

US EPA ARCHIVE DOCUMENT

Chemistry data review for the registration of a technical grade of active ingredient (TGAI) or an integrated system product (ISP).

Product Chemistry Data Requirements

(UNDATED)

Submission Number / DP Bar Code: 2003-0839

Registration Number: Not yet assigned

Source Code / PC Code: MTN-BAZ-31

Manufacturing Plant Location:

BASF Corporation
Agricultural Products Group
P.O. Box 13528
Research Triangle Park, NC
27709-3528
Phone: 919-547-2000

Applicant's / Registrant's Name and address:

BASF Canada Inc.
345 Carlingview Drive
Toronto, Ontario
M9W 6N9
Phone: 416-674-3611

Guarantee: On the label:
BAS 670H.....99.2%

On the SPSF:
BAS 670H Technical, [3-(4,5-dihydro-isoxazol-3-yl)-4-methylsulfonyl-2-methylphenyl](5-hydroxy-1-methyl-1 H-pyrazol-4-yl)methanone...99.2% (97.0 - 100%)

Reviewer: B. Boutin-Muma

INTRODUCTION:

The purpose of this Category A submission is to register a new technical herbicide for corn, containing the active ingredient BAS 670 H. In support of the registration, Part 0-Index, Part 1- label, the Product Statement of Specification Form and Part 2 (in V:\Subs-E-Info\2003 subs\2003-0839\BAS H, 2nd set), have been submitted.

| Table 1. Product Identity of BAS 670 H: | | |
|---|------------|------------------|
| DACO # / GLN | Title | Data/Information |
| 2.3 / 830.1000 | Trade Name | To be assigned |
| 2.3.1 / 830.1000 | Other Name | BAS 670H |

| Table 1. Product Identity of BAS 670 H: | | |
|---|---------------------|---|
| DACO # / GLN | Title | Data/Information |
| 2.4 / 830.1550 | Common Name | To be assigned |
| 2.5 / 830.1550 | IUPAC Chemical Name | [3-(4,5-dihydro-isoxazol-3-yl)-4-methylsulfonyl-2-methylphenyl](5-hydroxy-1-methyl-1 H-pyrazol-4-yl)methanone |
| | CAS Chemical Name | Methanone, [3-(4,5-dihydro-3-isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl](5-hydroxy-1-methyl-1 H-pyrazol-4-yl)- |
| 2.6 / 830.1550 | CAS Number | 210631-68-8 |
| 2.7 / 830.1550 | Structural Formula | |
| 2.8 / 830.1550 | Molecular Formula | C ₁₆ H ₁₇ N ₃ O ₅ S |
| 2.9 / 830.1550 | Molecular Weight | 363.39 |

SUMMARY OF FINDINGS:

BAS 670 H is synthesized in a pilot plant at BASF Ludwigshafen, Germany by a process involving several steps. Each step of the process has been described in detail and supported by chemical reactions. A discussion on the formation of the impurities occurring at each step was provided.

The TGAI is guaranteed to contain the active ingredient at a nominal concentration of 99.2% with lower and upper limits of 97 and 100%. Impurities including [redacted] and [redacted] were specified. Of the [redacted] impurities, [redacted] and two below [redacted]. The specifications are based on a pilot plant production batch data.

Five representative batches of BAS 670 H technical grade active ingredient were analyzed for the active ingredient and the content of impurities including [redacted]. The level of the active ingredient ranged between 99.0 % and 99.5 % with an average value of 99.2%. The mean closure for the five batches examined was reported to be 100.1%.

The identity of the active ingredient, (BAS 670H) has been confirmed by UV, NMR, IR and MS-spectrometry. The proposed structure is consistent with the spectra. Identity of BAS 670 H TGAI and structurally related impurities has been confirmed by LC retention time comparison with corresponding reference standards.

The chemical and physical properties were either provided or are not applicable.

CONCLUSIONS: The chemistry requirements are not complete. The following requirements remain to be addressed.

DACO Title 1.0
Label

Deficiencies A BASF code "BAS 670 H" is used for the active ingredient instead of the common name.

Required Data: An ISO common name should be used on the label once one is accepted. This issue can be addressed at the level E review stage.

DACO Title 2.2
Manufacturer's Name and Office Address and
Manufacturing Plant's Name and Address

Deficiencies The manufacturing plant location is listed as "BASF, Research Triangle Park, NC" under DACO 2.2 in the chemistry data package and as "BASF, Germany" in box 6 of the SPSF.

Required Data: The applicant is required to confirm the correct plant location where the TGAI is manufactured.

DACO Title 2.13.3
Batch data

Deficiencies: The data submitted in support of the specifications of the TGAI, manufactured at the BASF Ludwigshafen, are based on five batches of the TGAI produced in pilot scale.

Required Data: Analytical data from five batches of the TGAI from full scale production are required when available, to support the specifications as per the requirements of DIR 98-04.

The requirement of full scale batch data can be addressed at the level E review stage. In the interim, the applicant is required to provide the expected date of such data.

DACO Title: 2.15
Sample of Chemical Standard

Deficiencies: A 2.5 g analytical standard of the active ingredient was not submitted.

Required Data: As per Dir98-04, a 2.5 g analytical standard of the active ingredient is required. It should be sent directly to:

Laboratory Services
Pest Management Regulatory Agency
Health Canada
Laboratory Services Building, No. 22
Central Experimental Farm
Ottawa, Ontario
K1A 0C6
Attn: Mary O'Neil

Review status: C1-passed.

Good Laboratory Practices Compliance Statement:

The studies contained within this report were conducted in accordance with the Good Laboratory Practice Standards as specified in 40 CFR 160 or equivalent.

yes

no

not stated / applicable

OECD Principles of Good Laboratory practice and the GLP Principles of the German "Chemikaliengesetz"(Chemicals Act) were used.

1. Chemical and Physical Properties: See Table 2.

Reference:

1. Roland Kastel, July 25, 200, Physical and chemical Properties of the Technical Active Ingredient of BAS 670 H, PCP02480

2. Summary of Chemical and Physical Properties, Anonymous, August 24, 2000; K II A 2.16 Other Studies/Data (Data #1 in V:drive).

| Table 2. Chemical & physical properties. | | | | | |
|--|-------------------------------------|---------------------------|---|---------------------|-----------------------------------|
| DACO # / GLN | Title | Test substance purity (%) | MRID / Report # | Status ¹ | Result ² or Deficiency |
| ¹ A = Acceptable; N = Unacceptable (see Deficiency); N/A = Not applicable. ² For example, "brown" for 830.6302; "155°C" for 830.7200. | | | | | |
| 2.14.1 / 830.6302 | Colour | | Ansgar Daum November 2, 1999 PCP02480 | A | White |
| 2.14.2 / 830.6303 | Physical state | | Ansgar Daum November 2, 1999 PCP02480 | A | Solid |
| 2.14.3 / 830.6304 | Odour | | Ansgar Daum November 2, 1999 PCP02480 | A | Odourless |
| 2.14.4 / 830.7200 | Melting point/range | 99.8 | Ansgar Daum November 2, 1999 PCP05410 OECD Test Guideline102 | A | 220.9°C - 222.2°C. |
| 2.14.5 / 830.7220 | Boiling point/range | | | N/A | The product is a solid |
| 2.14.6 / 830.7300 | Density or specific gravity at 20°C | 99.7 | Roland Kastel, September 20, 1999 OECD Test Guideline 109 | A | 1.425 g/cm ³ |

Table 2. Chemical & physical properties.

| DACO # / GLN | Title | Test substance purity (%) | MRID / Report # | Status ¹ | Result ² or Deficiency | | | | | | | | | | | | | | | | |
|--|--|---------------------------|--|---------------------|---|-------------------------|---|---------|------------------------|--------------|------------------------|-----------------|----------|-----------------------|------------|---------------|-------|-----------------|-------|---|--|
| ¹ A = Acceptable; N = Unacceptable (see Deficiency); N/A = Not applicable. ² For example, "brown" for 830.6302; "155°C" for 830.7200. | | | | | | | | | | | | | | | | | | | | | |
| 2.14.7 / 830.7840 | Water solubility at 20°C | 99.7 | Ansgar Daum, October 4, 1999 PCP05405 OECD 105 | A | <table border="0"> <tr> <td><u>pH</u></td> <td><u>Solubility</u></td> </tr> <tr> <td>3</td> <td>0.06 g/L</td> </tr> <tr> <td>5</td> <td>0.98 g/L</td> </tr> <tr> <td>7</td> <td>15g/L</td> </tr> <tr> <td>9</td> <td>23.4 g/L</td> </tr> </table> | <u>pH</u> | <u>Solubility</u> | 3 | 0.06 g/L | 5 | 0.98 g/L | 7 | 15g/L | 9 | 23.4 g/L | | | | | | |
| <u>pH</u> | <u>Solubility</u> | | | | | | | | | | | | | | | | | | | | |
| 3 | 0.06 g/L | | | | | | | | | | | | | | | | | | | | |
| 5 | 0.98 g/L | | | | | | | | | | | | | | | | | | | | |
| 7 | 15g/L | | | | | | | | | | | | | | | | | | | | |
| 9 | 23.4 g/L | | | | | | | | | | | | | | | | | | | | |
| 2.14.8 / 830.7860 | Solvent solubility at 20°C | 99.9 | Ansgar Daum, January 13, 2000 PCP05408 | A | <table border="0"> <tr> <td><u>Solvent</u></td> <td><u>Solubility (g/100mL)</u></td> </tr> <tr> <td>Acetone</td> <td>< 1.0</td> </tr> <tr> <td>Acetonitrile</td> <td>< 1.0</td> </tr> <tr> <td>Dichloromethane</td> <td>2.5 -2.9</td> </tr> <tr> <td>N,N-dimethylformamide</td> <td>11.4 -13.3</td> </tr> <tr> <td>Ethyl acetate</td> <td>< 1.0</td> </tr> <tr> <td>Other solvents*</td> <td>< 1.0</td> </tr> <tr> <td colspan="2">*N-heptane, methanol, 1-octanol, olive oil, 2-propanol, and toluene are each < 1.0.</td> </tr> </table> | <u>Solvent</u> | <u>Solubility (g/100mL)</u> | Acetone | < 1.0 | Acetonitrile | < 1.0 | Dichloromethane | 2.5 -2.9 | N,N-dimethylformamide | 11.4 -13.3 | Ethyl acetate | < 1.0 | Other solvents* | < 1.0 | *N-heptane, methanol, 1-octanol, olive oil, 2-propanol, and toluene are each < 1.0. | |
| <u>Solvent</u> | <u>Solubility (g/100mL)</u> | | | | | | | | | | | | | | | | | | | | |
| Acetone | < 1.0 | | | | | | | | | | | | | | | | | | | | |
| Acetonitrile | < 1.0 | | | | | | | | | | | | | | | | | | | | |
| Dichloromethane | 2.5 -2.9 | | | | | | | | | | | | | | | | | | | | |
| N,N-dimethylformamide | 11.4 -13.3 | | | | | | | | | | | | | | | | | | | | |
| Ethyl acetate | < 1.0 | | | | | | | | | | | | | | | | | | | | |
| Other solvents* | < 1.0 | | | | | | | | | | | | | | | | | | | | |
| *N-heptane, methanol, 1-octanol, olive oil, 2-propanol, and toluene are each < 1.0. | | | | | | | | | | | | | | | | | | | | | |
| 2.14.9 / 830.7950 | Vapour pressure at 20°C | 99.7 | Roland Kastel, September 20, 1999 | A | <table border="0"> <tr> <td><u>Temperature (°C)</u></td> <td><u>Vapor pressure (mbar)</u></td> </tr> <tr> <td>20</td> <td>< 1x 10⁻¹²</td> </tr> <tr> <td>25</td> <td>< 1x 10⁻¹²</td> </tr> </table> | <u>Temperature (°C)</u> | <u>Vapor pressure (mbar)</u> | 20 | < 1x 10 ⁻¹² | 25 | < 1x 10 ⁻¹² | | | | | | | | | | |
| <u>Temperature (°C)</u> | <u>Vapor pressure (mbar)</u> | | | | | | | | | | | | | | | | | | | | |
| 20 | < 1x 10 ⁻¹² | | | | | | | | | | | | | | | | | | | | |
| 25 | < 1x 10 ⁻¹² | | | | | | | | | | | | | | | | | | | | |
| 830.7 | pH | | Roland Kastel, July, 2000 PCP02480 CIPAC MT 75 | A | 2.9 (1% de-ionized water) | | | | | | | | | | | | | | | | |
| 2.14.10 / 830.7370 | Dissociation constant (pK _a) | 99.7 | Ansgar Daum, September 21, 1999 PCP05406, OECD 112 Dissociation | A | 4.06 | | | | | | | | | | | | | | | | |
| 2.14.11 / 830.7550 830.75608 30.7570 | Octanol/water partition coefficient (K _{ow}) at 20°C | 99.9 | Ansgar Daum, August 24, 2000 PCP05828 OECD 107 | A | <table border="0"> <tr> <td><u>pH</u></td> <td><u>log Kow</u></td> </tr> <tr> <td>4</td> <td>-0.81</td> </tr> <tr> <td>7</td> <td>-1.52</td> </tr> <tr> <td>9</td> <td>-2.34</td> </tr> </table> | <u>pH</u> | <u>log Kow</u> | 4 | -0.81 | 7 | -1.52 | 9 | -2.34 | | | | | | | | |
| <u>pH</u> | <u>log Kow</u> | | | | | | | | | | | | | | | | | | | | |
| 4 | -0.81 | | | | | | | | | | | | | | | | | | | | |
| 7 | -1.52 | | | | | | | | | | | | | | | | | | | | |
| 9 | -2.34 | | | | | | | | | | | | | | | | | | | | |
| 2.14.12 / 830.7050 | UV/visible absorption spectrum (indicate conditions, if any) | 99.7 | Ansgar Daum, January 13, 2000 PCP05409 OECD 101 | A | <table border="0"> <tr> <td><u>λ, nm</u></td> <td><u>ε, mol⁻¹cm⁻¹</u></td> </tr> <tr> <td>207</td> <td>27077</td> </tr> <tr> <td>272</td> <td>8601</td> </tr> <tr> <td>300</td> <td>5800</td> </tr> <tr> <td>410</td> <td>410</td> </tr> </table> | <u>λ, nm</u> | <u>ε, mol⁻¹cm⁻¹</u> | 207 | 27077 | 272 | 8601 | 300 | 5800 | 410 | 410 | | | | | | |
| <u>λ, nm</u> | <u>ε, mol⁻¹cm⁻¹</u> | | | | | | | | | | | | | | | | | | | | |
| 207 | 27077 | | | | | | | | | | | | | | | | | | | | |
| 272 | 8601 | | | | | | | | | | | | | | | | | | | | |
| 300 | 5800 | | | | | | | | | | | | | | | | | | | | |
| 410 | 410 | | | | | | | | | | | | | | | | | | | | |
| 2.14.13 / 830.6313 | Stability (temperature, metals, sunlight) | Not provided | R. Yacoub November 1, 2002 FR0221 | A | Stable to normal and elevated temperatures 54°C for 14 days, in the presence of aluminum, aluminum acetate and iron filings. The test substance may not be stable in the presence of iron acetate after 14 days at elevated temperature. | | | | | | | | | | | | | | | | |

| Table 2. Chemical & physical properties. | | | | | |
|--|-------------------|---------------------------|--|---------------------|--|
| DACO # / GLN | Title | Test substance purity (%) | MRID / Report # | Status ¹ | Result ² or Deficiency |
| ¹ A = Acceptable; N = Unacceptable (see Deficiency); N/A = Not applicable. ² For example, "brown" for 830.6302; "155°C" for 830.7200. | | | | | |
| 2.14.14 / 830.6317 | Storage stability | | Wemer Konig March 7, 2002 PCF02075 | A | After 24 months at 20°C and 30°C no significant change in active ingredient concentration (less than 5%) was observed. |

Data Submitted: See Table 3.

| Table 3. Identity and Composition Data for BAS 670 H TGAI | | | | |
|---|--|-----------------|---------------------|--|
| DACO # / GLN | Title | MRID / Report # | Status ¹ | Details and/or Deficiency ² |
| 2.12.2 / 830.1550 | Product Identity and Disclosure of Ingredients | | A | No deficiencies |
| 2.11.2, 2.11.3 / 830.1600 830.1620 | Starting Materials & Manufacturing Process | | A | No deficiencies |
| 2.11.4 / 830.1670 | Discussion of Impurities | | A | No deficiencies |
| 2.13.3 / 830.1700 | Preliminary Analysis | | N | The specifications are based on batches from a pilot plant production. |
| 2.12.1 / 830.1750 | Certification of Limits | | A | No deficiencies |
| 2.13.1 / 830.1800 | Enforcement Analytical Methods | | A | No deficiencies |
| ¹ A = Acceptable; N = Unacceptable (see Deficiency); N/A = Not applicable. ² Refer to CBI Appendix A for details | | | | |

ATTACHMENT: CONFIDENTIAL APPENDIX

Chem Data Review for the Reg of TGAJ ORAW.

Page _____ is not included in this copy.

Pages 7 through 17 are not included.

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.
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The information not included is generally considered confidential by product registrants. If you have any questions, please contact the individual who prepared the response to your request.
