TEST PLAN FOR CARBONIC ACID, OXYDIETHYLENE DIALLYL ESTER (CAS NO. 142-22-3)

OVERVIEW

Great Lakes Chemical Corporation and PPG Industries, Inc. jointly agree to sponsor CARBONIC ACID, OXYDIETHYLENE DIALLYL ESTER (CAS NO. 142-22-3) (DAC) under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. A common synonym for this chemical is diallyl diglycol carbonate, which is the chemical name that will be utilized throughout this document. The companies hereby submit a test plan for this substance. It is the intent of the sponsoring companies to use existing data combined with planned new studies specified in the test plan to fulfill the Screening Information Set (SIDS) endpoints for environmental fate, ecotoxicity and human health effects.

CAS No. 142-22-3	Information Available	Acceptable	New Testing Required
ENDPOINT	Y/N	Y/N	Y/N
PHYSICAL CHEMISTRY			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Density	Y	Y	N
Vapor Pressure	Y	Y	N
Water Solubility	Y	Y	N
Kow	Y	Y	N
ENVIRONMENTAL FATE			
Photodegradation	Y	Y	N
Stability in Water	N	N	Y
Biodegradation	Y	Y	N
Transport between Environmental Compartments (Fugacity)	Y	Y	N
ECOTOXICITY			
Acute Toxicity to Fish	Y	Y	N
Acute Toxicity to Aquatic Invertebrates	Y	Y	N
Toxicity to Aquatic Plants	Y	Y	N
TOXICOLOGICAL DATA			
Acute Toxicity	Y	Y	N
Repeated Dose Toxicity	Y	N	Y
Genetic Toxicity-Mutation	Y	Y	N
Genetic Toxicity-Chromosomal Aberrations	N	N	Y
Toxicity to Reproduction	N	N	Y
Developmental Toxicity	Y	Y	N

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1. Sponsoring Companies

Great Lakes Chemical Company and PPG Industries, Inc. are the United States manufacturers of Diallyl diglycol carbonate (DAC) and are the joint sponsors of this substances in the U. S. Environmental Protection Agency's HPV Chemical Challenge Program. The technical contacts at these companies are:

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2. Identity of Sponsored Substance

Diallyl diglycol carbonate (CAS No. 142-22-3) is a single chemical substance. It's primary use is as an industrial intermediate (a monomer), which is polymerized into allyl resins to make optical lenses. Its molecular structure is as follows:

$$CH_2=CHCH_2OC(=O)OCH_2CH_2OCH_2CH_2OC(=O)OCH_2CH=CH_2$$

DAC is a clear, colorless liquid at room temperature, with a melting point of –4 to 0 degrees C and a boiling point of 160 degrees C at 2.7 hPa.

3. Criteria for Determining Adequacy of Data

All relevant studies were reviewed and assessed for adequacy according to the standards of Klimisch et al. (1997). Studies receiving a Klimisch rating of 1 or 2 were considered to be adequate.

4. Test Plan

4.1 Physical/Chemical Properties

Data are available for melting point, boiling point, density and water solubility (PPG Industries, 2001)(see below). Data for vapor pressure and partition coefficient (Kow) are estimated (calculated) using a model approach. No testing is recommended.

Melting point:	-4 to 0 degrees C
Boiling point:	160 degrees C @ 2.7 hPa
Density:	1.14-1.15 g/cm^3 @ 20 degrees C
Water solubility:	< 0.1 g/l @ 20 degrees C
Vapor pressure:	0.00146 hPa @ 25 degrees C
Log Pow:	1.543

4.2 Environmental Fate/Pathways

Results of an OECD guideline study indicate that DAC is readily biodegradable. Data for photodegradation and environmental transport are estimated (calculated) using the EPIWIN/AOP Program. The estimated photodegradation hydroxyl radical rate constant is estimated to be 73.2806 E-12 cm^3/molecule-sec with an atmospheric half-life calculated to be 0.146 days. Mackay Level III Fugacity modeling indicates that DAC should partition primarily to water (46.7%) and soil (52.9%), with smaller percentages in air (0.23%) and sediment (0.115%) under hypothetical equilibrium conditions. The EPIWIN/HYDROWIN program cannot be used to model stability in water because DAC possesses a carbonate ester bond. Therefore, an experimental study to determine stability in water is warranted.

4.3 Ecotoxicity

4.3.1 Acute Toxicity to Fish

This endpoint is filled from data from two adequate fish toxicity tests (Sousa, 1982; Ward, 1982b). The LC_{50} values for DAC in freshwater and saltwater species are 0.57 mg/l and 0.707 mg/l, respectively. No testing is recommended.

4.3.2 Acute Toxicity to Aquatic Invertebrates

This endpoint is filled from data from one study in *Daphnia magna* (Suprenant et al., 1982) and another in *Mysidopsis bahia* (mysid shrimp) (Ward, 1982a). The 48-hour EC_{50} values for DAC in these species are 18 mg/l and 70.7 mg/l, respectively. No testing is recommended.

4.3.3 Acute Toxicity to Aquatic Plants

This endpoint is filled from data from one study in *Selenastrum capricornutum* (freshwater algae) (Maziarz, 1983a) and another in *Skeletonema costatum* (saltwater algae) (Maziarz, 1983b). The no observable effect concentration for DAC in both of these species is 10 mg/l (highest concentration used in the study). No testing is recommended.

4.4 Human Health Data

4.4.1 Acute Mammalian Toxicity

This endpoint is filled by two sufficient oral toxicity studies in rats (Ebbens, 1971; Kingery and Mahew, 1981a) and three dermal toxicity studies in rabbits (Ebbens, 1971; Kingery and Mahew, 1981b,c). The oral LD_{50} values for DAC in rats range from 349.5 – 515 mg/kg, and the dermal LD_{50} values range from 3038 - 10250 mg/kg. No testing is recommended.

4.4.2 Repeated Dose Mammalian Toxicity

Data from two 14-day dermal toxicity tests in rats were summarized (Lequire et al., 1980; McGahan and Mahew, 1980). Results of the study by McGahan and Mahew (1980) indicate a NOEL of 0.4 ml/kg/day. A NOEL was not determined in the study by Lequire et al., as effects

were noted at the only dose tested. An additional, longer term test is recommended, since a 14 day exposure period may be of insufficient length to adequately predict repeated dose toxicity over a longer duration.

4.4.3 Genetic Toxicity

4.4.3.1 Mutagenicity

DAC has been tested for mutagenicity in *S. typhimurium* strains TA98, TA100, TA1535, TA1537 and TA1538 in the absence and presence of a metabolic activation system (Schectman et al., 1980) and in an unscheduled DNA synthesis assay in cultured rat hepatocytes (Myhr and Brusick, 1980). Results of both studies were negative (with the exception of a positive result in Salmonella strain TA98). The positive result in strain TA98 is questionable, since it was not dose-dependent and did not occur in other strains with frame-shift mutations (TA1537 and TA1538). No further testing is required as a chromosomal aberration study is planned.

4.4.3.2 Chromosomal aberration

There are no data to fill this endpoint. Testing is recommended.

4.4.4 Reproductive Toxicity

There are no data to fill this endpoint. Testing is recommended.

4.4.5 Developmental Toxicity

Data from a well-conducted study in rabbits shows that DAC is not a developmental toxicant (Robinson et al., 1986). Effects in pups only occurred at doses that caused maternal toxicity. The NOEL for developmental toxicity was 0.1 ml/kg/day. No testing is recommended.

4.5 Additional Data

4.5.1 Metabolism

Data are available which show that DAC undergoes hydrolysis under biological conditions (Subak and Beauregard, 1981).

4.5.2 Eye and Skin Irritation

Adequate studies in rabbits have shown that DAC causes skin irritation (of varying degrees of severity) (Ebbens, 1971; Lacroix et al., 1976; Reddington, 1979) and is slightly irritating to eyes (Ebbens, 1971).

4.5.3 Sensitization

Adequate studies have shown that the skin irritation caused by dermal exposure of rabbits to DAC is not allergic in nature (Humphrey, 1979; Reddington, 1979).

4.5.4 Human Experience

Adequate studies in humans have shown that DAC causes irritant contact dermatitis (Lacroix et al., 1976; Lovell et al., 1988).

5. Proposed Testing

5.1 Stability in Water

The panel intends to perform a study on the stability of DAC in water as a function of pH to satisfy this endpoint

5.2 Repeated Dose and Reproductive Toxicity

The panel intends to perform a 90-day repeated dose oral or dermal toxicity study with DAC in the rat that incorporates histological examination of testes and ovaries. Examination of testes and ovaries from existing 90-day studies has been accepted as meeting the requirements for the reproductive toxicity endpoint in the OECD/SIDS high production volume chemical programs. Results from these studies will satisfy the repeated dose and reproductive toxicity endpoints.

5.3 Chromosomal Effects

The panel intends to perform a mammalian cell chromosomal toxicity test on diallyl diglycol carbonate. This will satisfy the chromosomal aberrations endpoint.

6. Summary

In summary, valid data are present to satisfy all physical/chemistry, ecotoxicity, and environmental endpoints (with the exception of water stability). Additionally, existing studies on acute and developmental toxicity are sufficient to satisfy these human health endpoints. Data for eye and skin irritation and sensitization are summarized (although not required). Existing studies on repeated dose toxicity (14 days) are not sufficient. The test plan recommends conductance of a repeated dose toxicity study of a 90-day duration, which will incorporate toxicity to reproductive organs. As no studies exist on stability in water, or chromosomal toxicity, studies will be performed which address these endpoints.

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