

201-15483A

EPA High Production Volume Program

Test Plan for

IRGANOX 1330 / ETHANOX 330

1,3,5-trimethyl-2, 4,6-tris (3,5-di-t-butyl-4-hydroxybenzyl) benzene

CAS No. 1709-70-2

July 30, 2004

Submitted by:

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And

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## Executive Summary

### A. Introduction

An important objective of EPA's High Production Volume (HPV) chemical challenge program is the gathering and public release of basic hazard information on chemicals imported or manufactured at high volumes in the United States. Ciba Specialty Chemicals and Albemarle Corporation have agreed to participate in this program and here submit for review and public comment the available data and test plan for Irganox 1330 / Ethanox 330.

### B. General Substance Information

Chemical Name: 1,3,5-trimethyl-2, 4,6-tris (3,5-di-t-butyl-4-hydroxybenzyl) benzene

Appearance: White solid

Typical Commercial Purity: 98 – 100%

Chemical abstract Service Registry Number: CAS # 1709-70-2

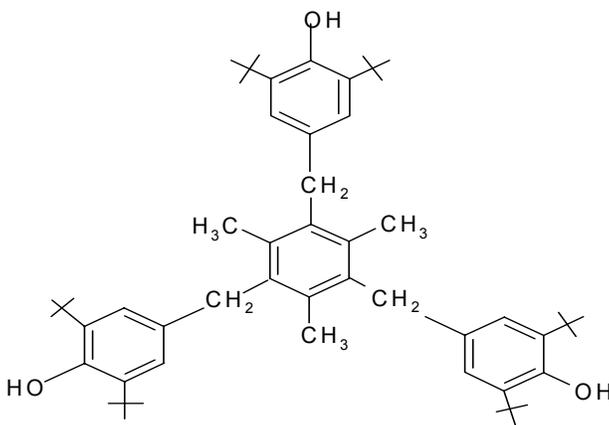
Trade Names: IRGANOX 1330 (Ciba)  
ETHANOX 330 (Albemarle)

Other Synonyms / Trade Names: Ionox 330, Ethyl 330, Ethyl Antioxidant 330, AO 40

Chemical Formula: C<sub>54</sub>H<sub>78</sub>O<sub>3</sub>

Molecular weight: 775.22

Structure:



### C. General Use Information

1,3,5-trimethyl-2,4,6-tris(3,5-di-*t*-butyl-4-hydroxybenzyl)benzene, commercially known as Irganox 1330 and Ethanox 330, is a sterically hindered phenolic antioxidant that protects organic substrates against thermo-oxidative degradation.

Irganox 1330 / Ethanox 330 is used in polyolefins (e.g., polyethylene, polypropylene, polybutene) for the stabilization of pipes, molded articles, wires and cables, dielectric films and in other polymers such as engineering plastics like linear polyesters, polyamides, and styrene homo- and copolymers. It may also be used in PVC, polyurethanes, elastomers, adhesives, and other organic substrates.

This product has been regulated by the FDA for use in all polymers at a maximum level of 0.5% except for nylon resins where the maximum use level is 1%. The resultant polymers would conceivably contact all food types with no temperature restrictions.

Sales of Irganox 1330 / Ethanox 330 are to industrial users only. The polymer industry has a record of safe use of additives such as Irganox 1330 / Ethanox 330 and worker exposures are considered minimal. Industrial Hygiene programs and Responsible Care® practices are the norm throughout the industry and it is the experience of Ciba Specialty Chemicals and Albemarle Corporation that customers handle such products in a careful and conscientious manner. Material Safety Data Sheets (MSDS) are distributed that present detailed hazard data and provide directions for safe handling. After Irganox 1330 / Ethanox 330 is incorporated in the polymer matrix it is relatively immobile and release-exposure to humans or the environment is considered minimal.

#### Environmental Endpoints:

Ecotoxicology testing for Irganox 1330 / Ethanox 330 indicates the compound has low toxicity to fish, aquatic plants and aquatic invertebrates. Aquatic toxicity testing was conducted with water loadings well above the solubility limits of the compound; these test conditions provide a worst-case challenge to the test organisms and indicate that there is low concern for environmental effects. Furthermore, under environmental conditions the low solubility of the material (< 1mg/L) should preclude the occurrence of acutely toxic exposures. The compound has a calculated *n*-octanol-water coefficient (log *P*<sub>ow</sub>) of > 6. Based on this and its other physical-chemical properties, the substance in the environment is likely to bind to the soil and sediment where it is expected to be immobile and have limited bioavailability. The material is not readily biodegradable. Based on its present commercial use, environmental release and exposures are expected to be negligible.

## Toxicology Endpoints:

Available mammalian acute toxicity data indicates the compound has very low toxicity by oral, dermal, or inhalation exposure. In a 28-day toxicity study in the rat, there are no adverse effects up to 1000 mg/kg bw per day. In subchronic 15-week toxicity studies with rats and dogs, there are no significant effects observed and a dietary NOEL greater than 5000 ppm was indicated. In 2-year carcinogenicity studies, neither tumors nor lesions were observed with dietary exposures ranging from 400 to 10,000 ppm. Repeat dose testing consistently shows that Irganox 1330 / Ethanox 330 does not have adverse effects on reproductive organs, even at relatively high exposure levels, and multi-generation reproduction testing did not demonstrate significant toxicity or teratogenic potential. Genetic toxicity testing has shown that the compound is not mutagenic. Chromosomal aberration testing is not available, however, multiple chronic studies, that are discussed in detail in the robust summary document, show that the compound does not induce tumors and is not carcinogenic. Therefore, there is no need to conduct a chromosome aberration test at this time. Furthermore, available genetic toxicity testing with other hindered phenols has indicated a low potential for mutagenic or clastogenic effects (see HPV Hindered Phenol submission, American Chemistry Council, 2003). All toxicological endpoints are fulfilled.

## Conclusions

The available data are sufficient to meet the requirements of the HPV challenge program and no additional testing is proposed.

### SUMMARY TABLE

| CAS NO. 1709-70-2                               | DATE         | RESULTS  | FULFILLS REQUIREMENT |
|---|--------------|--|----------------------|
| <b>PHYSICAL/CHEMICAL ELEMENTS</b>               |              |  |                      |
| Melting Point                                   | 2003         | 240 - 245 °C   | Yes                  |
| Boiling Point                                   | 2004         | 821.96 °C  | Yes                  |
| Vapor Pressure                                  | 2004         | 3.14 x 10 <sup>-22</sup> mm Hg (estimated)<br>1.3 x 10 <sup>-12</sup> Pa (measured)  | Yes                  |
| Partition Coefficient                           | 2004<br>1988 | log Kow > 17.17 (estimated)<br>log Kow > 6.0 (measured)  | Yes                  |
| Water Solubility                                | 1992<br>2003 | < 1 mg / liter (measured)<br>9.11 x 10 <sup>-14</sup> mg/ L (estimated)  | Yes                  |
| <b>ENVIRONMENTAL FATE AND PATHWAYS ELEMENTS</b> |              |  |                      |
| Photodegradation                                | 2004         | For reaction with hydroxyl radical,<br>predicted rate constant = 150.13 x 10 <sup>-12</sup><br>cm <sup>3</sup> /molecule-sec.<br>Predicted half-life = 0.855 hours | Yes                  |
| Stability in Water                              | 2004         | EPIWIN model could not evaluate this<br>structure. Experimental determination is<br>not practical due to low water solubility.                                     | Waiver               |
| Fugacity  | 2004         | Predicted distribution using Level III<br>fugacity model<br>Air 0.0134 %<br>Water 1.26 %<br>Soil 32.8 %<br>Sediment 66 %   | Yes                  |
| Biodegradation                                  | 1988         | Not biodegradable<br>10 mg/L: 6% in 28 days<br>20 mg/L: 16% in 28 days   | Yes                  |
| <b>ECOTOXICITY ELEMENTS</b>                     |              |  |                      |
| Acute Toxicity to Fish                          | 1988         | Zebra Fish : LC <sub>50</sub> (96 h) > 100 mg/L  | Yes                  |
| Toxicity to Aquatic Plants                      | 1988         | EC <sub>50</sub> (0-72 h) > 100 mg/L   | Yes                  |
| Acute Toxicity to Aquatic Invertebrates         | 1988         | EC <sub>50</sub> (24 h) > 100 mg/L   | Yes                  |

**SUMMARY TABLE (CONTINUED)**

| CAS No. 1709-70-2                               | DATE | RESULTS  | FULFILLS REQUIREMENT  |
|---|------|--|---|
| <b>HEALTH ELEMENTS</b>                          |      |  |   |
| Acute Toxicity                                  | 1965 | Rat: LD <sub>50</sub> (Oral) > 5,000 mg/kg   | Yes   |
|   | 1992 | Rabbit: LD <sub>50</sub> (Dermal) > 2,000 mg/kg  |   |
|   | 1983 | Rat: LD <sub>50</sub> (Inhalation) > 1,000 mg/ m <sup>3</sup>  |   |
| Genetic Toxicity<br>• Gene Mutation             | 1984 | Ames Test - Salmonella typhimurium: No increase in mutations with or without metabolic activation (at doses of 0, 0.05, 0.1, 0.2, 0.5, 1.0, and 2.0 mg/ plate) | Yes   |
| • Chromosome Aberration                         |      | No testing available   | Available chronic testing precludes the need for this study |
| Repeat Dose Toxicity<br>• Subchronic Toxicity   |      |  |   |
| i ) 15 Week oral toxicity study in rats         | 1966 | NOEL > 5000 ppm  | Yes   |
| ii ) 15 Week oral toxicity study in dogs        | 1966 | NOEL >5000 ppm   |   |
| • Chronic Toxicity Carcinogenicity              |      |  |   |
| i ) 2-Year Oral Toxicity Study in Rats and Mice | 1969 | NOEL = 5000 ppm<br>No tumors or lesions were observed  | Yes   |
| ii ) 2-Year Oral Toxicity Study in Dogs         | 1968 | NOEL = 10,000 ppm<br>No tumors or lesions were observed  |   |
| iii ) 2-Year oral toxicity study in rats        | 1968 | NOEL = 2000 ppm<br>NOAEL = 10000 ppm<br>No tumors or lesions were observed   |   |
| Reproductive and Developmental Toxicity         | 1970 | No significant effects on reproduction or development in a three-generation study.<br><br>NOEL = 5000 ppm  | Yes   |