivo 0 mg 1,1-dimethylhydrazine/kg n) IV EC hazard R40

s and bobwhite quail uegill sunfish 423 mg/l. i. Bees Not toxic to bees orms >632 ppm.

thylhydrazine. t residues becoming bound, with o longer recoverable after 17 h. No s detected. In soil under anaerobic a major products were bound the daminozide had disappeared ays for the degradation of

herbicide, insecticide

-ISO, WSSA, JMAF); tiazon (USSR) no-3,5-dimethyl-1,3,5-thiadiazine diazine-2-thione

CAS RN [533-74-4] EEC no. 208-576-7 Development codes N-521 (Stauffer Chemical Co.); fungicide 974 (Rhône-Poulenc); BAS 00 201N

PHYSICAL CHEMISTRY: Composition ≥94% pure. Mol. wt. 162.3 M.f. C₅H₁₀N₂S₂ Form Colourless crystals. M.p. 104–105°C (decomp.; tech. grade) V.p. 0.37 mPa at 20°C $\log P = -0.15$ (pH 7) Henry 2.00×10^{-5} Pa m³ mol⁻¹ (calc.) S.g./density 1.37 (tech.) Solubility In water 3 g/kg (20°C). In cyclohexane 400, chloroform 391, acetone 173, benzene 51, ethanol 15, diethyl ether 6 (all in g/kg, 20°C). Stability Stable at temperatures up to 35°C. Sensitive to temperatures >50°C, and to moisture. Hydrolysed in acidic media to carbon disulfide, formaldehyde, and methylamine.

COMMERCIALISATION: History Originally prepared by M. Delépine (Bull. Soc. Chim. Fr., 1897, 15, 891), later introduced as a soil fumigant. Manufacturers BASF.

APPLICATIONS: Biochemistry Non-selective inhibition of enzymes by degradation products. Mode of action A pre-planting soil fumigant, acting by decomposition to methyl isothiocyanate. Uses Soil sterilant, applied prior to planting out crops, at 200–600 kg/ha. Controls soil fungi (*Fusarium*, *Pythium*, *Rhizoctonia*, *Sclerotinia* and *Verticillium* spp. and *Colletotrichum coccodes* (*grammentium*)), nematodes, germinating weed seeds, and soil insects. Also used as a slimicide in pulp and paper manufacture, and as a preservative in adhesives and glues. Phytotoxicity Highly phytotoxic to all green plants. Treated soils should not be planted until shown to be free of dazomet and its degradation products. Formulation types DP; GR; WP. Selected tradenames 'Basamid' (BASF)

ANALYSIS: Product analysis by acid hydrolysis, absorption of the carbon disulfide produced and iodometric titration (CIPAC Handbook, 1985, 1C, 2074; H. A. Stansbury, Anal. Methods Pestic., Plant Growth Regul. Food Addit., 1964, 3, 119). Residues of parent compound in soil by hplc; of methyl isothiocyanate in crops by glc. Details available from BASF.

MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats 520, male mice 455, female mice 710; rabbits 320–620 mg/kg. Skin and eye Acute percutaneous LD₅₀ for rats >2000 mg/kg. DP formulation is a skin and eye irritant to rabbits. Inhalation LC₅₀ (4 h) for rats 8.4 mg/l air. NOEL in rats 20 mg/kg diet. Other Not oncogenic. Toxicity class WHO (a.i.) III; EPA (formulation) III EC hazard Xn; R22| Xi; R36| N; R50, R53

ECOTOXICOLOGY: Birds LD₅₀ for bobwhite quail 415 mg/kg b.w. LC₅₀ for bobwhite quail 1850, mallard ducks >5000 mg/kg diet. Fish LC₅₀ (96 h) 0.16 mg/l. Daphnia EC₅₀ (48 h) 0.3 mg/l. Algae EC₅₀ (96 h) for *Scenedesmus subspicatus* 1.0 mg/l. Other aquatic spp. EC₁₀ (17 h) for *Pseudomonas putida* 1.8 mg/l. Bees Not toxic to bees when used as directed.

ENVIRONMENTAL FATE: Plants Following application to strawberries, no residues of dazomet or of its degradation products methyl isothiocyanate, dimethyl- or monomethylthiourea were detected at >0.01 ppm in the fruit. Soil/Environment In soil, in the presence of moisture, undergoes degradation to methyl(methylaminomethyl)dithiocarbamic acid, which then undergoes further degradation to methyl isothiocyanate, formaldehyde, hydrogen sulfide, and methylamine. See N. Drescher & S. Otto, Residue Rev., 1968, 23, 49.

Main Entries