

Data Evaluation Report on the Photolysis of O-sulfamuron (IR5878) in Water

PMRA Submission Number {.....}

EPA MRID Number 46588509

Data Requirement: PMRA Data Code:
EPA DP Barcode: D319377
OECD Data Point:
EPA Guideline: 161-2

Test material:

Common name: O-Sulfamuron.

Chemical name:

IUPAC name: 1-(4,6-Dimethoxypyrimidin-2-yl)-3-[2-(dimethylcarbamoyl)phenylsulfamoyl]urea.

CAS name: 2-[[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]amino]-N,N-dimethylbenzamide.

CAS No.: 213464-77-8.

Synonyms Orthosulfamuron, IR5878.

Smiles string: CN(C(=O)c1cccc1NS(=O)(=O)NC(=O)Nc1nc(cc(n1)OC)OC)C (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 7/6/06.

Primary Reviewer: Leanne Ganser
Cambridge Environmental

Signature:
Date: 7/12/06

Secondary Reviewer: Kathleen Ferguson
Cambridge Environmental

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QC/QA Manager: Joan Gaidos
Cambridge Environmental

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Final Reviewer: Gregory Orrick
EPA Reviewer

Signature:
Date: 7/18/06



Company Code:

Active Code:

Use Site Category:

EPA PC Code: 108209

CITATION: Hennecke, D. 2002. Aquatic Photodegradation and Quantum Yield of IR5878. Unpublished study performed by Fraunhofer Institute for Molecular Biology and Applied Ecology, Schmallenberg, Germany; sponsored and submitted by ISAGRO S.p.A., Milan, Italy. GLP-Code: ISA-003/7-05. Experiment started July 26, 2002, and completed August 13, 2002. Final report issued November 8, 2002. 52 pp.



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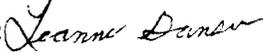
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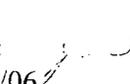
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EXECUTIVE SUMMARY

The aqueous phototransformation of unlabeled 1-(4,6-dimethoxypyrimidin-2-yl)-3-[2-(dimethylcarbamoyl) phenylsulfamoyl]urea (o-sulfamuron, purity 98.19%), at 10, 20 and 30 mg a.i./L, was studied in a pH 9 buffer (borate, molarity not reported) solution that was irradiated continuously using a filtered xenon lamp for 166 hours at 25°C. The nominal intensity of the lamp was 700 W/m²; the actual intensity was quantified using an actinometer. This experiment was conducted in accordance with the EC Commission Directive 94/37/EC and the draft OECD guideline "Phototransformation of Chemicals in Water-Direct and Indirect Photolysis", and in compliance with OECD and German GLP standards. The test system consisted of cylindrical glass trays (21 mm diameter, 10 mL volume) containing treated buffer solution. Three trays of each concentration were placed in the irradiation chamber and covered with quartz glass plates and maintained at 25 ± 5°C using a circulator. The dark controls were kept in a darkened incubator. Replicate samples of each concentration were collected at 0, 2, 4, 8, 16, 24, 32, 40, 48, 64, 87.5, 120, 144, and 166 hours posttreatment; sampling may have been done by collecting aliquots of the bulk irradiated solutions. The test solutions were analyzed for o-sulfamuron and its transformation products by HPLC. Compounds were identified by comparison to the retention times of unlabeled reference standards of o-sulfamuron, DOP urea, DBS acid, DOR amine, and DB amine. Volatiles were not collected.

The temperature of the irradiated solutions was maintained at 25 ± 5°C and of the dark controls at 25°; no supporting data provided. The pH of the buffer solutions and the sterility of the samples were not reported.

A material balance was not determined. The test material was not radiolabeled, and the test solution was analyzed only for o-sulfamuron.

O-Sulfamuron was relatively stable in the irradiated solutions, declining 4.9-5.6% of the applied during *ca.* 7 days of continuous irradiation. O-Sulfamuron was stable in the dark controls. No transformation products were isolated from either the irradiated samples or dark controls. Volatiles were not collected.

Using first order linear regression analysis (Excel 2003), o-sulfamuron dissipated with calculated half-lives of 85, 87, and 98 days, applied at 10, 20, and 30 mg a.i./L, respectively, yielding a calculated half-life (combined data) of 90 days based on the continuous irradiation used in the study. These half-lives are of uncertain value since they are extrapolated well beyond the 6.9-day duration of the study.

Since o-sulfamuron was stable in the dark control, the **phototransformation half-life** of o-sulfamuron is 2,150 hours (*ca.* 90 days) based on the continuous irradiation used in the study. Based on a 12-hour light/12-hour dark cycle, the calculated phototransformation half-life of o-sulfamuron is **180 days** (*ca.* 6 months).

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The **environmental phototransformation half-life** of o-sulfamuron could not be determined because the intensity of the artificial light was not compared to natural sunlight. Based on calculations using the quantum yield, the study author estimated an environmental phototransformation half-life of >6 months.

A transformation pathway was not provided and could not be developed since o-sulfamuron was relatively stable to photolysis and no transformation products were isolated.

The quantum yield of o-sulfamuron in pH 9 buffer was estimated to be an average of $1.56 \times 10^{-4} \pm 2.3 \times 10^{-5}$.

Results Synopsis

pH 9	Half-life	Transformation products	
		Major	Minor
<u>10 mg a.i./L</u>			
Irradiated	2,035 hours (84.8 days).	None.	None.
Dark	Stable.	None.	None.
<u>20 mg a.i./L</u>			
Irradiated	2,089 hours (87.0 days).	None.	None.
Dark	Stable.	None.	None.
<u>30 mg a.i./L</u>			
Irradiated	2,351 hours (98.0 days).	None.	None.
Dark	Stable.	None.	None.
<u>10, 20, 30 mg a.i./L (combined data)</u>			
Irradiated	2,150 hours (89.6 days).	None.	None.
Dark	Stable.	None.	None.

Study Acceptability: This study is classified as **supplemental**, as the study was terminated after *ca.* 7 days of continuous irradiation, at which time >94% of the applied o-sulfamuron remained undegraded. Furthermore, sterility was not confirmed, the intensity of the artificial light was not compared to natural sunlight, and raw sample concentration and temperature data were not reported.

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I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with the European Union Directive 94/37/EC, Section 2.9.2 and 2.9.3 (1994) and the draft OECD guideline "Phototransformation of Chemicals in Water-Direct and Indirect Photolysis" (2000, pp. 3, 4, 13). Significant deviations from the objectives of Subdivision N guidelines include:

The study was terminated after only 166 hours of continuous irradiation, at which time >94% of the applied o-sulfamuron remained undegraded. Subdivision N guidelines specify that a photodegradation study be conducted for 30 days (15 days if irradiation is continuous).

The artificial light intensity was not compared to natural sunlight, as specified by Subdivision N guidelines.

The sterility of the samples was not reported. Subdivision N guidelines specify that glassware should be sterilized to minimize the possibility of microbial degradation.

COMPLIANCE: This study was conducted in compliance with OECD (1997) and German GLP standards (2002; pp. 3, 4a, 4b, 13). Signed and dated Data Confidentiality, Certificate of Authenticity, GLP, and Quality Assurance statements were provided (pp. 2-4b, 10-11).

A. MATERIALS:

1. Test Material O-Sulfamuron (unlabeled; p. 15).

Chemical Structure: See DER Attachment 1.

Description: Whitish powder, technical grade (p. 15).

Purity: Radiochemical purity: The test material was not radiolabeled (p. 15).
Lot No.: 20689/27.
Analytical purity: 98.19%.
Specific activity: Not Applicable.
Location of the radiolabel: Not applicable.

Storage conditions of test chemicals: The test material was stored at 4-6°C in the dark (p. 16).

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Physico-chemical Properties of O-sulfamuron:

Parameter	Value	Comment
Molecular weight (g/mol)	Not reported.	
Chemical formula	C ₁₆ H ₂₀ N ₆ O ₆ S.	
Water Solubility	23.9 mg/L.	
Vapor Pressure/Volatility	Not reported.	
UV Absorption	914.1 L-mol/cm at 290 nm; no significant adsorption above 400 nm.	
Pka	Not reported.	
K _{ow} /log K _{ow}	Not reported.	
Stability of compound at room temperature.	Not reported.	

Data obtained from pp. 15-16, 32-33; Attachment 1, Figure 4, p. 41; and Attachment 4, Table 12, pp. 45-46 in the study report.

2. Buffer Solution

The following buffer solution was prepared:

Table 1: Description of buffer solutions.

pH	Type and molarity of buffer	Composition
9	Borate (Molarity not reported)	Prepared using Merck Titrisol ready-to-use buffer, which is comprised of boric acid, potassium chloride, and NaOH.

Data obtained from pp. 23, 25 in the study report.

3. Details of light source

Table 2: Artificial light source.

Property	Details
Nature of light source	Xenon lamp (Atlas/Hanau Suntest CPS+).
Emission wavelength spectrum	290-800 nm.
Light intensity	Nominal 700 W/m ² ; actual intensity measured using a p-nitroanisole/pyridine actinometer.
Filters used	Coated quartz and special UV glass.
Relationship to natural sunlight	The spectral energy distribution of the artificial light was reported to be comparable to the solar spectrum. A graphical representation of the wavelength distribution of only the artificial light is presented in Attachment 2, p. 42. A direct comparison of the intensity of the artificial light to sunlight was not provided by the study author.

Data obtained from pp. 24-25 and 27, and Attachment 2, Figure 5, p. 42 in the study report.



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B. EXPERIMENTAL CONDITIONS:

1. Preliminary Study: In order to select the pH at which to conduct the study and to determine UV adsorbance, o-sulfamuron was dissolved in buffer solutions of pH 5, 7, and 9 (p. 24). The absorption of the buffer solutions was determined by UV/VIS. No significant differences were observed, so it was concluded that absorption was not dependent upon pH (Attachment 1, Figure 4, p. 41). The definitive study was conducted at pH 9 where hydrolytic stability was highest.

2. Experimental Conditions

Table 3: Experimental Parameters.

Parameters		Details
Duration of the study		166 hours.
Test concentrations (mg a.i./L) Nominal: Measured:		10, 20, 30 10.05, 19.78, 30.33
Dark controls used (Yes/No)		Yes.
Replication	Dark	Not reported; possibly three. For each concentration, bulk solutions were prepared and transferred to three sample vessels. The sample vessels appear to have been subsampled throughout the study.
	Irradiated	
Preparation of the test medium:	Volume used/treatment	Bulk solutions were prepared and transferred into individual sample vessels.
	Method of sterilization:	The treated buffer solution was filtered (<0.45 µm).
	Co-solvent, if any:	None, the test substance was dissolved in water.
Test apparatus (Type/Material/Volume)		Irradiated: Cylindrical glass trays (10 mL volume, 21 mm diameter) containing treated buffer solution were placed in the irradiation chamber and covered with quartz glass plates. Every tray was stirred with a magnetic stirrer. The temperature was maintained at 25 ± 5°C using a circulating waterbath. Dark: The dark controls were incubated in identical glass trays and kept in an incubator at 25°C.
Details of traps for volatile compounds, if any		Volatiles were not trapped.
If no traps were used, is the test system closed/open		Closed.
Is there any indication of the test material adsorbing to the walls of the test apparatus?		No.
Experimental Conditions Temperature: Duration of light/darkness:		Irradiated: 25 ± 5°C; dark control: 25°C. Continuous.
Other details, if any		None.

Data obtained from pp. 25, 26 and 35, and Table 4, p. 25 in the study report.

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3. Supplementary experiments: To determine quantum yield, an actinometer consisting of p-nitroanisole/pyridine was prepared (p. 22). The p-nitroanisole/pyridine solutions were placed in cylindrical glass trays and irradiated with the test solutions (p. 25).

4. Sampling:

Table 4: Sampling details.

Observations	Details
Sampling intervals for the parent/transformation products	0, 2, 4, 8, 16, 24, 32, 40, 48, 64, 87.5, 120, 144 and 166 hours.
Sampling method	Three aliquots (50-100 µL) of the irradiated and dark controls were collected at all sampling intervals.
Method of sampling volatile compounds, if any	Volatiles were not collected.
Sampling intervals/times for: Sterility check pH measurement	Not reported. Not reported.
Sample storage before analysis, if any	Not reported.
Other observation, if any	None.

Data obtained from pp. 25-26 and Table 6, p. 35 in the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: The samples were diluted before HPLC analysis, but were otherwise analyzed without modification (p. 21).

Volatile residue determination: Volatiles were not collected.

Total ¹⁴C measurement: The test substance was not radiolabeled.

Derivatization method, if used: A derivatization method was not employed.

Identification and quantification of parent compound: Aliquots of each sample were analyzed by HPLC using the following operating conditions: ODS 3 Inertsil column (250 x 4.6 mm, 5 µm), a mobile phase gradient of (A) acetonitrile and (B) 0.004M KH₂PO₄ in water [percent A:B (v:v): 0-2 minutes, 30:70; 2-7 minutes, decreasing to 85:15; 7-10 minutes, 85:15; 10-12 minutes, increasing to 30:70; 12-18 minutes, hold at 30:70], flow rate 1.0 mL/minute; with UV detection (200-356 nm; pp. 20-21). O-Sulfamuron was identified by comparison to the relative retention time of the test substance (Rt ca. 9.7 minutes).

Identification and quantification of transformation products: Transformation products were separated and quantified using HPLC as described for the parent and were identified by comparison to the relative retention time of unlabeled reference standards of:



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Compound	Purity	Retention Time (minutes)
DOP urea	99.77%	6.4
DBS acid	100%	3.1
DOP amine	98%	6.6
DB amine	99.5%	5.3

Data obtained from pp. 16-19 and 21 of the study report.

Detection limits (LOD, LOQ) for the parent: The limit of detection (LOD) for the HPLC method was 0.034 mg/mL (p. 21). The limit of quantification (LOQ) was 0.111 mg/L.

Detection limits (LOD, LOQ) for the transformation: LOD and LOQ values were identical to those for the parent.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The temperature of the irradiated solutions was maintained at $25 \pm 5^\circ\text{C}$ and of the dark controls was 25°C ; no supporting data provided (pp. 25-26). The pH of the buffer solutions and the sterility of the samples were not reported.

B. MASS BALANCE: A material balance was not determined. The test material was not radiolabeled, and the test solution was analyzed only for o-sulfamuron.

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Table 5: Phototransformation of O-sulfamuron, Expressed as Percentage of the Applied Radioactivity, in pH 9 Buffer.

Compound	Sampling times (hours)														
	0	2	4	8	16	24	32	40	48	64	87.5	120	144	166	
10 mg a.i./L															
O-Sulfamuron	Irradiated	100.0	94.7	100.7	102.5	99.7	101.1	102.1	100.5	99.4	98.4	100.4	95.6	94.4	94.8
	Dark		95.1	98.9	103.1	113.7	103.1	101.3	102.4	101.3	104.1	103.7	102.8	101.5	101.5
Transformation Products	Irradiated	No transformation products were detected.													
	Dark														
CO ₂ and volatile organics	Irradiated	Volatiles were not addressed.													
	Dark														
Total recovery	Irradiated	Total recoveries were not determined; samples were analyzed only for o-sulfamuron.													
	Dark														
20 mg a.i./L															
O-Sulfamuron	Irradiated	100.0	96.9	101.2	102.0	104.7	102.7	101.3	102.1	100.0	101.4	102.1	97.2	97.2	94.3
	Dark		97.6	100.8	100.4	129.9	100.4	102.9	102.9	102.9	102.7	106.2	99.6	102.4	102.4
Transformation Products	Irradiated	No transformation products were detected.													
	Dark														
CO ₂ and volatile organics	Irradiated	Volatiles were not addressed.													
	Dark														
Total recovery	Irradiated	Total recoveries were not determined; samples were analyzed only for o-sulfamuron.													
	Dark														

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Compound	Sampling times (hours)													
	0	2	4	8	16	24	32	40	48	64	87.5	120	144	166
30 mg a.i./L														
O-Sulfamuron	Irradiated	98.2	100.6	100.6	100.2	99.9	99.0	99.1	97.9	99.1	100.3	96.5	95.1	95.2
	Dark	98.0	99.0	103.1	107.0	103.1	101.5	101.5	101.5	100.8	102.6	102.7	100.1	100.1
Transformation Products	Irradiated	No transformation products were detected.												
	Dark	No transformation products were detected.												
CO ₂ and volatile organics	Irradiated	Volatiles were not addressed.												
	Dark	Volatiles were not addressed.												
Total recovery	Irradiated	Total recoveries were not determined; samples were analyzed only for o-sulfamuron.												
	Dark	Total recoveries were not determined; samples were analyzed only for o-sulfamuron.												

Data obtained from p. 25 and Table 6, p. 35, in the study report. Averaged concentration data were converted to percent of applied, as no raw concentration or percent of applied data were provided in the MRID (DER Attachment 2).

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C. TRANSFORMATION OF PARENT COMPOUND: O-Sulfamuron was relatively stable in the irradiated solutions, declining 4.8-5.7% of the applied during *ca.* 7 days of continuous irradiation (p. 25; Table 6, p. 35; DER Attachment 2). O-Sulfamuron was stable in the dark controls.

In the irradiated solution treated at 10 mg a.i./L, o-sulfamuron ranged from 94.7 to 102.5% with no discernable pattern between 0 and 87.5 hours posttreatment, and from 94.4 to 95.6% between 120 and 166 hours (study termination). In the dark control, o-sulfamuron averaged 95.1% of the applied at 2 hours posttreatment and 101.5% at 166 hours posttreatment.

In the irradiated solution treated at 20 mg a.i./L, o-sulfamuron ranged from 96.9 to 104.7% with no discernable pattern between 0 and 87.5 hours posttreatment, averaged 97.2% at 120 to 144 hours, and 94.3% at 166 hours. In the dark control, o-sulfamuron averaged 97.6% of the applied at 2 hours posttreatment and 102.4% at 166 hours posttreatment.

In the irradiated solution treated at 30 mg a.i./L, o-sulfamuron ranged from 97.9 to 100.6% with no discernable pattern between 0 and 87.5 hours posttreatment, averaged 96.5% at 120 hours, and 95.1-95.2% at 166 hours. In the dark control, o-sulfamuron averaged 98.0% of the applied at 2 hours posttreatment and 100.1% at 166 hours posttreatment.

HALF-LIFE/DT₅₀/DT₉₀: Using first order linear regression analysis (Excel 2003), o-sulfamuron dissipated with calculated half-lives of 85, 87, and 98 days, applied at 10, 20, and 30 mg a.i./L, respectively, yielding a calculated half-life (combined data) of 90 days based on the continuous irradiation used in the study. These half-lives are of uncertain value since they are extrapolated well beyond the 6.9-day duration of the study. O-sulfamuron was stable in the dark controls.

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Half-lives/DT₅₀/DT₉₀

Treatment	First order linear			DT ₅₀ (days)	DT ₉₀ (days)
	Half-life (hours)	Regression equation	r ²		
10 mg/L					
Irradiated	2,035	y = -0.0003406x - 4.6119	0.4282	---	---
Dark	Stable			---	---
20 mg/L					
Irradiated	2,089	y = -0.0003319x + 4.6248	0.4146	---	---
Dark	Stable			---	---
30 mg/L					
Irradiated	2,351	y = -0.0002948x + 4.6079	0.6953	---	---
Dark	Stable			---	---
Combined					
Irradiated	2,150	y = -0.0003224x + 4.6149	0.4398	---	---
Dark	Stable			---	---

Calculated using data obtained from p. 25 and Table 6, p. 35 in the study report (DER Attachment 2).

Since o-sulfamuron was stable in the dark control, the **phototransformation half-life** of o-sulfamuron is 2,150 hours (ca. 90 days) based on the continuous irradiation used in the study. Based on a 12-hour light/12-hour dark cycle, the calculated phototransformation half-life of o-sulfamuron is **180 days** (ca. 6 months).

The **environmental phototransformation half-life** of o-sulfamuron could not be determined because the intensity of the artificial light was not compared to natural sunlight. Based on calculations using the quantum yield, the study author estimated an environmental phototransformation half-life of >6 months.

TRANSFORMATION PRODUCTS: No transformation products were isolated from either the irradiated samples or dark controls (p. 34).

VOLATIZATION: Volatiles were not collected.

TRANSFORMATION PATHWAY: A transformation pathway was not provided. O-sulfamuron was relatively stable to photolysis; no transformation products were isolated (p. 34).

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Based on the results of the study, the quantum yield of o-sulfamuron in pH 9 buffer was estimated to be an average of $1.56 \times 10^{-4} \pm 2.3 \times 10^{-5}$ (p. 37).

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III. STUDY DEFICIENCIES

1. The study was terminated after only 166 hours or *ca.* 6.9 days of continuous irradiation, at which time >94% of the initial o-sulfamuron remained undegraded. Subdivision N guidelines specify that a photodegradation study be conducted for 30 days (15 days if irradiation is continuous) or until the half-life of the parent is clearly established. Although the data suggest that the half-life of o-sulfamuron is >30 days, an additional 8 days of data would have provided greater confidence in the results from the half-life calculations.
2. Raw sample concentration data were not provided, nor were raw temperature data. Sample concentration data were reported as mean values of two parallel samples from up to three possible replicates. Raw data should be reported to confirm statistical calculations.
3. The study methods were poorly described. Three vessels of each concentration (nine total) plus three vessels containing the actinometer solution were placed in the irradiation apparatus at the same time. The volume of each vessel was 10 mL, but it was not certain that the vessel was completely filled. It could not be determined with any certainty whether each vessel was subsampled at each of the thirteen sampling intervals, whether random subsamples were collected (so that only duplicate samples were collected at each interval), or whether the experiment was repeated several times using different intervals and entire vessels were collected. The study author states that "...only 12 samples of the test solution could be irradiated simultaneously..." (p. 25) and also that data represent "...mean values of both parallel samples..." (Table 6, p. 35). "Parallel samples" may refer to irradiated vs dark control samples rather than replicate samples.
4. A direct comparison of the intensity of the artificial light to sunlight was not provided. Rather, several assumptions (water surface 100 m², depth 10 cm, zenith angle noon minus 1/6 of daylight; p. 32) and the quantum yield were used to predict the minimum, maximum and mean half-lives of o-sulfamuron at 52°N throughout the year (Table 10, p. 39). The half-life of o-sulfamuron in June was estimated to average 6.6 months, which is comparable to the photodegradation half-life.
5. The sterility of the samples was not reported. Subdivision N guidelines specify that the sterility of glassware should be confirmed to minimize the possibility of microbial degradation.

IV. REVIEWER'S COMMENTS

1. The molarity of the buffer solution was not reported. A commercial ready-to-use borate buffer was used in the study.



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2. The final sampling interval was reported to be as 160 hours (p. 26) in the text and 166 hours in the data table (Table 6, p. 35).

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-2. Photolysis studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.
2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.



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Attachment 1: Structures of Parent Compound and Transformation Products



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Orthosulfamuron [IR5878; S3]

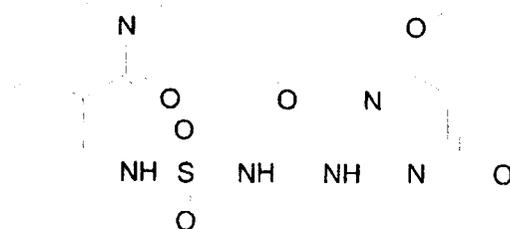
IUPAC Name: 1-(4,6-Dimethoxypyrimidin-2-yl)-3-[2-(dimethylcarbamoyl)phenylsulfamoyl]urea.

CAS Name: 2-[[[[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]amino]-N,N-dimethylbenzamide.

CAS Number: 213464-77-8.

SMILES String: CN(C(=O)c1cccc1NS(=O)(=O)NC(=O)Nc1nc(cc(n1)OC)OC)C
(ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 7/6/06.



Data Evaluation Report on the Photolysis of O-sulfamuron (IR5878) in Water

PMRA Submission Number {.....}

EPA MRID Number 46588509

Identified Compounds

17

Data Evaluation Report on the Photolysis of O-sulfamuron (IR5878) in Water

PMRA Submission Number {.....}

EPA MRID Number 46588509

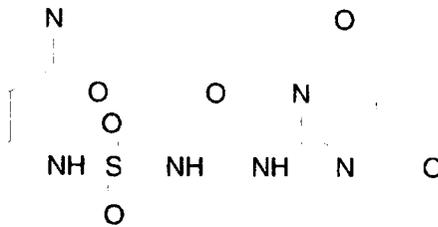
Orthosulfamuron [IR5878; S3]

IUPAC Name: 1-(4,6-Dimethoxypyrimidin-2-yl)-3-[2-(dimethylcarbamoyl)phenylsulfamoyl]urea.

CAS Name: 2-[[[[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]amino]-N,N-dimethylbenzamide.

CAS Number: 213464-77-8.

SMILES String: CN(C(=O)c1cccc1NS(=O)(=O)NC(=O)Nc1nc(cc(n1)OC)OC)C
(ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 7/6/06.



Data Evaluation Report on the Photolysis of O-sulfamuron (IR5878) in Water

PMRA Submission Number {.....}

EPA MRID Number 46588509

Unidentified Reference Compounds

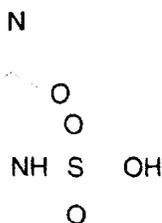
Data Evaluation Report on the Photolysis of O-sulfamuron (IR5878) in Water

PMRA Submission Number {.....}

EPA MRID Number 46588509

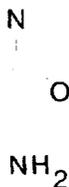
DBS acid [IR7863; S1]

IUPAC Name: (2-Dimethylcarbamoylphenyl)sulfamic acid.
CAS Name: Sodium (2-dimethylcarbamoylphenyl)sulfamate.
CAS Number: Not reported.



DB amine [S4]

IUPAC Name: 2-Amino-N,N-dimethylbenzamide.
CAS Name: Not reported.
CAS Number: Not reported.



Data Evaluation Report on the Photolysis of O-sulfamuron (IR5878) in Water

PMRA Submission Number {.....}

EPA MRID Number 46588509

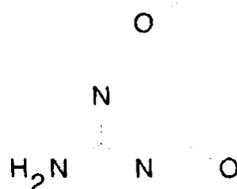
DOP amine [S13]

IUPAC Name: 4,6-Dimethoxypyrimidin-2-yl amine.

2-Amino-4,6-dimethoxypyrimidine.

CAS Name: Not reported.

CAS Number: Not reported.

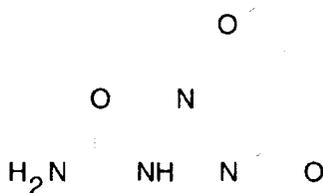


DOP urea [IR7825; S12]

IUPAC Name: N-(4,6-Dimethoxypyrimidin-2-yl)-urea.

CAS Name: 4,6-Dimethoxy-2-pyrimidinyl urea.

CAS Number: Not reported.



Attachment 2: Excel Spreadsheets

Chemical: O-sulfamuron
MRID: 46588509
PC Code: 108209
Guideline: 161-2

Phototransformation of o-sulfamuron in pH 9 buffer, expressed as mg a.i./L.

Irradiated Samples (mg/L)				Dark Controls (mg/L)			
Irradiation time (hr)	Concentration (mg/L)			irradiation time (hr)	Concentration (mg/L)		
	10	20	30		10	20	30
0	10.05	19.78	30.33	0	10.05	19.78	30.33
2	9.52	19.17	29.78	2	9.56	19.30	29.73
4	10.12	20.01	30.52	4	9.94	19.94	30.03
8	10.30	20.17	30.52	8	10.36	19.85	31.26
16	10.02	20.70	30.40	16	11.43	25.69	32.44
24	10.16	20.32	30.31	24	10.36	19.85	31.26
32	10.26	20.03	30.04	32	10.18	20.35	30.79
40	10.10	20.19	30.07	40	10.29	20.35	30.80
48	9.99	19.78	29.68	48	10.18	20.35	30.79
64	9.89	20.05	30.07	64	10.46	20.31	30.56
87.5	10.09	20.20	30.43	87.5	10.42	21.00	31.12
120	9.61	19.22	29.27	120	10.33	19.70	31.16
144	9.49	19.22	28.85	144	10.20	20.26	30.36
166	9.53	18.66	28.86	166	10.20	20.26	30.36

Data obtained from p. 25 and Table 6, p. 35 of study report. Only mean values reported by study author.

Phototransformation of o-sulfamuron in pH 9 buffer, expressed as % initial radioactivity.

Irradiated Samples (% of initial)				Dark Controls (% of initial)			
Irradiation time (hr)	Concentration (mg/L)			irradiation time (hr)	Concentration (mg/L)		
	10	20	30		10	20	30
0	100.0	100.0	100.0	0	100.0	100.0	100.0
2	94.7	96.9	98.2	2	95.1	97.6	98.0
4	100.7	101.2	100.6	4	98.9	100.8	99.0
8	102.5	102.0	100.6	8	103.1	100.4	103.1
16	99.7	104.7	100.2	16	113.7	129.9	107.0
24	101.1	102.7	99.9	24	103.1	100.4	103.1
32	102.1	101.3	99.0	32	101.3	102.9	101.5
40	100.5	102.1	99.1	40	102.4	102.9	101.5
48	99.4	100.0	97.9	48	101.3	102.9	101.5
64	98.4	101.4	99.1	64	104.1	102.7	100.8
87.5	100.4	102.1	100.3	87.5	103.7	106.2	102.6
120	95.6	97.2	96.5	120	102.8	99.6	102.7
144	94.4	97.2	95.1	144	101.5	102.4	100.1
166	94.8	94.3	95.2	166	101.5	102.4	100.1

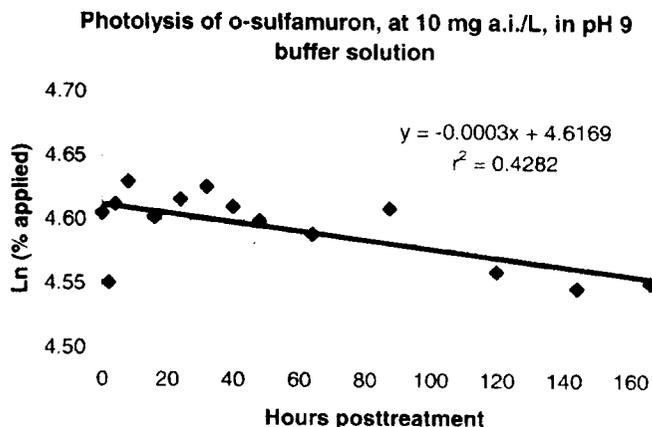
24

Chemical: O-sulfamuron
PC Code: 108209
MRID: 46588509
Guideline: 161-2

Irradiated, 10 mg a.i./L

Half life (hours): 2035.1 (84.8 days)

Hours posttreatment	O-sulfamuron	
	% applied	Ln (% applied)
0	100.0	4.6052
2	94.7	4.5510
4	100.7	4.6121
8	102.5	4.6297
16	99.7	4.6022
24	101.1	4.6161
32	102.1	4.6259
40	100.5	4.6101
48	99.4	4.5992
64	98.4	4.5891
87.5	100.4	4.6091
120	95.6	4.5604
144	94.4	4.5478
166	94.8	4.5520



Data obtained from p. 25 and Table 6, p. 35 of the study report and DER Attachment 2.

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.654386872
R Square	0.428222179
Adjusted R Squ	0.380574027
Standard Error	0.022585582
Observations	14

ANOVA

	df	SS	MS	F	Significance F
Regression	1	0.004584433	0.004584	8.987173	0.011111
Residual	12	0.006121302	0.00051		
Total	13	0.010705736			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.611948904	0.008603883	536.0311	1.2E-27	4.593203	4.630695	4.593203	4.630695
X Variable 1	-0.0003406	0.000113614	-2.997861	0.011111	-0.000588	-9.31E-05	-0.000588	-9.31E-05

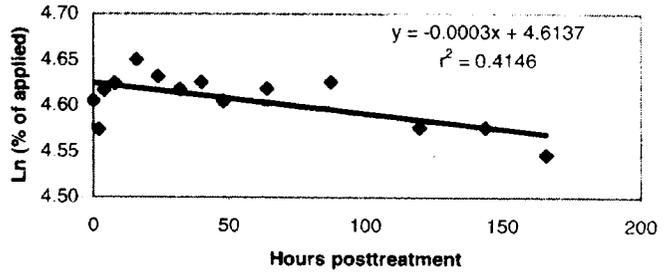
Chemical: O-sulfamuron
 PC Code: 108209
 MRID: 46588509
 Guideline: 161-2

Irradiated, 20 mg a.i./L

Half life (hours): 2088.6 (87.0 days)

Hours posttreatment	O-sulfamuron	
	% applied	Ln (% applied)
0	100	4.6052
2	96.9	4.5738
4	101.2	4.6167
8	102.0	4.6247
16	104.7	4.6506
24	102.7	4.6321
32	101.3	4.6177
40	102.1	4.6257
48	100.0	4.6052
64	101.4	4.6187
87.5	102.1	4.6262
120	97.2	4.5765
144	97.2	4.5765
166	94.3	4.5469

Photolysis of o-sulfamuron, at 20 mg a.i./L, in pH 9 buffer solution



Data obtained from p. 25 and Table 6, p. 35 of the study report and DER Attachment 2.

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.643880365
R Square	0.414581924
Adjusted R Squ	0.365797084
Standard Error	0.022630848
Observations	14

ANOVA

	df	SS	MS	F	Significance F
Regression	1	0.004352383	0.004352	8.498171	0.012956
Residual	12	0.006145863	0.000512		
Total	13	0.010498247			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.62479874	0.008621127	536.4494	1.19E-27	4.606015	4.643583	4.606015	4.643583
X Variable 1	-0.000331868	0.000113842	-2.915162	0.012956	-0.00058	-8.38E-05	-0.00058	-8.38E-05

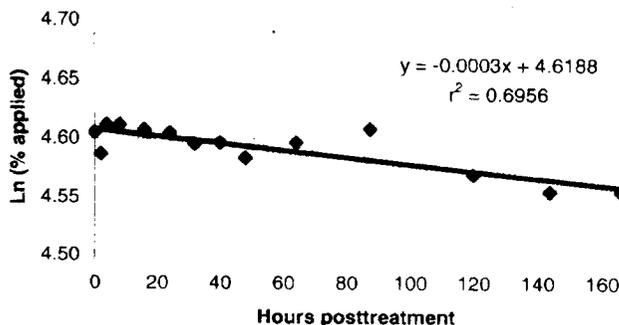
Chemical: O-sulfamuron
 PC Code: 108209
 MRID: 46588509
 Guideline: 161-2

Irradiated, 30 mg a.i./L

Half life (hours) 2351.1 (98.0 days)

Hours posttreatment	O-sulfamuron	
	% applied	Ln (% applied)
0	100	4.6052
2	98.2	4.5869
4	100.6	4.6114
8	100.6	4.6114
16	100.2	4.6075
24	99.9	4.6045
32	99.0	4.5956
40	99.1	4.5966
48	97.9	4.5835
64	99.1	4.5966
87.5	100.3	4.6085
120	96.5	4.5696
144	95.1	4.5551
166	95.2	4.5555

Photolysis of O-sulfamuron, at 30 mg a.i./L, in pH 9 buffer solution



Data obtained from p. 25 and Table 6, p. 35 of the study report and DER Attachment 2.

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.833821663
R Square	0.695258566
Adjusted R Squ	0.669863446
Standard Error	0.011201102
Observations	14

ANOVA

	df	SS	MS	F	Significance F
Regression	1	0.003434928	0.003435	27.37764	0.00021
Residual	12	0.001505576	0.000125		
Total	13	0.004940504			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.60789108	0.004267013	1079.887	2.68E-31	4.598594	4.617188	4.598594	4.617188
X Variable 1	-0.000294822	5.63459E-05	-5.232365	0.00021	-0.000418	-0.000172	-0.000418	-0.000172

97

Chemical: O-sulfamuron
PC Code: 108209
MRID: 46588509
Guideline: 161-2

Irradiated, 10, 20 and 30 mg a.i./L

Half life (hours): **2149.8** (89.6 days)

Hours posttreatment	O-sulfamuron % applied	Ln (% applied)
0	100.0	4.6052
2	94.7	4.5510
4	100.7	4.6121
8	102.5	4.6297
16	99.7	4.6022
24	101.1	4.6161
32	102.1	4.6259
40	100.5	4.6101
48	99.4	4.5992
64	98.4	4.5891
87.5	100.4	4.6091
120	95.6	4.5604
144	94.4	4.5478
166	94.8	4.5520
0	100.0	4.6052
2	96.9	4.5738
4	101.2	4.6167
8	102.0	4.6247
16	104.7	4.6506
24	102.7	4.6321
32	101.3	4.6177
40	102.1	4.6257
48	100.0	4.6052
64	101.4	4.6187
87.5	102.1	4.6262
120	97.2	4.5765
144	97.2	4.5765
166	94.3	4.5469
0	100.0	4.6052
2	98.2	4.5869
4	100.6	4.6114
8	100.6	4.6114
16	100.2	4.6075
24	99.9	4.6045
32	99.0	4.5956
40	99.1	4.5966
48	97.9	4.5835
64	99.1	4.5966
87.5	100.3	4.6085
120	96.5	4.5696
144	95.1	4.5551
166	95.2	4.5555

Data obtained from p. 25 and Table 6, p. 35 of the study report and DER Attachment 2.

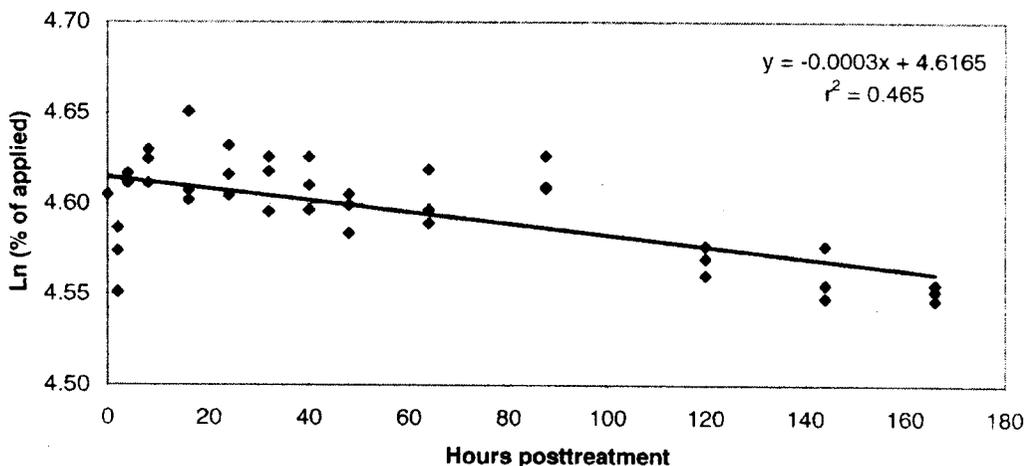
90

Chemical: O-sulfamuron
 PC Code: 108209
 MRID: 46588509
 Guideline: 161-2

Irradiated, 10, 20 and 30 mg a.i./L

Half life (hours): 2149.8 (89.6 days)

Photolysis of o-sulfamuron, at 10-30 mg a.i./L, in pH 9 buffer



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.663205562
R Square	0.439841617
Adjusted R Square	0.425837658
Standard Error	0.01980942
Observations	42

ANOVA					
	df	SS	MS	F	Significance F
Regression	1	0.012325058	0.012325	31.40837527	1.69993E-06
Residual	40	0.015696524	0.000392		
Total	41	0.028021582			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.614879575	0.004356867	1059.22	1.37928E-90	4.606074017	4.623685	4.606074	4.623685
X Variable 1	-0.00032243	5.75324E-05	-5.604318	1.69993E-06	-0.000438707	-0.000206	-0.000439	-0.000206

Attachment 3: Comparison of Artificial Light to Natural Sunlight

DER for MRIO # 46588509

Page 31 is not included in this copy.

Pages _____ through _____ are not included in this copy.

The material not included contains the following type of information:

- _____ Identity of product inert ingredients.
- _____ Identity of product impurities.
- _____ Description of the product manufacturing process.
- _____ Description of quality control procedures.

- _____ Identity of the source of product ingredients.
- _____ Sales or other commercial/financial information.
- _____ A draft product label.
- _____ The product confidential statement of formula.
- _____ Information about a pending registration action.
- FIFRA registration data.
- _____ The document is a duplicate of page(s) _____.
- _____ The document is not responsive to the request.
- _____ Internal deliberative information.
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