Date: August 18, 2004

SUBJECT: VOLFEE. Product Chemistry Review of Chlorothalonil Technical Fungicide

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DP BARCODE: D302851 & 303004
EPA REG. NO.: 74601-R
PRODUCT: Chlorothalonil Technical Fungicide
PCC: 081901
REGISTRANT: VISCHIM, S. R. L
USE: Fungicide

INTRODUCTION:

Technology Sciences Group, on behalf of Vischim S.R.L., has submitted an application for me-too registration of chlorothalonil technical fungicide. The Reregistration Eligibility Document (RED, April 1997) for chlorothalonil required that all technical and manufacturing use products containing chlorothalonil must certify a maximum level of HCB in these products of 40 ppm by January 1, 2003. Vischim recently conducted a five batch analysis (assigned MRID No. 459430-01) to address this requirement, which must be used in place of the original report (MRID No. 457102-01) submitted with the original application. Based on the five batch analysis, a revised CSF for basic formulation (dated June 4, 2003) has been submitted. The preliminary analysis also indicated a higher nominal concentration of the active ingredient than claimed in the original application (99.4% versus 99.0% in original). The revised CSF and the label reflect these results. The original data were assigned the MRID Nos. 457102-01 and 457102-02; the new five batch analysis study has been assigned the MRID No. 457102-01. The registrant has claimed that the proposed product is substantially similar to the registered product with Reg. No. 50534-7. The TRB has been asked to evaluate the product chemistry data submitted for Chlorothalonil technical produced in Italy and determine its similarity to the registered product from chemistry point of view.

SUMMARY OF FINDINGS:

1. The registrant has submitted a revised Confidential Statement of Formula for alternate formulation (dated 06-04-03) for chlorothalonil technical based on the recent 5 batch analysis study. The average purity of the technical chlorothalonil was 99.4%, as determined by the five batch analysis. The proposed certified limits for the chlorothalonil are not in accordance with standard limits as described in 40 CFR§158.175(b)(2), but are based on expected production variability. The product chemistry data submitted corresponding to guideline reference 830.1550 (product identity & composition) and 830.1750 (certified limits) satisfy the data requirements of 40 CFR§158.155 and 158.175 respectively. [MRID No. 459430-01 & 457102-01]

2. The product chemistry data submitted corresponding to guideline reference 830.1600 (description of material used to produce the product) satisfy the data requirements of 40 CFR§ 158.160. The registrant has provided product specifications data on all the starting materials used for the production of this technical. [MRID No. 457102-01]

3. The product chemistry data submitted corresponding to guideline reference 830.1620 (description of production process) satisfy the data requirements for 40 CFR§158.162. The active ingredient was produced by continuous process which has been described in details including the quality assurance steps to obtain consistency of the product. [MRID No. 457102-01]
4. The product chemistry data submitted corresponding to guideline reference 830.1670 (discussion on the 
formation of impurities) satisfy the data requirements for 40CFR§158.167. The registrant has listed 
impurities including the hexachlorobenzene (HCB). The impurities were determined by 
[MRID No. 459430-01] The determination of HCB at very low concentrations required 

5. The data submitted corresponding the guideline reference 830.1700 (preliminary analysis) satisfy the 
data requirements of 40CFR§158.170. Five representative batches of the technical were analyzed for 
percent active ingredient by GC with internal standard using the FID. The determination of HCB at very low 
concentrations required [MRID No. 459430-01] 

6. The data submitted corresponding the guideline reference 830.1800 (enforcement analytical method) satisfy 
the data requirements of 40CFR§158.180. The method described in Item # 5 above was used to assay the 
active ingredient in the technical product and was non-confidential. The method is based on comparison of 
the ratio of chlorothalonil analytical standard peak area versus to the dibutyl phthalate standard (IS) peak area 
and the same ratio in the sample with a known amount of IS added. The method was validated for accuracy, 
linearity, and precision. [MRID No. 459430-01 & 457102-01] 

7. The data submitted corresponding to 830 series subgroup B (physical-chemical properties) satisfy the data 
requirements of 40CFR§158.190. The applicant has stated that the studies corresponding to guidelines 
830.6317 (one year storage stability) and 830.6320 (corrosion characteristics) are in progress. [MRID No. 
457102-02] 

CONCLUSIONS: 

The TRB has reviewed the product chemistry data submitted for chlorothalonil technical and has concluded 
that: 

1. All the product chemistry data submitted corresponding to 830 Series Subgroup A & Subgroup B satisfy 
the data requirements of 40CFR§158.155 to 158.190 and are acceptable, except for storage stability & 
corrosion characteristics studies. 

2. The CSF for basic formulation (dated 06-04-03 ) is acceptable. 

3. The results of one year storage stability (830.6317) and corrosion characteristics (830.6320) must be 
submitted to the Agency on completion. 

4. The proposed product was determined to be substantially similar to the registered product with Reg. No. 
50534-7 from product chemistry point of view. The amount of toxic impurity (HCB) reported on the CSF of 
the proposed product is less than the amount present in the registered product. 

*Quality control process information may be entitled to confidential treatment*
Common Name: Chlorothalonil

Chemical name:

CAS Name: 2,4,5,6-Tetrachloro-1,3-benzodicarbonitrile

IUPAC Name: Tetrachloroisophthalonitrile

CAS No.: 1897-45-6

PC Code No.: 081901

Empirical formula: C₆Cl₄N₂

Molecular Weight: 265.93

Structural formula:
Table 1: Manufacturing and Impurity Data for Chlorothalonil Technical

<table>
<thead>
<tr>
<th>GLN</th>
<th>Requirement</th>
<th>MRID</th>
<th>Status</th>
<th>Details and/or Deficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>830.1550</td>
<td>Product identity and composition</td>
<td>Basic CSF (06-04-03)</td>
<td>A</td>
<td>The NC of AI (99.4%) is supported by 5 batch analysis &amp; agree with the label claim NC. Impurities are listed on the CSF.</td>
</tr>
<tr>
<td>830.1600</td>
<td>Description of materials used to produce product</td>
<td>457102-01</td>
<td>A</td>
<td>The product specification sheets (MSDS) for all the starting materials have been provided by the registrant.</td>
</tr>
<tr>
<td>830.1620</td>
<td>Description of production process</td>
<td>457102-01</td>
<td>A</td>
<td>The production process has been described in full details. The production process is a continuous process. The reaction conditions are given, and the amounts of the reagents used in each step have been provided. The QA steps involved in each step have been described.</td>
</tr>
<tr>
<td>830.1670</td>
<td>Discussion of formation of impurities</td>
<td>457102-01 459430-01</td>
<td>A</td>
<td>The registrant has provided the complete mechanisms of formation, quantification and identification of all the impurities. The HCB has been reported with maximum of</td>
</tr>
<tr>
<td>830.1700</td>
<td>Preliminary analysis</td>
<td>457102-01 459430-01</td>
<td>A</td>
<td>Registrant has provided 5 batch analysis for the TGA. The AI was assayed by using GC/FID with internal standard. The analytical method was validated for precision, linearity &amp; accuracy.</td>
</tr>
<tr>
<td>830.1750</td>
<td>Certified limits</td>
<td>Basic CSF (06-04-03)</td>
<td>A</td>
<td>The proposed certified limits for the AI and impurities are not based on the standard certified limits, but are based on the expected production variability.</td>
</tr>
<tr>
<td>830.1800</td>
<td>Enforcement analytical method</td>
<td>457102-01</td>
<td>A</td>
<td>The GC/FID with internal standard method was used for the assay of the AI in technical. The method validated for linearity, accuracy and precision.</td>
</tr>
</tbody>
</table>

A = Acceptable; N = Unacceptable (see Deficiency); N/A = Not Applicable; G = Data gap; I = In progress or need upgrade; U = Up-grade (additional information required)
### Table 2: Physical and Chemical Properties of Chlorothalonil Technical

<table>
<thead>
<tr>
<th>GLN</th>
<th>Requirement</th>
<th>MRID</th>
<th>Status</th>
<th>Result or Deficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>830.6302</td>
<td>Color</td>
<td>457102-02</td>
<td>A</td>
<td>White</td>
</tr>
<tr>
<td>830.6303</td>
<td>Physical state</td>
<td>&quot; &quot; &quot;</td>
<td>A</td>
<td>Crystalline solid</td>
</tr>
<tr>
<td>830.6304</td>
<td>Odor</td>
<td>&quot; &quot; &quot;</td>
<td>A</td>
<td>Odorless</td>
</tr>
<tr>
<td>830.6313</td>
<td>Stability to normal and elevated</td>
<td>&quot; &quot; &quot;</td>
<td>A</td>
<td>known to be stable at higher temperatures; no data submitted on stability to metal &amp; metal ions</td>
</tr>
<tr>
<td></td>
<td>temperatures, metals, and metal ions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>830.6314</td>
<td>Oxidation/reduction: chemical</td>
<td>&quot; &quot; &quot;</td>
<td>W</td>
<td>waiver accepted</td>
</tr>
<tr>
<td></td>
<td>incompatibility</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>830.6315</td>
<td>Flammability</td>
<td></td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td>830.6316</td>
<td>Explosibility</td>
<td></td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td>830.6317</td>
<td>Storage stability</td>
<td></td>
<td>I</td>
<td>one year study is in progress</td>
</tr>
<tr>
<td>830.6319</td>
<td>Miscibility</td>
<td></td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td>830.6320</td>
<td>Corrosion characteristics</td>
<td></td>
<td>I</td>
<td>one year study in progress along with storage stability</td>
</tr>
<tr>
<td>830.7000</td>
<td>pH</td>
<td>457102-02</td>
<td>A</td>
<td>5-6 at 20°C (1% suspension in water)</td>
</tr>
<tr>
<td>830.7050</td>
<td>UV/Visible absorption</td>
<td>&quot; &quot; &quot;</td>
<td>A</td>
<td>222 nm (ε=62390), 312 nm (ε=1116), &amp; 324 nm (ε=1507)</td>
</tr>
<tr>
<td>830.7100</td>
<td>Viscosity</td>
<td></td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td>830.7200</td>
<td>Melting point</td>
<td>457102-02</td>
<td>A</td>
<td>252.6 to 254.5°C (PAI)</td>
</tr>
<tr>
<td>830.7220</td>
<td>Boiling point</td>
<td>&quot; &quot; &quot;</td>
<td>A</td>
<td>boils at 350°C</td>
</tr>
<tr>
<td>830.7300</td>
<td>Relative Density</td>
<td>&quot; &quot; &quot;</td>
<td>A</td>
<td>1.7315 @ 20°C</td>
</tr>
<tr>
<td>830.7370</td>
<td>Dissociation constants in water</td>
<td>&quot; &quot; &quot;</td>
<td>W</td>
<td>DC could not be measured. The TS is neither acid nor basic character</td>
</tr>
<tr>
<td>830.7550</td>
<td>Partition coefficient</td>
<td>&quot; &quot; &quot;</td>
<td>A</td>
<td>Log P_{ow} = 2.93 at 22°C</td>
</tr>
<tr>
<td>830.7840</td>
<td>Water solubility</td>
<td></td>
<td>A</td>
<td>5.42 x 10^{-4} g/l (0.542 ppm or mg/l at 20°C; solubility in organic solvents: See Note 1</td>
</tr>
<tr>
<td>830.7950</td>
<td>Vapor pressure</td>
<td></td>
<td>A</td>
<td>2.2 x 10^{-4} Pa at 25°C</td>
</tr>
</tbody>
</table>

A = acceptable, N = Not acceptable, U = Upgrade required, I = In progress or incomplete, W = waiver, G = Data gap, NA = Not applicable.

**Note 1.** Solubility in organic solvents (g/l): acetone (16.1), dichloromethane (25.8), ethyl acetate (9.63), hexane (0.124), methanol (1.36), toluene (48.4).
The AI, chlorothalonil, was determined by GC/FID method. The weighed amount of chlorothalonil was dissolved in acetone with a known concentration of dibutyl phthalate (IS). Calibrants were prepared similarly, using measured amounts of reference standard chlorothalonil dissolved in acetone, also with a known concentration of dibutyl phthalate. The test solution and the calibrants were analyzed using capillary GC equipped with FID. The level of chlorothalonil in chlorothalonil technical was calculated from the relative responses of chlorothalonil and dibutyl phthalate in the test solution and the calibrants. The method is applicable for levels of chlorothalonil between 90% w and 100% w.

Instrument & Parameters:

GC: Gas chromatograph equipped with FID

Column: DB-5, 30 m x 0.53 mm, film thickness 1.5 μm
Column temperature: 150°C (5 min) to 250°C (5°C/min)
Injector temperature: 240°C
Detector temperature: 280°C
Column head pressure: 70 kPa at 150°C
Total helium pressure: 130 kPa
Injection volume: 1 μL, splitless 0.5 min
Retention time: chlorothalonil - 12 min; dibutyl phthalate - 15 min

The analytical method was validated for precision, accuracy, and linearity.
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.
___ Proprietary information pertaining to the chemical composition of an inert ingredient provided by the source of the ingredient.
___ Attorney-Client Privilege.
___ Claimed Confidential by submitter upon submission to the Agency.
___ Internal Deliberative Information.

* 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.