TEXT SEARCHABLE DOCUMENT

Data Evaluation Record on the photolysis of chloropicrin in water

PMRA Submission Number {.....}

EPA MRID Number 42900201

Data Requirement:

PMRA Data Code:

EPA DP Barcode: D314391

OECD Data Point: EPA Guideline: 161-2

Test material:

Common name:

Chloropicrin.

Chemical name:

IUPAC name:

Trichloronitromethane. Trichloronitromethane.

CAS name: CAS No.:

76-06-2.

Synonyms

Smiles string:

O=N(=O)C(Cl)(Cl)Cl (EPI Suite, v3.12 SMILES).

Primary Reviewer: Leanne Ganser

Cambridge Environmental

Signature: Leanne Dans

Date: 05/16/07

Secondary Reviewer: Joan Gaidos

Cambridge Environmental

Signature:

Date: 05/16/07

QC/QA Manager: Joan Gaidos

Cambridge Environmental

Signature:

Date: 05/16/07/

Final Reviewer: Faruque Khan

EPA Reviewer

Signature:

Date: 👝 🛵

Company Code:

Active Code:

Use Site Category: EPA PC Code: 081501

CITATION: Moreno, T. and H. Lee. 1993. Photohydrolysis of chloropicrin. Unpublished study performed by Bolsa Research Associates, Inc., Hollister, California, and submitted by Chloropicrin Manufacturers Task Force. Laboratory Project ID No.: BR389.1:93. Experiment start date and completion date not reported. Final report issue date not reported.

EXECUTIVE SUMMARY

The aqueous phototransformation of unlabeled trichloronitromethane (chloropicrin; purity 99.7%), at a nominal concentration of 164 mg a.i./L, was studied in sterile pH 7 buffer (0.05 M phosphate) irradiated on a 12 hour light/12 hour dark cycle using a xenon arc lamp (filters not reported) for 7 days, and continuously for the final 24 hours (108 total hours of irradiation; equivalent to 9 days 12 hour light/dark) at 25°C. The average intensity of the lamp was 1290-1310 lumens/m² and was approximately twice the intensity of natural sunlight in April in Hollister, California. Guidelines followed and compliance with GLP standards were not reported. The test system consisted of Kimble vials (material unspecified) completely filled with treated buffer solution (12 mL), which were pressure-sealed with Teflon-lined screw tops. The irradiated samples were maintained in a circulating water bath at 25°C in a photochamber. Dark controls were wrapped in foil and maintained at 25°C. Single irradiated samples and dark controls were collected at 0, 12, 24, 36, 48, 60, 72, 84 and 108 hours of irradiation. The test solutions were analyzed directly by GC/FID. Samples were analyzed for carbon dioxide by GC/MS.

The temperature was maintained at 25°C (supporting data not provided). The sterility of the samples was not reported. In the irradiated samples, the pH was 6.774-7.043 and in the dark controls was 6.847-6.998.

Overall recoveries were only reported for irradiated samples. The material balances ranged from 59.0-112.2% for chloropicrin plus chloride, 63.2-117.3% for chloropicrin plus nitrate and nitrite, and 62.8-112.1% for chloropicrin plus carbon dioxide and bicarbonate.

Chloropicrin degraded quickly in the irradiated samples, with a reviewer-calculated half-life (first order linear, Excel 2003) of 30 hours (1.3 days) based on the 12-hour light/12-hour dark cycle used in the study (all data). The observed DT50 was *ca.* 40 hours. In the irradiated solutions, chloropicrin decreased from 0.00090-0.00134 M (89-132% of the applied) at 0-12 hours of irradiation to 0.00057-0.000077 M (56-76% of the applied) at 24-36 hours to 0.00022-0.00036 M (22-35% of the applied) at 60 hours of irradiation and was 0.00004-0.00012 M (4-12% of the applied) at 108 hours of irradiation. Chloropicrin was stable in the dark controls, ranging from 0.00075-0.00122 M (74-120% of the applied) with no pattern of decline throughout the study; however, chloropicrin was 0.00159-0.00229 M (156-225% of the applied) at 12 hours of irradiation posttreatment.

In the irradiated samples, two major transformation products were identified as chloride and bicarbonate and two minor transformation products were identified as nitrate and nitrate. In the dark controls, chloride, bicarbonate, nitrate and nitrate were identified as minor transformation products.

In the irradiated samples, chloride increased from $0.214\text{-}0.287 \times 10^{-4} \text{ M}$ (0.7-1.0% of the applied) at time 0 to $12.5\text{-}24.0 \times 10^{-4} \text{ M}$ (42-80% of the applied) at 108 hours of irradiation (study termination). Bicarbonate, estimated from carbon dioxide concentration, increased from $0.04 \times 10^{-4} \text{ M}$

PMRA Submission Number {.....}

EPA MRID Number 42900201

 10^{-4} M at time 0 to 5.73 x 10^{-4} M at 108 hours of irradiation. Nitrate increased from 0.131-0.194 x 10^{-4} M at 0-12 hours of irradiation to 0.654-1.12 x 10^{-4} M at 108 hours of irradiation. Nitrite increased from 0.001-0.003 x 10^{-4} M at time 0 to Carbon dioxide totaled 1.20-1.43 x 10^{-4} M (12.0-14.3% of the applied) at 72-108 hours of irradiation. Volatile organics were not reported.

In the dark controls, chloride ranged from $1.33-9.34 \times 10^{-5} \text{ M}$ (0.4-3.1% of the applied) at 12-72 hours of irradiation and was $0.7-1.1 \times 10^{-5} \text{ M}$ (0.2-0.4% of the applied) at 84-108 hours of irradiation. Bicarbonate, estimated from carbon dioxide concentration, was $\leq 3.24 \times 10^{-5} \text{ M}$ throughout the study. Nitrate ranged from $0.524-1.85 \times 10^{-5} \text{ M}$ throughout the study. Nitrite ranged from $0.225-2.46 \times 10^{-6} \text{ M}$ throughout the study. Carbon dioxide was $\leq 0.81 \times 10^{-5} \text{ M}$ (≤ 0.81 of the applied) throughout the study. Volatile organics were not reported.

Since chloropicrin was stable in the dark control, the phototransformation half-life is equivalent to the half-life observed in the irradiated samples. The **phototransformation half-life** of chloropicrin is 30 days based on the 12-hour light/12-hour dark cycle used in this study.

The study author stated that irradiation with the artificial light was approximately twice the intensity of natural sunlight in April in Hollister, California. Assuming, one day of artificial light is equivalent to two days of natural sunlight, the **environmental phototransformation half-life** of chloropicrin is expected to be *ca.* 60 days.

A transformation pathway was not presented by the study authors. Chloropicrin degrades into chloride, nitrate, bicarbonate and carbon dioxide.

Results Synopsis

| pH 7 | Half-life | Transformation products | | | | |
|------------|-----------------|--|---|--|--|--|
| | (hours) | Major | Minor | | | |
| Irradiated | 30.0 (1.3 days) | Chloride. Bicarbonate. CO ₂ . | Nitrate. Nitrite. | | | |
| Dark | Stable. | None. | Chloride. Bicarbonate. Nitrate. Nitrite. CO _{2.} | | | |

Study Acceptability: This study is classified as supplemental. This study was previously (DER 10/20/94) determined to be unacceptable. The following significant deviation was noted: it was not possible to ascertain if the material balances were complete (material balances were calculated by the study authors from information provided in summary tables); however, various results within the summary tables differed considerably from the results reported in the raw data. Even though the study shows a number of deficiencies, some useful information can be derived from it.

PMRA Submission Number {.....}

EPA MRID Number 42900201

The study was determined to be upgradable if the study authors can verify the material balances. As part of the verification, the study author must adequately address: discrepancies between some of the average chloride and chloropicrin results reported in the summary tables and the average results reported within the raw data; the discrepancies between the nitrate and nitrate results reported in the raw data and those reported in the summary tables; and the accuracy of the carbon dioxide results.

This DER is primarily a reformatting of the DER for MRID 42900201 dated 10/20/94 and signed by Stephanie Syslo. Unless otherwise noted, all page numbers refer to the 10/20/94 DER.

The Chloropicrin Manufacturers' Task Force responded to several EPA questions (pp. 37-38 of Comments on USEPA's Chloropicrin Risk Assessment Phase 3, February 28, 2007; FRL: 8087-4; EPA-HQ-OPP-2006-0661). EPA concluded that the study provided only limited supplemental information on photohydrolysis of chloropicrin due to problems in the study related to the material balance. The registrant responded that the results of this study were comparable to other available data on aqueous photolysis and reported the following examples. Castro and Belser (1981) determined that the photohydrolytic half-life of a 10⁻³M solution of chloropicrin was ca. 5 hours (Castro, C.E., and N.O.Belser. 1981. Photohydrolysis of methyl bromide and chloropicrin. J. Agric. Food Chem. 29:1005-1008).

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED:

Guidelines followed were not reported. A significant deviation from the objectives of Subdivision N guidelines was noted:

It was not possible to ascertain if the material balances were complete (material balances were calculated by the study authors from information provided in summary tables); however, various results within the summary tables differed considerably from the results reported in the raw data.

COMPLIANCE:

Compliance with GLP was not reported. Signed and dated Data Confidentiality, GLP, Certificate of Authenticity, and Quality Assurance statements not were provided.

A. MATERIALS:

1. Test Material

Chloropicrin.

Chemical Structure:

See DER Attachment 1.

Description:

Unlabeled.

PMRA Submission Number {.....}

EPA MRID Number 42900201

Purity:

Radiochemical purity: Radiolabel not reported.

Lot/Batch No.: Not reported. Analytical purity: 99.7%.

Specific activity: Not applicable.

Location of the radiolabel: Radiolabel not reported.

Storage conditions of

test chemicals:

Not reported.

Physico-chemical properties of Chloropicrin:

| Parameter | Value | Comment |
|--|---------------|---------|
| Molecular weight (g/mol) | Not reported. | |
| Chemical formula | Not reported. | * |
| Water Solubility | Not reported. | |
| Vapor Pressure/Volatility | Not reported. | |
| UV Absorption | Not reported. | |
| pKa | Not reported. | |
| K _{ow} /log K _{ow} | Not reported. | |
| Stability of compound at room temperature, if provided | Not reported. | |

2. Buffer Solution

The following buffer solution was prepared:

Table 1: Description of buffer solutions

| pН | Type and molarity of buffer | Composition |
|----|-----------------------------|------------------------------|
| 7 | 0.05M Phosphate | No information was provided. |

Data obtained from p. 2.2 in the 10/20/94 DER.

PMRA Submission Number {.....}

EPA MRID Number 42900201

3. Details of light source

Table 2: Artificial light source

| Property | Details |
|----------------------------------|--|
| Nature of light source | Xenon arc lamp (Heraeus Suntest CPS). |
| Emission wavelength spectrum | 300-800 nm. |
| Light intensity | 1290-1310 lumens/m ² . |
| Filters used | Not reported; however, Appendix II, Figure 1, p. 32 of the study report indicates than irradiance <290 nm was negligible for the artificial light source. |
| Relationship to natural sunlight | A graphical comparison of the artificial light to sunlight is presented in Appendix II, Figures 1-2, pp. 32-33 of the study report. The average intensity of the artificial light was equivalent to <i>ca</i> . 2 times the intensity of natural sunlight in April in Hollister, California. |

Data obtained from pp. 2.2, 2.5 in the 10/20/94 DER and pp. 32-33 in MRID 42900201.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary Study: No preliminary studies were described.

2. Experimental Conditions

Table 3: Experimental Parameters

| Parameters | | Details | | | |
|--|--|---|--|--|--|
| Duration of the study | | 0-7 days, 12 hour light/dark; Day 8, 24 hours continuous irradiation. | | | |
| Test concentrations (mg a.i./L) Nominal: Measured: | | 164. Not reported. | | | |
| Dark controls used (| Yes/No) | Yes. | | | |
| Replication Dark | | 3-5 vials were collected from each treatment at each interval. | | | |
| Replication | Irradiated | 3-5 vials were collected from each treatment at each interval. | | | |
| Duomonation of the | Volume used/treatment | 12 mL. | | | |
| Preparation of the test medium: | Method of sterilization: | Buffers were sterilized by autoclaving. | | | |
| | Co-solvent (name/concentration), if any: | Not reported. | | | |
| Test apparatus (Type/Material/Volume) | | Kimble vials (material unspecified) were filled completely with no headspace with treated buffer solution (12 mL), pressure-sealed with Teflon-lined screw tops and maintained in a circulating water bath at 25°C in a photochamber. | | | |
| | | The dark controls were wrapped in aluminum foil and incubated at 25°C. | | | |

PMRA Submission Number {.....}

EPA MRID Number 42900201

| Parameters | Details | | | | |
|--|---|--|--|--|--|
| Details of traps for volatile compounds, if any | No traps were used. | | | | |
| 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? | Not reported.1 | | | | |
| Experimental Conditions Temperature; Duration of light/darkness: | 25°C. 12 hour light/dark at 0-7 days; continuous at day 8. | | | | |
| Other details, if any | None. | | | | |

Data obtained from pp. 2.2-2.3, 2.5 in the 10/20/94 DER and Table 1, p. 24; Table 4, p. 27 of MRID 42900201. 1 The possible adsorption of chloropicrin to the Kimble vials was not addressed. The study authors of a hydrolysis study (Accession No. 260211) stated that chloropicrin readily adsorbed to glass surfaces.

3. Supplementary experiments: No supplementary studies were described.

4. Sampling:

Table 4: Sampling details

| Observations | Details | | | | |
|--|--|--|--|--|--|
| Sampling intervals for the parent/transformation products | 0, 12, 24, 36, 48, 60, 72, 84 and 108 hours of irradiation. ¹ | | | | |
| Sampling method | 3-5 vials from each treatment were collected at each interval. | | | | |
| Method of sampling volatile compounds, if any | Not reported. | | | | |
| Sampling intervals/times for: Sterility check pH measurement | Not reported. At each sampling interval. | | | | |
| Sample storage before analysis, if any | Not reported. | | | | |
| Other observation, if any | None. | | | | |

Data obtained from p. 2.2 in the 10/20/94 DER and Table 1, p. 24; Table 4, p. 27 of MRID 42900201.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: The samples were analyzed directly, without extraction or concentration (p. 2.2).

Volatile residue determination: Aliquots of selected samples were analyzed directly for carbon dioxide using GC/MS in darkness (method not described; p. 2.2).

Total ¹⁴C **measurement:** Test substance not radiolabeled. A mass balance was performed by summing the concentration of the parent with the individual transformation products (p. 2.4; MRID 42900201, Table 5, p. 28).

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

¹ The study author reported all results based on hours of irradiation.

PMRA Submission Number {.....}

EPA MRID Number 42900201

Identification and quantification of parent compound: Aliquots of the buffer were analyzed by GC/FID using a DB624 megabore column in darkness (not further described; p. 2.2).

Identification and quantification of transformation products: Transformation products were identified as described for the parent compound and using ion-selective electrodes (p. 2.2).

Detection limits (LOD, LOQ) for the parent: Not reported.

Detection limits (LOD, LOQ) for the transformation: Not reported.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The temperature was maintained at 25°C (supporting data not provided; p. 2.2). The sterility of the samples was not reported. In the irradiated samples, the pH was 6.774-7.043 and in the dark controls was 6.847-6.998 (MRID 42900201, Table 1, p. 24; Table 4, p. 27).

B. MASS BALANCE: Overall recoveries were only reported for irradiated samples. The material balances ranged from 59.0-112.2% for chloropicrin plus chloride, 63.2-117.3% for chloropicrin plus nitrate and nitrite, and 62.8-112.1% for chloropicrin plus carbon dioxide and bicarbonate (p. 2.4; MRID 42900201, Table 5, p. 28; Reviewer's Comment 1).

PMRA Submission Number {.....}

EPA MRID Number 42900201

Table 5: Phototransformation of chloropicrin, expressed as concentration (Mol/L), in pH 7 buffer (mean, $n=3,5^1$)

| Compound | Compound | | Sampling times (hours of irradiation) | | | | | | | | | | |
|-------------------------------------|------------|---------------------------|---------------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--|--|--|
| Сотроина | | 0 | 12 | 24 | 36 | 48 | 60 | 72 | 84 | 108 | | | |
| Chloropicrin | Irradiated | - 10.2 x 10 ⁻⁴ | 10.6 x 10 ⁻⁴ | 6.82 x 10 ⁻⁴ | 6.64 x 10 ⁻⁴ | 3.78 x 10 ⁻⁴ | 3.06 x 10 ⁻⁴ | 2.20 x 10 ⁻⁴ | 2.60 x 10 ⁻⁴ | 0.90 x 10 ⁻⁴ | | | |
| Cinoropicini | Dark | | 18.5 x 10 ⁻⁴ | 10.1 x 10 ⁻⁴ | 9.82 x 10 ⁻⁴ | 10.7 x 10 ⁻⁴ | 9.04 x 10 ⁻⁴ | 10.0 x 10 ⁻⁴ | 8.36 x 10 ⁻⁴ | 10.5 x 10 ⁻⁴ | | | |
| Chloride Irradi | Irradiated | 0.249 x 10 ⁻⁴ | 1.83 x 10 ⁻⁴ | 6.99 x 10 ⁻⁴ | 6.97 x 10 ⁻⁴ | 9.09 x 10 ⁻⁴ | 12.3 x 10 ⁻⁴ | 11.0 x 10 ⁻⁴ | 19.4 x 10 ⁻⁴ | 20.5 x 10 ⁻⁴ | | | |
| Cinoride | Dark | 0.249 X 10 | 0.294 x 10 ⁻⁴ | 0.501 x 10 ⁻⁴ | 0.234 x 10 ⁻⁴ | 0.408 x 10 ⁻⁴ | 0.304 x 10 ⁻⁴ | 0.226 x 10 ⁻⁴ | 0.094 x 10 ⁻⁴ | 0.074 x 10 ⁻⁴ | | | |
| Nitrate ² Irradiate Dark | Irradiated | 1.63 x 10 ⁻⁵ | 1.46 x 10 ⁻⁵ | 2.35 x 10 ⁻⁵ | 3.05 x 10 ⁻⁵ | 3.19 x 10 ⁻⁵ | 6.13 x 10 ⁻⁵ | 7.70 x 10 ⁻⁵ | 9.99 x 10 ⁻⁵ | 9.23 x 10 ⁻⁵ | | | |
| | Dark | | 0.577 x 10 ⁻⁵ | 0.524 x 10 ⁻⁵ | 1.33 x 10 ⁻⁵ | 0.617 x 10 ⁻⁵ | 1.85 x 10 ⁻⁵ | -1.30-x 10 ⁻⁵ | 1.16 x 10 ⁻⁵ | 0.986 x 10 ⁻⁵ | | | |
| Nitrite ² | Irradiated | 0.023 x 10 ⁻⁵ | 1.45 x 10 ⁻⁵ | 1.89 x 10 ⁻⁵ | 3.64 x 10 ⁻⁵ | 3.41 x 10 ⁻⁵ | 3.73 x 10 ⁻⁵ | 3.88 x 10 ⁻⁵ | 3.93 x 10 ⁻⁵ | 10.6 x 10 ⁻⁵ | | | |
| Nume | Dark | | 0.242 x 10 ⁻⁵ | 0.246 x 10 ⁻⁵ | 0.140 x 10 ⁻⁵ | 0.130 x 10 ⁻⁵ | 0.119 x 10 ⁻⁵ | 0.126 x 10 ⁻⁵ | 0.127 x 10 ⁻⁵ | 0.120 x 10 ⁻⁵ | | | |
| CO_2 | Irradiated | 0.100 x 10 ⁻⁵ | 1.20 x 10 ⁻⁵ | 7.40 x 10 ⁻⁵ | 6.40 x 10 ⁻⁵ | 7.46 x 10 ⁻⁵ | 6.42 x 10 ⁻⁵ | 12.0 x 10 ⁻⁵ | 12.7 x 10 ⁻⁵ | 14.3 x 10 ⁻⁵ | | | |
| CO_2 | Dark | | 0 | 0.810 x 10 ⁻⁵ | 0 | 0 | 0.810 x 10 ⁻⁵ | 0.408 x 10 ⁻⁵ | 0 | 0.810 x 10 ⁻⁵ | | | |
| Bi- | Irradiated | 0.400×10^{-5} | 4.80 x 10 ⁻⁵ | 29.6 x 10 ⁻⁵ | 25.6 x 10 ⁻⁵ | 29.9 x 10 ⁻⁵ | 25.7 x 10 ⁻⁵ | 48.2 x 10 ⁻⁵ | 50.7 x 10 ⁻⁵ | 57.3 x 10 ⁻⁵ | | | |
| carbonate ³ | Dark | 0.400 X 10 | 0 | 3.24 x 10 ⁻⁵ | 0 | 0 | 3.24 x 10 ⁻⁵ | 1.63 x 10 ⁻⁵ | 0 | 3.24 x 10 ⁻⁵ | | | |
| Volatile | Irradiated | Not reported. | | | | | | | | | | | |
| organics | Dark | Not reported. | | | | | | | | | | | |
| Total | Irradiated | See Reviewer' | s Comment 1. | | | | | | | | | | |
| recovery | Dark | Not reported. | | | | | | | | | | | |

Reviewer-calculated means using data obtained from Table 1, p. 24; Table 4, p. 27; Appendices III-VI, Tables 6-44, pp. 35-73 in MRID 42900201 (Reviewer's Comment 1-3). The reviewer did not convert the data presented by the study author in terms of Mol/L into % of applied as discrepancies existed in the reported data.

¹ At sampling intervals time 0 and 12 hours, n = 3, otherwise, n = 5.

² Discrepancies between the concentration of the calibration standards reported in the narrative evaluation of the study and those listed in the raw data and discrepancies within the raw data between the cover pages and the individual data pages made it unclear which of the appendices corresponded to the nitrate results and which corresponded to the nitrite results (Reviewer's Comment 3).

³ The concentration of the bicarbonate ion was calculated by multiplying the measured concentration of carbon dioxide by 4 (Reviewer's Comment 4).

PMRA Submission Number {.....}

EPA MRID Number 42900201

C. TRANSFORMATION OF PARENT COMPOUND: In the irradiated solutions, chloropicrin decreased from 0.00090-0.00134 M (89-132% of the applied) at 0-12 hours of irradiation to 0.00057-0.000077 M (56-76% of the applied) at 24-36 hours of irradiation to 0.00022-0.00036 M (22-35% of the applied) at 60 hours of irradiation and was 0.00004-0.00012 M (4-12% of the applied) at 108 hours of irradiation (MRID 42900201, Appendix III, Tables 6-14, pp. 35-43 and DER Attachment 2). In the dark control, chloropicrin ranged from 0.00075-0.00122 M (74-120% of the applied) with no pattern of decline throughout the study; however, chloropicrin was 0.00159-0.00229 M (156-225% of the applied) at 12 hours of irradiation posttreatment.

HALF-LIFE/DT50/DT90: Based on first order linear regression analysis (Excel 2003), chloropicrin dissipated from the irradiated samples with a reviewer-calculated half-life of 30 hours, based on the 12-hour light/12-hour dark cycle used in the study (DER Attachment 2). The observed DT50 was *ca.* 40 hours. Chloropicrin was stable in the dark controls.

The study author calculated a half-life of 31.1 hours (p. 2.3).

Half-lives/DT50/DT90

| T | | DE 50 ² | D/T00 | | | |
|------------|-------------------|-----------------------|----------------|------------------------------|----------------|--|
| Treatment | Half-life (hours) | Regression equation | r ² | DT50 ² (hours) | DT90 (days) | |
| Irradiated | 30.0 | y = -0.0231x + 4.8087 | 0.8755 | 31.1 | | |
| Dark | Stable | , | | | | |

¹ Calculated by the reviewer using individual % applied data reviewer-calculated using data obtained from MRID 42900201, Appendix III, Tables 6-14, pp. 35-43 and DER Attachment 2.

Since chloropicrin was stable in the dark control, the phototransformation half-life is equivalent to the half-life observed in the irradiated samples. The **phototransformation half-life** of chloropicrin is 30 days based on the 12-hour light/12-hour dark cycle used in this study.

The study author stated that irradiation with the artificial light was approximately twice the intensity of natural sunlight in April in Hollister, California (p. 2.2). Assuming, one day of artificial light is equivalent to two days of natural sunlight, the **environmental phototransformation half-life** of chloropicrin is expected to be *ca.* 60 days.

TRANSFORMATION PRODUCTS: In the irradiated samples, two major transformation products were identified as chloride and bicarbonate and two minor transformation products were identified as nitrate and nitrate. In the dark controls, chloride, bicarbonate, nitrate and nitrate were identified as minor transformation products.

In the irradiated samples, chloride increased from 0.214-0.287 x 10⁻⁴ M (0.7-1.0% of the applied) at time 0 to 12.5-24.0 x 10⁻⁴ M (42-80% of the applied) at 108 hours of irradiation (study termination; p. 2.3; MRID 42900201, Appendix IV, Tables 15-23, pp. 45-53). Bicarbonate,

² Calculated by the study author using mean molar concentration data first order linear regression techniques (MRID 42900201, Table 3, p. 26).

PMRA Submission Number {.....}

EPA MRID Number 42900201

estimated from carbon dioxide concentration, increased from 0.04×10^{-4} M at time 0 to 5.73 x 10^{-4} M at 108 hours of irradiation (MRID 42900201, Table 1, p. 24). Nitrate increased from 0.131- 0.194×10^{-4} M at 0-12 hours of irradiation to 0.654- 1.12×10^{-4} M at 108 hours of irradiation (MRID 42900201, Appendix V, Tables 24-32, pp. 55-63). Nitrite increased from 0.001- 0.003×10^{-4} M at time 0 to 0.776- 1.87×10^{-4} M at 108 hours of irradiation (MRID 42900201, Appendix VI, Tables 33-44, pp. 65-73).

In the dark controls, chloride ranged from $1.33-9.34 \times 10^{-5}$ M (0.4-3.1% of the applied) at 12-72 hours of irradiation and was $0.7-1.1 \times 10^{-5}$ M (0.2-0.4% of the applied) at 84-108 hours of irradiation (p. 2.3; MRID 42900201, Appendix IV, Tables 15-23, pp. 45-53). Bicarbonate, estimated from carbon dioxide concentration, was $\leq 3.24 \times 10^{-5}$ M throughout the study (MRID 42900201, Table 4, p. 27). Nitrate ranged from $0.524-1.85 \times 10^{-5}$ M throughout the study (MRID 42900201, Appendix V, Tables 24-32, pp. 55-63). Nitrite ranged from $0.225-2.46 \times 10^{-6}$ M throughout the study (MRID 42900201, Appendix VI, Tables 33-44, pp. 65-73).

Table 6: Chemical names and CAS numbers for the transformation products of chloropicrin.

| Applicants Code Name | CAS Number | Chemical Name | Chemical Formula | Molecular Weight (g/mol) | Smiles String |
|--------------------------|------------|---------------|---------------------|-----------------------------|------------------|
| Chloride | <u></u> | | <u></u> | | |
| Nitrate | | - | | | |
| Nitrite | | | ′ | | |
| Bicarbonate ¹ | | | | | |

Data obtained from p. 2.3 in the 10/20/94 DER.

VOLATIZATION: In the irradiated samples, CO₂ totaled 1.20-1.43 x 10^{-4} M (12.0-14.3% of the applied) at 72-108 hours of irradiation (p. 2.3; MRID 42900201, Table 1, p. 24). In the dark controls, CO₂ was $\leq 0.81 \times 10^{-5}$ M (≤ 0.81 of the applied) throughout the study (MRID 42900201, Table 4, p. 27). Volatile organics were not reported.

TRANSFORMATION PATHWAY: A transformation pathway was not presented by the study authors. Chloropicrin degrades into chloride, nitrate, bicarbonate and carbon dioxide.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: No supplementary experiments were described.

III. STUDY DEFICIENCIES

It was not possible to ascertain if the material balances were complete (material balances were calculated by the study authors from information provided in summary tables); however, various results within the summary tables differed considerably from the results reported in the raw data.

¹ Estimated from carbon dioxide concentration.

^{--:} Not reported.

IV. REVIEWER'S COMMENTS

- 1. Based on the information provided in the study, it was not possible to verify that the material balance was complete. Material balances reported by the study authors in Table 5 (p. 28) reflect the sums of the parent with the individual degradates and were reported only for the irradiated samples. However, since the material balances reported were calculated from the summary tables and various results within the summary tables differed considerably from the results reported in the raw data (see points below), the reviewer did not include total recovery in the data table.
- 2. Some of the average chloropicrin and chloride results reported in the summary tables differed considerably from the average results reported within the raw data; therefore, the reviewer presented means calculated from the raw data. The study authors did not provide explanation for these discrepancies.
- 3. Due to discrepancies between the raw data and the summary tables for nitrate and nitrite results, the reviewer presented means calculated from the raw data. The results reported in Mol/L in the raw data were calculated from the numerical results designated in units of mg of nitrogen per L, while results reported in the summary tables were calculated from the same numerical results designated in units of mg of nitrate or nitrite per L. Additionally, discrepancies between the concentration of the calibration standards reported in the narrative evaluation of the study and those listed in the raw data and discrepancies within the raw data between the cover pages and the individual data pages made it unclear which of the appendices corresponded to the nitrate results and which corresponded to the nitrite results.
- 4. The concentration of the bicarbonate ion was calculated from the measured concentration of free carbon dioxide and was based on the equilibrium relationship between pH and the percent of total carbon dioxide as the bicarbonate ion, the carbonate ion and free carbon dioxide (MRID 42900201, Figure 2, p. 16). Based on this relationship, at pH 7, at 20% concentration of free carbon dioxide is in equilibrium with 80% bicarbonate. The concentration of the bicarbonate ion was apparently not confirmed by directly analysis at any sampling interval.
- 5. The reviewer calculated percent of chloropicrin applied with the formula: concentration recovered on day X/concentration recovered on day 0.
- 6. The reviewer also calculated the half-life using only the first 7 day (0-84 hours) 12 hour light/dark cycle and excluding the last 24 hour continuous irradiation between 84 and 108 hours. Based on first-order linear regression analysis, the half-life was 34.1 hours ($r^2 = 0.8577$), which is very similar to the half-life using all data (30.0 hours).

PMRA Submission Number {.....}

EPA MRID Number 42900201

Table 7: Phototransformation of chloropicrin, expressed as percentage of the applied, in pH 7 buffer (mean \pm sd, n= 3.5¹)

| Compound | | · | Sampling times (hours) | | | | | | | |
|--------------|------------|---------|------------------------|---------------|---------------|--------------|---------------|----------------|---------------|----------------|
| | | 0 | 12 | 24 | 36 | 48 | 60 | 72 | 84 | 108 |
| Chloropicrin | Irradiated | 100.0 ± | 104.3 ± 23.9 | 67.1 ± 7.7 | | 37.2 ± 6.2 | 30.1 ± 7.3 | 21.6 ± 3.8 | 25.6 ± 3.0 | 8.9 ± 3.7 |
| | Dark | 8.9 | 182.0 ± 37.7 | 99.2 ± 3.6 | 96.6 ± 4.6 | 105.3 ± 14.5 | 88.9 ± 7.7 | 98.4 ± 16.7 | 82.2 ± 6.4 | 102.9 ± 3.6 |

Data obtained from Appendix III, Tables 6-14, pp. 35-43 in MRID 42900201.

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.

¹ At sampling intervals time 0 and 12 hours, n = 3, otherwise, n = 5.

| Data Evaluation | Record on | the photoly | ysis of | chloropicrin | in water |
|------------------------|-----------|-------------|---------|--------------|----------|
|------------------------|-----------|-------------|---------|--------------|----------|

| PMRA Submission Number {} | EPA MRID Number 42900201 |
|--------------------------------|--|
| ivite i Submission i vanibor j | 211111122 1100310 11 12 10 10 10 10 10 10 10 10 10 10 10 10 10 |

Attachment 1: Structures of Parent Compound and Transformation Products

PMRA Submission Number {.....}

EPA MRID Number 42900201

Chloropicrin

IUPAC Name:

Trichloronitromethane.

CAS Name:

Trichloronitromethane.

CAS Number:

76-06-2.

SMILES String:

O=N(=O)C(Cl)(Cl)Cl (EPI Suite, v3.12 SMILES).

$$\begin{array}{c} \text{Cl} \\ \text{Cl} \\ \text{Cl} \end{array}$$

| PMRA Submission Number { | EPA MRID Number 429002 | 20 |
|--------------------------|------------------------|----|
| | | |

Identified Compounds

PMRA Submission Number {.....}

EPA MRID Number 42900201

Chloropicrin

IUPAC Name:

Trichloronitromethane.

CAS Name:

Trichloronitromethane.

CAS Number:

76-06-2.

SMILES String:

O=N(=O)C(Cl)(Cl)Cl (EPI Suite, v3.12 SMILES).

Nitrate

IUPAC Name:

Not reported.

CAS Name:

Not reported.

CAS Number:

Not reported.

Nitrite.

IUPAC Name:

Not reported.

CAS Name:

Not reported.

CAS Number:

Not reported.

PMRA Submission Number {.....}

EPA MRID Number 42900201

Bicarbonate

IUPAC Name:

Not reported.

CAS Name:

Not reported.

CAS Number:

Not reported.

HO O

Chloride

IUPAC Name:

Not reported.

CAS Name:

Not reported.

CAS Number:

Not reported.

 Cl^-

Carbon Dioxide

IUPAC Name:

Not reported.

CAS Name:

Not reported.

CAS Number:

Not reported.

o=c=o

PMRA Submission Number {.....}

EPA MRID Number 42900201

Attachment 2: Excel Spreadsheets

PMRA Submission Number {.....}

EPA MRID Number 42900201

Chemical: PC Code: MRID: Guideline Chloropicrin 081501 42900201 161-2

Irradiated

| Hours | Chlore | |
|---------------|--------|----------------|
| posttreatment | | Ln (% applied) |
| 0 | 101.31 | |
| 0 | 90.49 | |
| 0 | 108.2 | |
| 12 | 88.52 | 4.4832 |
| . 12 | 92.46 | |
| 12 | 131.8 | |
| 24 | 69.84 | 4.2462 |
| 24 | 62.95 | 4.1423 |
| . 24 | 56.07 | 4.0266 |
| 24 | 70.82 | 4.2601 |
| 24 | 75.74 | 4.3273 |
| 36 | 63.93 | |
| 36 | 71.8 | |
| 36 | 60 | 4.0943 |
| . 36 | 60.98 | 4.1105 |
| 36 | 69.84 | 4.2462 |
| 48 | 29.51 | 3.3847 |
| 48 | 39.34 | 3.6722 |
| 48 | 39.34 | |
| 48 | 32.46 | |
| 48 | 45.25 | |
| 60 | 21.64 | 3.0745 |
| 60 | 22.62 | 3.1188 |
| 60 | 35.41 | 3.5670 |
| . 60 | 35.41 | 3.5670 |
| 60 | 35.41 | 3.5670 |
| 72 | 20.66 | 3.0282 |
| 72 | 24.59 | |
| 72 | 17.7 | 2.8736 |
| 72 | 26.56 | 3.2794 |
| 72 | 18.69 | |
| 84 | 25.57 | |
| 84 | 27.54 | |
| 84 | 29.51 | 3.3847 |
| 84 | 22.62 | 3.1188 |
| 84 | 22.62 | 3.1188 |
| 108 | 11.8 | 2,4681 |
| 108 | 11.8 | 2.4681 |
| . 108 | 5.9 | 1.7750 |
| 108 | 3.93 | 1.3686 |
| 108 | 10.82 | 2.3814 |

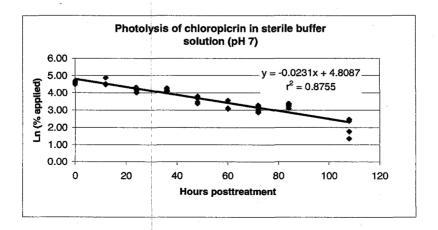
Half life (hours): 30.0

Data imported from calcs worksheet.

Chemical: PC Code: MRID:

Guideline

Chloropicrin 081501 42900201



PMRA Submission Number {.....

EPA MRID Number 42900201

Chemical: PC Code: Chloropicrin

PC Code: MRID: Guideline 081501 42900201 161-2

Irradiated

| $\overline{}$ | Hours | Chloro | nicrin |
|---------------|------------|----------------|------------------|
| pos | ttreatment | | Ln (% applied) |
| | 0 | 101.31 | 4.6182 |
| 1 | 0 | 90.49 | 4.5052 |
| 1 | 0 ' | 108.2 | 4.6840 |
| 1 | 12 | 88.52 | 4.4832 |
| | 12 | 92.46 | 4.5268 |
| | 12 | 131.8 | 4.8813 |
| | 24 | 69.84 | 4.2462 |
| ı | 24 | 62.95 | 4.1423 |
| 1 | 24 | 56.07 | 4.0266 |
| | 24 | 70.82 | 4.2601 |
| | 24 | 75.74 | 4.3273 |
| | 36 | 63.93 | 4.1578 |
| | . 36 | 71.8 | 4.2739 |
| 1 | 36 | 60 | 4.0943 |
| 1 | 36 | 60.98 | 4.1105 |
| 1 | 36 | 69.84 | 4.2462 |
| 1 | 48 | 29.51 | 3.3847 |
| 1 | 48 | 39.34 | 3.6722 |
| | 48 | 39.34 | 3.6722 |
| | 48 | 32.46 | 3.4800 |
| | 48 | 45.25 | 3.8122 |
| 1 | 60 | 21.64 | 3.0745 |
| | 60 | 22.62 | 3.1188 |
| 1 | 60 | 35.41 | 3.5670 |
| 1 | 60 | 35.41 | 3.5670 |
| | 60 | 35.41 | 3.5670 |
| ł | 72 | 20.66 | 3.0282 |
| 1 | 72 | 24.59 | 3.2023 |
| 1 | 72 | 17.7 | 2.8736 |
| 1 | 72 | 26.56 | 3.2794 |
| 1 | 72 | 18.69 | 2.9280 |
| 1 | 84 84 | 25.57 | 3.2414 |
| 1 | 84 84 | 27.54 29.51 | 3.3156 3.3847 |
| 1 | 84 | 29.51 | 3.3847 |
| ŀ | 84 | 22.02 | 3.1100 |

Half life (hours):

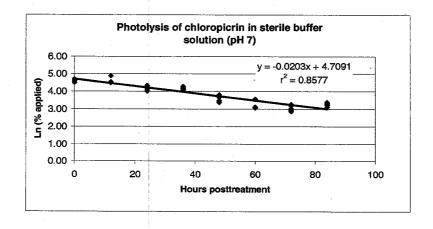
34.1

Data imported from calcs worksheet.

Chemical:

Chloropicrin

PC Code: MRID: Guideline 081501 42900201 161-2



PMRA Submission Number {..

EPA MRID Number 42900201

Chemical: PC Code: MRID:

Chloropicrin 081501 42900201 161-2

Guideline Irradiated

| Hours | Chlorop | |
|---------------|---------|------------|
| posttreatment | Mol/L | Ln (Mol/L) |
| 0 | 0.00103 | -6.8782 |
| 0 | 0.00092 | -6.9911 |
| 0 | 0.0011 | -6.8124 |
| 12 | 0.0009 | -7.0131 |
| 12 | 0.00094 | -6.9696 |
| 12 | 0.00134 | -6.6151 |
| 24 | 0.00071 | -7.2502 |
| 24 | 0.00064 | -7.3540 |
| 24 | 0.00057 | -7.4699 |
| 24 | 0.00072 | -7.2363 |
| 24 | 0.00077 | -7.1691 |
| 36 | 0.00065 | -7.3385 |
| 36 | 0.00073 | -7.2225 |
| 36 | 0.00061 | -7.4021 |
| 36 | 0.00062 | -7.3858 |
| 36 | 0.00071 | -7.2502 |
| 48 | 0.0003 | -8.1117 |
| 48 | 0.0004 | -7.8240 |
| 48 | 0.0004 | -7.8240 |
| 48 | 0.00033 | -8.0164 |
| 48 | 0.00046 | -7.6843 |
| 60 | 0.00022 | -8.4219 |
| 60 | 0.00023 | -8.3774 |
| 60 | 0.00036 | -7.9294 |
| 60 | 0.00036 | -7.9294 |
| 60 | 0.00036 | -7.9294 |
| 72 | 0.00021 | -8.4684 |
| 72 | 0.00025 | -8.2940 |
| 72 | 0.00018 | -8.6226 |
| 72 | 0.00027 | -8.2171 |
| 72 | 0.00019 | -8.5685 |
| 84 | 0.00026 | -8.2548 |
| 84 | 0.00028 | -8.1807 |
| 84 | 0.0003 | -8.1117 |
| 84 | 0.00023 | -8.3774 |
| 84 | 0.00023 | -8.3774 |
| 108 | 0.00012 | -9.0280 |
| 108 | 0.00012 | -9.0280 |
| 108 | 0.00006 | -9.7212 |
| 108 | 0.00004 | -10.1266 |
| . 108 | 0.00011 | -9.1150 |

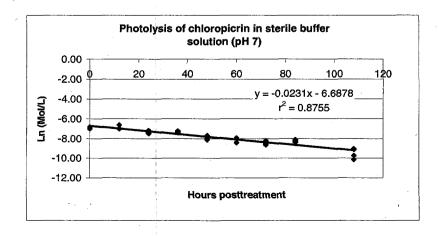
Half life (hours):

30.0

Data imported from calcs worksheet.
Chemical: Chloropicrin
PC Code: 081501
MRID: 42900201

Guideline

161-2



PMRA Submission Number {.....}

EPA MRID Number 42900201

Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2

| Chlorop | oicrin | | | Chlorop | icrir | 1 | |
|----------|--------|----------|-----------|---------|-------|----------|-----------|
| Irradiat | ed | | | Dark | | | |
| Hours | N | Mol/L | % applied | Hours | | Mol/L | % applied |
| | 0 | 0.001017 | 100.00 | • | 0 | 0.001017 | 100.00 |
| | 12 | 0.00106 | 104.23 | | 12 | 0.001849 | 181.81 |
| | 24 | 0.000681 | 66.96 | | 24 | 0.001005 | 98.82 |
| | 36 | 0.000664 | 65.29 | | 36 | 0.000984 | 96.76 |
| | 48 | 0.000378 | 37.17 | | 48 | 0.001067 | 104.92 |
| | 60 | 0.000306 | 30.09 | • | 60 | 0.000906 | 89.09 |
| | 72 | 0.000222 | 21.83 | | 72 | 0.000999 | 98.23 |
| | 84 | 0.000259 | 25.47 | | 84 | 0.000838 | 82.40 |
| • | 108 | 0.000033 | 3 24 | 1 | กล | 0.001044 | 102 65 |

PMRA Submission Number {

EPA MRID Number 42900201

Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2

Mol/L Average 0 0.00103 0.001017 0 0.00092 0 0.0011

| Chloropicrin | | | | | | | Chloropics | in | | | |
|---------------|-----------|---------------|-------------|--------|--------|-----------------|------------|---------|----------|----|------|
| Irradiated | | | % applied | | | | Irradiated | | | | |
| | /lol/L | % applied | | SD | | | Hours | Mol/L | Average | SD | |
| 0 | 0.00103 | 101.31 | 100.00 | - 1 | 8.93 | | C | | 1.02E-03 | | 0.00 |
| 0 | 0.00092 | 90.49 | | | | | | | | | |
| 0 | 0.0011 | 108.20 | | | | | C | 0.0011 | | | |
| 12 | 0.0009 | 88.52 | 104.26 | 2 | 3.93 | | 12 | | 1.06E-03 | | 0.00 |
| 12 | 0.00094 | 92.46 | | | | | 12 | | | | |
| 12 | 0.00134 | 131.80 | | | | | 12 | 0.00134 | | | |
| 24 | 0.00071 | 69.84 | 67.08 | | 7.66 | | 24 | 0.00071 | 6.82E-04 | | 0.00 |
| 24 | 0.00064 | 62.95 | | | | | - 24 | | | | |
| 24 | 0.00057 | 56.07 | | | | | 24 | | | | |
| 24 | 0.00072 | 70.82 | | | | | 24 | | | | |
| 24 | 0.00077 | 75.74 | | | | | 24 | | | | |
| 36 | 0.00065 | 63.93 | | | 5.28 | | 36 | | 6.64E-04 | | 0.00 |
| 36 | 0.00073 | 71.80 | | | | | 36 | | | | |
| 36 | 0.00061 | 60.00 | | | | | . 36 | | | | |
| 36 | 0.00062 | 60.98 | | | | | 36 | | | | |
| 36 | 0.00071 | 69.84 | | | | | 36 | | | | |
| 48 | 0.0003 | 29.51 | | | 6,24 | | 48 | | 3.78E-04 | | 0.00 |
| 48 | 0.0004 | 39.34 | | | | | 48 | 0.0004 | | | |
| 48 | 0.0004 | 39.34 | | | | | 48 | | | | |
| 48 | 0.00033 | 32.46 | | | | | 48 | | | | |
| 48 | 0.00046 | 45.25 | | | | | 48 | 0.00046 | | | |
| 60 | 0.00022 | 21.64 | | | 7.28 | | 60 | | 3.06E-04 | | 0.00 |
| 60 | 0.00023 | 22.62 | | | | | 60 | 0.00023 | | | |
| - 60 | 0.00036 | 35.41 | | | | | 60 | | | | |
| 60 | 0.00036 | 35.41 | | | | | 60 | | | | |
| 60 | 0.00036 | 35.41 | | | • | | 60 | | | | |
| 72 | 0.00021 | 20.66 | 21.64 | | 3.81 | | 72 | | 2.20E-04 | | 0.00 |
| 72 | 0.00025 | 24.59 | | | | | 72 | | | | |
| 72 | 0.00018 | 17.70 | | | | | 72 | | | | |
| 72 | 0.00027 | 26.56 | | | | | 72 | 0.00027 | | | |
| 72 | 0.00019 | 18.69 | | | | | 72 | 0.00019 | | | |
| 84 | 0.00026 | 25.57 | 25.57 | | 3.03 | | 84 | 0.00026 | 2.60E-04 | | 0.00 |
| 84 | 0.00028 | 27.54 | | | | | 84 | 0.00028 | | | |
| 84 | 0.0003 | 29.51 | | | | | 84 | | | | |
| 84 | 0.00023 | 22.62 | | | | | 84 | | | | |
| 84 | 0.00023 | 22.62 | | | | | 84 | 0.00023 | | | |
| 108 | 0.00012 | 11.80 | 8.85 | | 3.68 | | 108 | | 9.00E-05 | | 0.00 |
| 108 | 0.00012 | 11.80 | | | | | 108 | | | | |
| 108 | 0.00006 | 5.90 | | | | | 108 | | | | |
| 108 | 0.00004 | 3.93 | | | | | 108 | | | | |
| 108 | 0.00011 | 10.82 | | | | | 108 | 0.00011 | | | |
| Data obtaine | d from Ap | pendix III, T | ables 6-14, | pp. 35 | -43 of | MRID 429 | 900201 | | | | |
| Chemical: Cl | | | | | | | | | | | |
| MRID: 42900 | | | | | | | | | | | |
| PC Code: 08 | | | | | | | | | | | |
| Guideline: 16 | 51-2 | | | | | | | | | | |

Mol/L Average
0 0.00103 0.001017
0 0.00092
0 0.0011

| Chlorop Dark | oicrin | | | : | pplied | Ch Da | loropicr | in | | | |
|-----------------|--------|-----------|----------------|-------------|-------------|--------------|-----------|------------------|---------------------|----|------|
| Hours | | Aol/L | % applied | | SD | | urk | B.4-18 | | SD | |
| riouis | ۰, | 0.00103 | | 100.00 | | no | iuis O | Mol/L 0.00103 | Average 1.02E-03 | | 0.00 |
| | ŏ | 0.00092 | | 100.00 | 0.93 | | ä | | 1.025-03 | | 0.00 |
| | ő | 0.00092 | 108.20 | | | | Ö | | | | |
| | 12 | 0.00229 | | | 37.69 | | 12 | | 1.85E-03 | | 0.00 |
| | 12 | 0.00229 | | 101.97 | 37.09 | | 12 | | 1.855-03 | | 0.00 |
| | 12 | 0.00159 | | | | | 12 | | | | |
| | 24 | 0.00159 | 98.36 | 99.15 | 3.64 | | 24 | | 1.01E-03 | | 0.00 |
| | 24 | 0.00101 | 99.34 | | 3.04 | | 24 | | 1.01E-03 | | 0.00 |
| | 24 | 0.00107 | 105.25 | | | | 24 | | | | |
| | 24 | 0.00098 | 96.39 | | | | 24 | | | | |
| | 24 | 0.00098 | | | | | | | | | |
| | 36 | 0.00091 | 96.39 89.51 | 96.59 | 4.58 | | 24 36 | | 9.82E-04 | | 0.00 |
| | 36 | 0.00098 | 96.39 | 90.58 | 4.50 | | 36 | | 9.626-04 | | 0.00 |
| | 36 | 0.00099 | | | | | 36 | | | | |
| | 36 | 0.00099 | 97.38 | | | | 36 | | | | |
| | 36 | 0.00099 | | | | | 36 | | | | |
| | 48 | 0.00104 | 120.00 | | | • | | | 4 075 00 | | |
| | 48 | | | 105.25 | 14.47 | | 48 | | 1.07E-03 | | 0.00 |
| | | 0.00107 | | | | | 48 | | | | |
| | 48 | 0.00108 | 106.23 | | | | 48 | 0.00108 | | | |
| | 48 | 0.00115 | | | | | 48 | | | | |
| | 48 | 0.00083 | 81.64 | | | | 48 | | | | |
| | 60 | 0.00082 | 80.66 | 88.92 | 7.67 | | 60 | | 9.04E-04 | | 0.00 |
| | 60 | 0.00098 | 96.39 | | | | 60 | | | | |
| | 60 | 0.00096 | | | | | 60 | | | | |
| | 60 | 0.00082 | | | | | 60 | | | | |
| | 60 | 0.00094 | 92.46 | i | | | 60 | | | | |
| | 72 | 0.00112 | | 98.36 | 16.69 | | 72 | | 1.00E-03 | | 0.00 |
| | 72 | 0.00076 | | 1 | | | 72 | | | | |
| | 72 | 0.00096 | | | | | 72 | | | | |
| | 72 | 0.00096 | | | | | 72 | | | | |
| | 72 | 0.0012 | | | | | 72 | | | | |
| | 84 | 0.00084 | 82.62 | 82.23 | 6.40 | | 84 | | 8.36E-04 | | 0.00 |
| | 84 | 0.00075 | 73.77 | | | | 84 | | | | |
| | 84 | 0.0008 | 78.69 | i | | | 84 | | | | |
| | 84 | 0.00087 | 85.57 | İ | | | 84 | | | | |
| | 84 | 0.00092 | 90.49 | i | | | 84 | | | | |
| | 108 | 0.00107 | 105.25 | 102.89 | 3.59 | | 108 | 0.00107 | 1.05E-03 | | 0.00 |
| | 108 | 0.001 | 98.36 | į | | | 108 | | | | |
| | 108 | 0.00109 | 107.21 | i | | | 108 | | | | |
| | 801 | 0.00102 | 100.33 | į. | | | 108 | | | | |
| | 801 | 0.00105 | 103.28 | į | | | 108 | 0.00105 | | | |
| Data ob | taine | d from Ac | nendîx III. T | lables 6-14 | no. 35,43 c | F MRID 42900 | 201 | | | | |

PMRA Submission Number {...

EPA MRID Number 42900201

Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2 Chloride . Chloride Dark Hours Mol/L 0.000214 0.000287 0.000287 0.000285 0.000285 0.000285 0.000289 0.000249 0.000048 0.000084 0.000093 0.000013 0.0000142 0.0000249 0.0000249 Average 2.49E-05 0.00 0 0 12 12 2.94E-05 0.00 24 24 24 24 36 36 36 36 48 48 48 48 60 60 60 72 72 72 72 84 84 84 84 84 84 81 108 81 108 5.01E-05 0.00 2.34E-05 0.00 0.000244 0.0000386 0.000026 0.000025 0.000038 0.000038 0.00008 0.000029 0.000033 0.000031 0.000031 4.08E-05 0.00 3.04E-05 0.00

0.000007 0.000008 ed from Appendix IV, Tables 15-23, pp. 45-53 of MRID 42900201

2.26E-05

9.40E-06

7.40E-06

0.00

0.00

0.00

0.000017 0.000016 0.000018 0.000019

0.000019 0.000043 0.000009 0.000009 0.00001 0.00007 0.000007

Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2

| Nitrate | | | |
|------------|--------------|-------------------|-------------------------|
| Irradiated | | | |
| Hours | Mol/L | Average SD | 0.00 |
| 0 | 0.0000194 | 1.63E-05 | 0.00 |
| 0 | 0.0000161 | | |
| 12 | | 1.46E-05 | 0.00 |
| 12 | | 1.466-05 | 0.00 |
| 12 | | | |
| 24 | | 2.35E-05 | 0.00 |
| 24 | | 2.350-05 | 0.00 |
| 24 | | | |
| 24 | | | |
| 24 | | | |
| 36 | | 3.05E-05 | 0.00 |
| 36 | | 0.002.00 | 0.00 |
| 36 | | | |
| 36 | | | |
| 36 | | | |
| 48 | | 3.19E-05 | 0.00 |
| 48 | | | |
| 48 | | | |
| 48 | | | |
| 48 | | | |
| 60 | | 6.13E-05 | 0.00 |
| 60 | | | |
| 60 | | | |
| 60 | 0.000065 | | |
| 60 | 0.0000698 | | |
| 72 | 0.0000675 | 7.70E-05 | 0.00 |
| 72 | 0.0000675 | | |
| 72 | 0.0000724 | | |
| 72 | 0.0000887 | | |
| 72 | 0.0000887 | | |
| 84 | 0.000105 | 9.99€-05 | 0.00 |
| 84 | 0.000109 | | |
| 84 | 0.000102 | | |
| 84 | 0.0000797 | | |
| 84 | 0.000104 | | • |
| 108 | 0.000109 | 9.23E-05 | 0.00 |
| 108 | 0.000112 | | |
| 108 | 0.0000805 | | |
| 108 | 0.0000654 | | |
| 108 | | | |
| | | endix V, Tables 2 | 4-32, pp. 55-63 of MRII |
| | Chloropicrin | | |
| MRID: 429 | | | |
| PC Code: (| 081501 | | |
| | | | |

ID 42900201

Guideline: 161-2

| Nitrate Dark | | | | |
|-----------------|----------|------------|------------|------|
| Hours | | Mol/L | Average SD | |
| | 0 | 0.0000194 | 1.63E-05 | 0.00 |
| | 0 | 0.0000161 | | |
| | 0 | 0.0000133 | | |
| | 12 | | | 0.00 |
| | 12 | | | |
| | 12 | | | |
| | 24 | | 5.24E-06 | 0.00 |
| | 24 | | | |
| | 24 | | | |
| | 24 | | | |
| | 24 | | | |
| | 36 | | 1.33E-05 | 0.00 |
| | 36 | | | |
| | 36 | | | |
| | 36 | 0.000013 | | |
| | 36 | 0.0000146 | 0.475.00 | 2.00 |
| | 48 | 0.00000806 | 6.17E-06 | 0.00 |
| | 48 | 0.00000511 | | |
| , | 48 | 0.0000052 | | |
| | 48 | 0.00000645 | | |
| | 48 | 0.00000603 | | |
| | 60 | 0.0000221 | 1.85E-05 | 0.00 |
| | 60 | 0.0000175 | | |
| | 60 | 0.0000191 | | |
| | 60 | 0.0000152 | | |
| | 60 | 0.0000188 | | |
| | 72 72 | | 1.30E-05 | 0.00 |
| | | | | |
| | 72 72 | | | |
| | 72 | | | |
| | 84 | | 1.16E-05 | 0.00 |
| | 84 | | 1.162-05 | 0.00 |
| | 84 | 0.0000106 | | |
| | 84 | 0.00000997 | | |
| | 84 | | | |
| | 108 | | 9.86E-06 | 0.00 |
| | 108 | | 3.00E-00 | 0.00 |
| | 108 | 0.0000102 | | |
| | | 0.00000102 | | |

108 0.00000906 108 0.0000976 Data obtained from Appendix V, Tables 24-32, pp. 55-63 of MRID 42900201

PMRA Submission Number {.....}

EPA MRID Number 42900201

Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2

| Nitrite | | | | |
|----------|-------|------------------|------------------|-----------|
| irradiat | ed | | | |
| Hours | | Mol/L | Average SD | |
| | 0 | 0.000000276 | 2.25E-07 | 0.00 |
| | 0 | 0.000000123 | | |
| | 0 | 0.000000276 | | |
| | 12 | 0.0000144 | 1.45E-05 | 0.00 |
| | 12 | 0.0000147 | | |
| | 12 | . 0.0000144 | | |
| | 24 | 0.0000186 | 1.89E-05 | 0.00 |
| | 24 | 0.000017 | | |
| | 24 | 0.0000226 | | |
| | 24 | 0.0000183 | | |
| | 24 | 0.000018 | | |
| | 36 | 0.0000394 | 3.64E-05 | 0.00 |
| | 36 | 0.0000374 | | |
| | 36 | 0.0000334 | | |
| | 36 | 0.0000389 | Ì | |
| | 36 | 0.0000329 | | |
| | 48 | 0.0000351 | 3.41E-05 | 0.00 |
| | 48 | 0.000029 | İ | |
| | 48 | 0.0000448 | | |
| | 48 | 0.0000334 | | |
| | 48 | 0.0000281 | | |
| | 60 | 0.0000265 | 3.73E-05 | 0.00 |
| | 60 | 0.0000391 | | |
| | 60 | 0.0000418 | | |
| | 60 | 0.000034 | | |
| | 60 | 0.0000449 | | |
| | 72 | 0.0000406 | 3.88E-05 | 0.00 |
| | 72 | 0.0000398 | | |
| | 72 | 0.0000328 | | |
| | 72 | 0.000043 | | |
| | 72 | 0.0000377 | | |
| | 84 | 0.0000425 | 3.93E-05 | 0.00 |
| | 84 | 0.0000496 | | |
| | 84 | 0.0000238 | | |
| | 84 | 0.000052 | | |
| | 84 | 0.0000286 | | |
| | 108 | 0.0000776 | 1.06E-04 | 0.00 |
| | 108 | 0.0000776 | | |
| | 108 | 0.0000794 | | |
| | 108 | 0.000107 | | |
| | 108 | 0.000187 | | |
| Data ob | otain | ed from Appendix | VI. Tables 33-44 | 1. pp. 65 |

Data obtained from Appendix VI, Tables 33-44, pp. 65-73 of MRID 42900201

Data obtained from App Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2

| LAIGHTE |
|---------|
| Dark |
| Hours |
| |
| |
| |

| | /Iol/L | Average SD | |
|-----------|--------------------------|------------|------|
| 0 | 0.000000276 | 2.25E-07 | 0.00 |
| 0 | 0.000000123 | | |
| 0 | 0.000000276 | | |
| 12 | 0.0000022 | 2.42E-06 | 0.00 |
| 12 | 0.0000022 | | |
| 12 | 0.00000286 | | |
| 24 | 0.00000286 | 2.46E-06 | 0.00 |
| 24 | 0.0000022 | | |
| 24 | 0.00000253 | | |
| 24 | 0.00000253 | | |
| 24 | 0.0000022 | | |
| 36 | 0.00000135 | 1.40E-06 | 0.00 |
| 36 | 0.00000135 | | |
| 36 | 0.00000135 | | |
| 36 | 0.0000016 | | |
| 36 | 0.00000135 | | |
| 48 | 0.00000148 | 1.30E-06 | 0.00 |
| 48 | 0.00000126 | | |
| 48 | 0.00000126 | | |
| 48 | 0.00000126 | | |
| 48 | 0.00000126 | | |
| 60 | 0.00000126 | 1.19E-06 | 0.00 |
| 60 | 0.00000126 | | |
| 60 | 0.00000126 | | |
| 60 . | 0.00000103 | | |
| 60 | 0.00000114 | | |
| 72 | 0.00000128 | 1.26E-06 | 0.00 |
| 72 | 0.00000101 | | |
| 72 | 0.00000101 | | |
| 72 | 0.00000115 | : | |
| 72 | 0.00000183 | | |
| 84 | 0.00000141 | 1.27E-06 | 0.00 |
| 84 | 0.00000127 | | |
| 84 | 0.00000127 | | |
| 84 | 0.00000127 | | |
| 84 108 | 0.00000114 0.00000124 | 1.20E-06 | 0.00 |
| 108 | 0.00000124 | 1.200-06 | 0.00 |
| 108 | 0.00000124 | | |
| 108 | 0.00000114 | ! | |
| 100 | 0.00000124 | | |

108 0.00000114

Data obtained from Appendix VI, Tables 33-44, pp. 65-73 of MRID 42900201

PMRA Submission Number {.....}

EPA MRID Number 42900201

Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2

Carbon dioxide

Irradiated

| Hours | | Mol/L | | | | | | | |
|---------|-------|----------|-----------|---|----|----|-----|-------|----|
| | 0 | 1 | .00E-06 | | | | | | |
| | 12 | 1 | .20E-05 | | | | | | |
| | 24 | 7 | .40E-05 | | | | | | |
| | 36 | 6 | .40E-05 | | | | | | |
| | 48 | 7 | .46E-05 | | | | | | |
| | 60 | 6 | .42E-05 | | | | | | |
| | 72 | 1 | .20E-04 | | | | | | |
| | 84 | 1 | .27E-04 | | | | | | |
| | 108 | 1 | .43E-04 | | | | | | |
| Data al | atair | and from | m Toble 1 | _ | 24 | ٥f | MOI | 7 420 | 20 |

Data obtained from Table 1, p. 24 of MRID 42900201

Carbon dioxide

| Dark |) | а | r | k |
|------|---|---|---|---|
|------|---|---|---|---|

| Hours | Mol/L | | |
|-------|-------|----------|--|
| | 0 | 1.00E-06 | |
| | 12 | 0.00E+00 | |
| | 24 | 8.10E-06 | |
| | 36 | 0.00E+00 | |
| | 48 | 0.00E+00 | |
| | 60 | 8.10E-06 | |
| | 72 | 4.08E-06 | |
| | 84 | 0.00E+00 | |
| | 108 | 8.10E-06 | |

Data obtained from Table 4, p. 27 of MRID 42900201

PMRA Submission Number {.....}

EPA MRID Number 42900201

Chemical: Chloropicrin MRID: 42900201 PC Code: 081501 Guideline: 161-2

Bicarbonate

Irradiated

| Hours | Mol/L | |
|-------|-------|---------|
| | 0 4 | .00E-06 |
| 13 | 2 4 | .80E-05 |
| 2 | 4 2 | .96E-04 |
| 3 | 6 2 | .56E-04 |
| 4 | 8 2 | .99E-04 |
| 6 | 0 2 | .57E-04 |
| 7: | 2 4 | .82E-04 |
| 84 | 4 5 | .07E-04 |
| 108 | 8 5 | .73E-04 |

Data obtained from Table 1, p. 24 of MRID 42900201

Bicarbonate

Dark

| Dark | | | |
|-------|-----|-------|---------|
| Hours | | Mol/L | |
| | 0 | 4 | .00E-06 |
| | 12 | 0. | 00E+00 |
| | 24 | 3 | .24E-05 |
| | 36 | 0. | 00E+00 |
| • | 48 | 0. | 00E+00 |
| | 60 | 3 | .24E-05 |
| | 72 | 1 | .63E-05 |
| | 84 | 0. | 00E+00 |
| | 108 | 3 | .24E-05 |

Data obtained from Table 4, p. 27 of MRID 42900201

PMRA Submission Number {.....}

EPA MRID Number 42900201

Attachment: Comparison of Artificial Light to Natural Sunlight

