ANNEX 5-1: Case studies (US EPA , New chemicals)

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Category: Acid Chlorides Environmental Toxicity

Definition. This category includes carbonyl chlorides (R-C[=O]Cl) and sulfochlorides (R-S[=O]Cl) where R may be either aliphatic or aromatic. Toxicity is limited by the fact that this class of compounds hydrolyzes and also, probably, if the octanol/water partition coefficient (Kow) is above a log Kow value of 8. It has been assumed that these compounds need to be absorbed to be toxic, therefore, compounds with MWs > 1000 will probably be excluded in the future once this assumption is confirmed with toxicity information. However, toxicity information is needed to confirm this assumption.

Hazard Concerns. Acute toxicity for three members of this category are available and all have been shown to be moderately toxic to aquatic organisms (i.e., acute toxicity values between 1 and 100 mg/L): benzoyl chloride, fish 96-h LC50 = 35.0 mg/L, an aromatic dicarboxyl dichloride, fish 96-h LC50 = 6.2 mg/L, and benzene sulfochloride, fish 48-h LC50 = 3.0 mg/L. All of these tests have been done with the static method using nominal concentrations. It is unclear just how acid chlorides are toxic to aquatic organisms. It is known that acid chlorides hydrolyze to the carboxylic/sulfonic acid and HCl. It is not known if the toxic effect is the result of (1) absorption of the acid chloride and hydrolysis within the membrane, or (2) the HCl produced from the hydrolysis. It is known that the carboxylic/sulfonic-acid hydrolysis products are of low toxicity.

Boundaries. There are no known lower boundaries. The upper boundaries will be based on K_{ow} and MW when enough information is obtained. In general, when the log K_{ow} value is < 8, the environmental base set of tests will be requested for aquatic releases and the terrestrial base set of tests will be recommended for terrestrial exposures. When the log K_{ow} is > 8, testing will be requested until enough information is obtained to determine whether these compounds will have no toxic effects at saturation. Generally, members of this category will have MWs of less than 1000 but testing of members with a MW > 1000 may be requested to confirm whether acid chlorides have to be absorbed to be toxic.

General Testing Strategy. The testing strategy for acid chlorides will consist of two steps. (1) Hydrolysis as a function of pH at 25 C (40 CFR 796.3500) will be recommended. Depending on the outcome of this environmental fate testing and reassessment, (2) the aquatic base set of environmental toxicity tests will be recommended for aquatic exposures with the fish acute toxicity test done once or twice.

Chronic toxicity testing for aquatic organisms include: the fish early life state toxicity test, the daphnid partial life cycle toxicity test and the algal toxicity test.

The terrestrial base set of environmental toxicity tests (i.e., the early seeding growth test, the earthworm acute toxicity test and the soil microbial community bioassay) will be recommended for terrestrial exposures. Chronic toxicity testing for terrestrial organisms include: the plant whole life cycle test, the plant uptake test, and the soil microbial community bioassay.

October, 1990

Category: Acid Dyes and Amphoteric Dyes Environmental Toxicity

Definition. Organic dyes are divided into four classes depending on the type of electronic charge of the dye: nonionic (neutral dyes); anionic (negative charge or acid dyes); cationic (positive charge) dyes; and amphoteric (mixture of positive and negative charges on same molecule) dyes. Nonionic or neutral dyes are assessed as neutral organic chemicals for which there is a separate category description, and cationic dyes also have a separate category description. Amphoteric dyes are assessed either as cationic or anionic dyes depending on dominant net charge.

Hazard Concerns. Analysis of over 200 acid dyes (Auer et al. 1990, Nabholz 1990, Sigman et al. 1983, Tonogai et al. 1979, Little and Lamb 1972, ADMI 1974) have indicated that some monoacid and diacid dyes can show moderate to high toxicity (i.e., acute values < 100 mg/L and < 1 mg/L) to fish and aquatic organisms. Dyes with three or more acid groups showed low toxicity (i.e., acute values > 100 mg/L) towards fish and invertebrates. Some metal chelated dyes, i.e., Al, Co, Cr, Fe, have shown moderate toxicity towards fish and daphnids and the toxicity has not been explained by the residual free (un-chelated) metal ion in the dye product. All acid dyes showed moderate toxicity towards green algae. Analysis of available data (Auer et al. 1990, Nabholz 1990) has suggested that effects to algae were not the result of direct toxicity but represented an indirect effect due to shading. Senior regulatory decision-makers in OPPT (then OTS) decided in 1988 that the risk to algae from indirect (shading) toxicity was not an unreasonable risk for two main reasons: (1) algae grew quickly as soon as the dye was diluted, and (2) the release of colored effluents in the U. S. generally results in immediate complaints by citizens to their local authorities, e.g., county and state governments. The rapid response by the public generally results in quick regulatory action by local officials.

Since there is no SAR for acid dyes (Auer et al. 1990), hazard profiles for monoacid dyes are developed using measured data or data for the nearest analog(s).

Boundaries. Acids dyes must have some water solubility and molecular weights generally need to be near or below 1000.

General Testing Strategy.

I. Release to Aquatic Ecosystems:

Tier 1. Because of the above boundary conditions, and the need to assess human exposure as well as environmental toxicity, if there is insufficient knowledge about the water solubility of the dye, then it should be measured (40 CFR §796.1860). The fish and daphnid acute toxicity tests from the aquatic base set of environmental toxicity tests will be recommended for aquatic exposures. The acute toxicity tests for fish (40 CFR §797.1400) and daphnids (40 CFR §797.1300) will be done using the flow-through method with measured concentrations, and effective concentrations will be based on 100% active ingredients (AI) and mean measured concentrations.

If there is no significant risk from the PMN after the results of the fish and daphnid acute toxicity tests have been integrated into the risk assessment, then no further testing is recommended. However, if there is a significant risk, then go to Tier 2.

Tier 2. Direct and Indirect Photolysis Screening Test (40 CFR 796.3765). If $t_{1/2} \leq 2$ days, go to Tier 3; if $t_{1/2}$ > 2 days, go to Tier 4.

Tier 3a. If $t_{1/2} \leq 2$ days and photolysis products are known and/or identified, then assess photolysis products for environmental hazards.

Tier 3b. If t½ ≤ 2 days and photolysis products are not known and/or identifiable, then prepare a stock solution of PMN using the standard humic-containing solution described in the direct and indirect photolysis screening test [40 CFR 796.3765 (b)(2) and (c)(2)], expose to sunlight for at least 6 half-lives (t½), and test photolysis products for toxicity with most sensitive species from environmental base set.

Tier 4. Fish chronic toxicity testing, i.e., fish early life stage (ELS) toxicity testing (40 CFR 797.1600), with flow-through methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; and statistical analysis of effective concentrations at days 7, 14, 21, and 28.

Daphnid chronic toxicity testing (40 CFR 797.1330), with flow-through methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; statistical analysis of effective concentrations at days 7, 14, and 21.

Aerobic biodegradability according to any one of the following test guidelines (listed in order of preference):

Aerobic Aquatic Biodegradation 40 CFR 796.3100

Modified Sturm Test 40 CFR 796.3260

Closed Bottle Test 40 CFR 796.3200

Modified OECD Screening Test 40 CFR 796.3240

Modified MITI Test (I) 40 CFR 796.3220

Modified AFNOR Test 40 CFR 796.3180

II. Release to Terrestrial Ecosystems:

The terrestrial base set of environmental toxicity tests (i.e., the early seeding growth test, the earthworm toxicity test and the soil microbial community bioassay) will be recommended for terrestrial exposures. Chronic toxicity testing for terrestrial organisms include: the plant whole life cycle test, the plant uptake test, and the soil microbial community bioassay.

References.

American Dye Manufacturers Institute, Inc. (ADMI), 1974, "Dyes and the Environment: Reports on Selected Dyes and Their Effects," Vol. II, ADMI, New York.

Auer, C.M., Nabholz, J.V. and Baetcke, K.P., 1990, "Mode of Action and the Assessment of Chemical Hazards in the Presence of Limited Data: Use of Structure-Activity Relationships (SAR) under TSCA, Section 5," Environmental Health Perspectives, Vol. 87, pp. 183-197.

Little, L.W. and Lamb J.C., III, 1972, "Acute Toxicity of 46 Selected Dyes to the Fathead Minnow, Pimephales promelas,"Final Report to the American Dye Manufacturers Institute,Inc., UNC Wastewater Research Center, Department of Environmental Sciences and Engineering, School of Public Health, University of North Carolina, Chapel Hill, NC.

Nabholz, J.V., 1990, "The OTS PMN ECOTOX Data Base: a Confidential Business Information (CBI) Collection of Environmental Toxicity Data from New Chemical Submissions Under Sec. 5," Unpublished, Environmental EffectsBranch, Health and Environmental Review Division (TS-796),U. S. Environmental Protection Agency, Washington, DC.

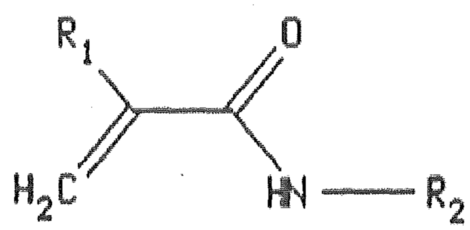
Sigman, C.C., Helms, C.T., Papa, P.A., Atkinson, D.L., Doeltz, M.K. and Winship-Ball, A., Jan. 1983, "Anthraquinone Dyes and Related Chemicals: Review and Assessment of Potential Environmental and Health Aspects," Final Report to the Dyes Environmental and Toxicology Organization, Inc., SRI International, Menlo Park, CA.

Tonogai, Y., Ito, Y., Iwaida, M., Tati, M., Ose, Y. and Sato, T., 1979, "Studies on the Toxicity of Coal-Tar Dyes. II. Examination of the Biological Reaction of Coal-Tar Dyes to Vital Body," The Journal of Toxicological Sciences, Vol. 4, pp. 211-219.

July, 1991; revised June, 1994

Category: Acrylamides Human Health and Environmental Toxicity

Definition. Any new chemical with the following structure is considered to be a member of the category:



R1 = H (acrylamides)

= CH3 (methacrylamides)

R2 = anything

A typical acrylamide in the new chemical program is used as a monomer and has a molecular weight of ≤500. The acrylamides of greatest concern are those with a labile substituent, e.g., methylol acrylamides, that may release acrylamide *per se* under metabolic conditions. For toxicity to aquatic organisms, there is a concern for all substituted acrylamides with molecular weights of <1000 and log Kow of <8.0.

Hazard Concerns. Based on analogy to acrylamide *per se*, members of the class are considered potential carcinogens, heritable mutagens, reproductive and developmental toxicants, and toxic to aquatic organisms. Acrylamides are also potential neurotoxins based on data for a number of low molecular weight acrylamides.

Boundaries. Structures with an acrylamide equivalent weight of ≥5,000 are presumed not to pose a hazard under any conditions. Typically, concerns are confined to those species with molecular weights <1,000 whenever inhalation (or environmental) exposure is expected, and to species <500 when dermal, but not inhalation, exposure to humans is expected.

Occupational Exposure Controls. Because acrylamides are expected to be absorbed via the dermal route, glove permeation testing conducted in accordance with standard ASTM testing protocols may be required, depending upon estimated workplace exposures and the hazard identified for the particular acrylamide submitted as a PMN.

General Testing Strategy.

Tier 1. To properly assess human and environmental toxicity or exposure, certain physical-chemical or environmental fate properties need to be measured:

water solubility (40 CFR §796.1860)

Kow (40 CFR §796.1570 or 40 CFR §796.1550)

vapor pressure (40 CFR §796.1950)

melting point-melting range (OECD 102 or OPPTS 830.7200)

Aerobic biodegradability can be determined using one of the following test guidelines, listed in approximate order of preference:

Aerobic aquatic biodegradation 40 CFR 796.3100

Modified Sturm test 40 CFR 796.3260

Closed bottle test 40 CFR 796.3200

Modified OECD screening test 40 CFR 796.3240

Modified MITI test (I) 40 CFR 796.3220

Modified AFNOR test 40 CFR 796.3180

The physical state and electronic charge of the PMN substance should also be reported.

Tier 2. EPA considers the following tests to be the most appropriate for acrylamides found to pose an unreasonable risk to human health:

- 90-day subchronic toxicity (40 CFR §798.2650) with functional observational battery (40 CFR §798.6050) and neuropathology (40 CFR §798.6400).

- A rodent dominant lethal assay (40 CFR §798.5450). If positive, a rodent heritable translocation test (40 CFR §798.5460) would be the appropriate followup test.

- A 2-year carcinogenicity test (40 CFR §798.3300) in rats and mice.

To address environmental toxicity concerns, the following testing is recommended, for acrylamides with log Kow <5: acute aquatic toxicity testing in algae, daphnid, and fish. The acute toxicity tests for fish (40 CFR 797.1400) and daphnids (40 CFR 797.1300) will be done using the flow-through method with measured concentrations; effective concentrations will be based on 100% active ingredients (AI) and mean measured concentrations; measured TOC of dilution water in the control <2 mg TOC/L; the highest treatment concentration on a mean measured-basis should equal the aqueous solubility limit; and solvent can be used to assist the PMN to reach its aqueous solubility limit quicker, but cannot be used to artificially enhance the water solubility of the PMN beyond its aqueous solubility limit.

The algal toxicity testing (40 CFR 797.1050), should be done with static methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; statistical analysis of effective concentrations at 24, 48, 72, and 96 hours; test medium with at least 0.300 mg/L EDTA as a final concentration; and the highest treatment concentration on a mean measured-basis equal to the aqueous solubility limit. Solvent can be used to assist the PMN substance to reach its aqueous solubility limit quicker, but cannot be used to artificially enhance the water solubility of the PMN substance beyond its aqueous solubility limit.

For acrylamides with log Kow >5 and <8, aquatic toxicity testing should be for chronic effects only: (1) fish chronic toxicity testing, i.e., fish early life stage (ELS) toxicity testing with rainbow trout (40 CFR 797.1600), with flow-through methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; and statistical analysis of effective concentrations at days 30, 45, 60, 75, and 90; (2) daphnid chronic toxicity testing (40 CFR 797.1330), with flow-through methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; statistical analysis of effective concentrations at days 7, 14, and 21; and

(3) algal toxicity testing (40 CFR 797.1050), with static methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; statistical analysis of effective concentrations at 24, 48, 72, and 96 hours; test medium with at least 0.300 mg/L EDTA as a final concentration; and the highest treatment concentration on a mean measured-basis equal to the aqueous solubility limit. Solvent can be used to assist the PMN substance to reach its aqueous solubility limit quicker, but cannot be used to artificially enhance the water solubility of the PMN substance beyond its aqueous solubility limit.

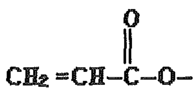
November 1990; revised July 1993; revised October 1995

Category: **Acrylates/Methacrylates** Environmental Toxicity

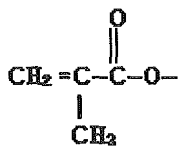
(Human Health, case-by-case)

Definition. Any molecular structure containing one or more of the following reactive groups is considered to be a member of the class:

– acrylate,



– methacrylate,



Hazard Concerns.

Human Health: As a result of testing conducted under an agreement between the Agency and the Specialty Acrylates and Methacrylates (SAM) Panel of the Chemical Manufacturers Association (CMA), EPA no longer controls new chemical acrylates or methacrylates as a category based on health concerns. However, if a new acrylate is structurally similar to a substance for which EPA has positive toxicity data, EPA may regulate that substance under TSCA section 5(e) based on its potential unreasonable risk. This will be done on a case-by-case basis and is expected to effectively eliminate most regulation of acrylates, especially higher molecular weight and polymeric substances. Despite the fact that EPA no longer expects to make a potential unreasonable risk to human health finding for many of the new acrylates, EPA still recommends the use of engineering controls or personal protective equipment to reduce exposures in the workplace in recognition of their potential as irritants and sensitizers.

Environmental Toxicity: The ecotoxicity of acrylates and methacrylates is a function of the octanol-water partition coefficient. They exhibit simple narcosis at log P's >5, but display excess toxicity at lower log P's. The toxicity of acrylates and methacrylates can be predicted by a QSAR (quantitative structure-activity relationship), although there are some members of the class such as allyl methacrylate that are significantly more toxic than predicted by the QSAR.

Boundaries. Typically, environmental toxicity concerns are confined to those species with molecular weights <1,000. Acute and chronic toxicity is possible at log P's <5, and chronic toxicity is possible at log P's <8.

General Testing Strategy

Tier 1. To properly assess environmental toxicity or exposure, certain physical-chemical or environmental fate properties need to be measured:

water solubility (40 CFR §796.1860)

log Kow (40 CFR §796.1570 or 40 CFR §796.1550)

vapor pressure (40 CFR §796.1950)

melting point-melting range (OECD 102 or OPPTS 830.7200)

aquatic biodegradation (40 CFR §796.3100).

The physical state and electronic charge of the PMN substance should also be reported.

Tier 2. To address environmental toxicity concerns, the following testing is recommended: acute aquatic toxicity testing in algae, daphnid, and fish (all tests using measured concentrations; algae: static method, daphnid and fish: flow-through method).

September, 1988; Revised July, 1993 and January, 1997.

Category: Aldehydes Environmental Toxicity

Aldehydes are a class of organic compounds characterized by the functional group R-C(=O)-H. Aldehydes are ionizable in water and exhibit excess aquatic toxicity in addition to narcosis. **Polyaldehydes** are more toxic than monoaldehydes to aquatic organisms and **acrylic/vinyl/allylic aldehydes**, e.g., acrolein, are more toxic than polyaldehydes. Vinyl/allylic/acrylic aldehydes are a class of organic compounds characterized by both the aldehyde, R-C(=O)-H, and vinyl, H_2C=C-R, or allylic, R-C=C-R, functional groups. Allylic and vinyl aldehydes, e.g., acrolein, C=CC(=O), exhibit excess toxicity.

It is assumed that aldehydes need to be absorbed to be toxic, therefore, aldehydes with MW >1000 will be excluded from this category. Acute toxicity for aldehydes is known to be limited by the octanol/water partition coefficient (K_{ow}). Above a log K_{ow} value of >6.0, aldehydes show no effects at saturation during 96-h exposures to fish. Aldehydes which are solids at room temperature may show no toxicity at saturation at lower K_{ow} values depending on the melting point, i.e., the higher the melting point at a given K_{ow}, the greater the likelihood that no toxicity will be observed at saturation. For solids, the no effects at saturation has to be determined on a case-by-case basis. There are no measured upper K_{ow} limits for chronic toxicity at this time, but it may not be much above a log K_{ow} = 8. Future testing will determine K_{ow} limits.

Hazard Concerns: The toxicity for aldehydes has been determined through SAR Analysis:

SARs for **monoaldehydes**:

log fish 96-h LC50 (moles/L) = -0.449 log K_{ow} -3.314

where n=54, R^2=0.53, CLOGP<6, MW<1000;

log daphnid 48-h LC50 (millimoles/L) = -0.059 -0.608 log K_{ow}

where n=5, R^2=1.0, CLOGP<6, MW<1000;

log green algal 96-h EC50 (mmol/L) = 0.994 -0.812 log K_{ow} (CLOGP)

where n=2, R^2=1.0, CLOGP<6.4, MW<1000;

log fish ChV (millimoles/L) = -0.810 -0.680 log K_{ow} (CLOGP)

where n=3, R^2=0.97, CLOGP<8, MW<1000;

log daphnid ChV (millimoles/L) = -1.090 -0.576 log K_{ow} (CLOGP) where n=2, R^2=1.0, CLOGP<8, MW<1000; and

log algal ChV (mmol/L) = 0.053 -0.644 log K_{ow} (CLOGP)

where n=5, R^2=0.99, CLOGP<8, MW<1000.

SARs for **polyaldehydes**:

log fish 96-h LC50 (millimoles/L) = -1.176 -0.371 log K_{ow} (CLOGP)

where n=2, R^2=1.0, CLOGP<6, MW<1000;

log fish 96-h LC50 (millimoles/L) = -1.021 -0.396 log K_{ow} (SRC)

where n=2, R^2=1.0, SRC<6, MW<1000;

log daphnid 48-h LC50 (mmol/L) = -1.059 -0.440 log K_{ow} (CLOGP)

where n=2, R^2=1.0, CLOGP<6, MW<1000;

log daphnid 48-h LC50 (mmol/L) = -0.875 -0.471 log K_{ow} (SRC)

where n=2, R^2=1.0, SRC<6, MW<1000;

log green algal 96-h EC50 (mmol/L)= -1.772 -0.364 log K_{ow} (CLOGP)

where n=3, R^2=0.99, CLOGP<6.4, MW<1000;

log green algal 96-h EC50 (mmol/L)= -1.620 -0.388 log K_{ow} (SRC)

where n=3, R^2=0.99, CLOGP<6.4, MW<1000;

log fish ChV (millimoles/L) = -2.298 -0.488 log K_{ow} (CLOGP)

where n=2, R^2=1.0, CLOGP<8, MW<1000;

log fish ChV (millimoles/L) = -2.092 -0.513 log K_{ow} (SRC)

where n=2, R^2=1.0, CLOGP<8, MW<1000;

log daphnid ChV (millimoles/L) = -1.798 -0.488 log K_{ow} (CLOGP)

where n=2, R^2=1.0, CLOGP<8, MW<1000;

log daphnid ChV (millimoles/L) = -1.592 -0.513 log K_{ow} (SRC)

where n=2, R^2=1.0, CLOGP<8, MW<1000;

log algal ChV (millimoles/L) = -2.313 -0.348 log K_{ow} (CLOGP)

where n=2, R^2=1.0, CLOGP<8, MW<1000; and

log algal ChV (millimoles/L) = -2.166 -0.367 log K_{ow} (SRC)

where n=2, R^2=1.0, CLOGP<8, MW<1000

SARs for **vinyl/allylic/acrylic aldehydes**:

log fish 96-h LC50 (mmoles/L) = -3.502 +0.017 log K_{ow} (CLOGP) where n=3, R^2=0.25, CLOGP<6, MW<1000; and

log fish ChV (millimoles/L) = -4.377 -0.228 log K_{ow} (CLOGP)

where n=2, R^2=1.0, CLOGP<8, MW<1000.

Environmental Fate:

Boundaries: MW <1000. Log K_{ow} <6.0 for acute toxicity to fish and aquatic invertebrates; log K_{ow} <6.4 for toxicity to green algae as a 96-h EC50; and log K_{ow} assumed to be <8.0 for chronic toxicity to aquatic organisms, but could be higher.

General Testing Strategy:

I. Release to Aquatic Ecosystems:

Tier 1. The aquatic base set of environmental toxicity tests will be recommended for aquatic exposures. The acute toxicity tests for fish (CFR §797.1400) and daphnids (CFR §797.1300) will be done using the flow-through method with measured concentrations; effective concentrations will be based on 100% active ingredients (AI) and mean measured concentrations; measured TOC of dilution water in the control; ideally, mean measured concentrations in the highest treatment concentration should be equal the aqueous solubility limit; and solvent can be used to assist the aldehyde to reach its aqueous solubility limit quicker, but cannot be used to artificially enhance the water solubility of the aldehyde beyond its aqueous solubility limit. Stock solutions in water should be adjusted to pH near 7.0.

The algal toxicity testing (CFR §797.1050), should be done with static methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; statistical analysis of effective concentrations at 24, 48, 72, and 96 hours; test medium with at least 0.300 mg/L EDTA as a final concentration; ideally, mean measured concentrations in the highest treatment concentration should be equal the aqueous solubility limit; and solvent can be used to assist the aldehyde to reach its aqueous solubility limit quicker, but cannot be used to artificially enhance the water solubility of the aldehyde beyond its aqueous solubility limit. Stock solutions in water should be adjusted to pH near 7.0.

If there is no significant risk from the aldehyde after the results of the environmental base set have been integrated into the risk assessment, then no further testing is recommended. However, if there is a significant risk, then go to Tier 2.

Tier 2. Aerobic biodegradability according to any one of the following test guidelines (listed in order of preference):

Aerobic Aquatic Biodegradation 40 CFR 796.3100

Modified Sturm Test 40 CFR 796.3260

Closed Bottle Test 40 CFR 796.3200

Modified OECD Screening Test 40 CFR 796.3240

Modified MITI Test (I) 40 CFR 796.3220

Modified AFNOR Test 40 CFR 796.3180

If there is no significant risk from the aldehyde after the results of biodegradation testing have been integrated into the risk assessment, then no further testing is recommended. However, if there is a significant risk, then go to Tier 3.

Tier 3. Fish chronic toxicity testing, i.e., fish early life stage (ELS) toxicity testing (CFR §797.1600), with flow-through methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; statistical analysis of effective concentrations at days

7, 14, 21, and 28; measured TOC of dilution water in the control; ideally, mean measured concentrations in the highest treatment concentration should be equal the aqueous solubility limit; solvent can be used to assist the PMN to reach its aqueous solubility limit quicker, but cannot be used to artificially enhance the water solubility of the PMN beyond its aqueous solubility limit; and the 7-d ELS stage toxicity test cannot be substituted for the 28-d ELS toxicity test because the 7-d ELS toxicity test may underestimate chronic toxicity measured by the 28-d ELS toxicity test when the Chronic Values are compared. Stock solutions in water should be adjusted to pH near 7.0.

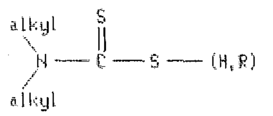
Daphnid chronic toxicity testing (CFR §797.1330), with flow-through methods; measured concentrations; effective concentrations based on 100% active ingredients (AI) and mean measured concentrations; statistical analysis of effective concentrations at days 7, 14, and 21; measured TOC of dilution water in the control; ideally, mean measured concentrations in the highest treatment concentration should be equal the aqueous solubility limit; solvent can be used to assist the PMN to reach its aqueous solubility limit quicker, but cannot be used to artificially enhance the water solubility of the PMN beyond its aqueous solubility limit; and the 7-d daphnid chronic toxicity test cannot be substituted for the 21-d toxicity test because the fish 7-d ELS toxicity test may underestimate chronic toxicity measured by the fish 28-d ELS toxicity test when the chronic values are compared.

II. Release to Terrestrial Ecosystems: The terrestrial base set of environmental toxicity tests (i.e., the early seeding growth test, the earthworm toxicity test and the soil microbial community bioassay) will be recommended for terrestrial exposures. Chronic toxicity testing for terrestrial organisms include: the plant whole life cycle test, the plant uptake test, and the soil microbial community bioassay.

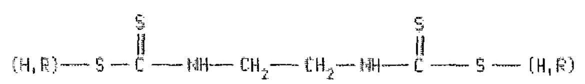
July, 1996

Category: Aliphatic Amines Environmental Toxicity

This category includes primary amines, secondary amines and tertiary amines; or monoalkyl amines, dialkly amines and trialkyl amines, respectively. This group includes alkanes, alkenes and alkynes; substitutions on carbon (alkyl) chains may include but not be limited to halogens and hydroxyls; insertions in alkyl chain may include but not be limited to ethoxys, propoxys, ethers, sulfides, disulfides and polysulfides; amine oxides are also included in this category; fatty polyamines (e.g., diamines, triamines, tetraamines, pentamines, etc) are also included; amines may either be un-ionized (free) or ionized; and strong ion pairs may also be included.



N,N-dialkyldithiocarbamate



ethylenebisdithiocarbamate

Hazard Concerns: Members of this category can be highly toxic to all groups of freshwater organisms (i.e., fish, aquatic invertebrates and green algae). Toxicity is related to the length of the hydrophobic carbon chains: the longer (or greater the number of carbons) the chain the more toxic to aquatic organisms when the number of amines is constant; and the greater the number of amines, the greater the toxicity given a constant carbon chain length. Small aliphatic amines are more toxic to algae than fish and invertebrates; higher molecular weight amines are equally toxic to all aquatic organisms. Small aliphatic amines which are un-ionized are more toxic to fish than when they are ionized; toxicity to algae appears to be unaffected by ionization. Strong ion pairs are generally much less toxic to fish and invertebrates because of solubility limitations, but remain highly toxic to green algae. The toxicity of each amine will be predicted using structure-activity relationships (SARs) and analogs contained in a generic standard environmental hazard review for aliphatic amines.

Boundaries: There are no lower boundaries and the upper boundary is unknown at this time. It is known that a C13-NH3 Cl is still toxic to fish at less than 1 mg/L. An upper boundary for carbon chain length will probably be about 20 carbons but more information is needed at this time. Generally, members of this category will have molecular weights less than 1000.

General Testing Strategy

Tier 1. The base set of environmental toxicity tests in clean dilution water and two fish acute toxicity tests done in the presence of humic acid (i.e., TOC) will be recommended. These test will be done under static methods with nominal concentrations. Smaller amines (e.g., Schiff bases) are expected to demonstrate less mitigation by humic acid (larger log P, greater mitigation; increase log P correlates to increased MW). If hydrolysis 1/2 life is less than one hour, test the hydrolysis product; if it is greater than one hour, test parent material.

Tier 2. If TOC significantly reduces the toxicity to water column species, then toxicity testing for toxicity to benthic organisms (i.e., organisms that ingest sediment) will be recommended; however, if TOC does not significantly reduce the toxicity to water column species, then chronic toxicity with fish and aquatic invertebrates will be recommended as well as aerobic biodegradation testing.

Aerobic biodegradability can be determined using one of the following test guidelines, listed in approximate order of preference:

Aerobic aquatic biodegradation 40 CFR 796.3100

Modified Sturm test 40 CFR 796.3260

Closed bottle test 40 CFR 796.3200

Modified OECD screening test 40 CFR 796.3240

Modified MITI test (I) 40 CFR 796.3220

Modified AFNOR test 40 CFR 796.3180

September 1988; revised November 1995.

Category: Alkoxysilanes Human Health

Environmental Toxicity

Definition. Any molecular structure containing one or more of the following reactive groups is considered to be a member of the category.

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 |  |
-C-O-Si-
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The "typical" new chemical of concern is a polymer with a substantial fraction of species with molecular weights <1000 and pendant trimethoxy- or triethoxysilane groups.

Hazard Concerns.

Health - Concern for lung toxicity from inhalation of vapors or aerosols is based on data for a number of low-molecular-weight alkoxysilanes. Trimethoxysilane (TMS) is clearly the most toxic member of the class causing irreversible lung effects at low doses, but the Agency does not consider it appropriate to use TMS as a regulatory benchmark for all alkoxysilanes.

For trimethoxysilane monomers and polymers with a low trimethoxysilyl equivalent weight, a NOAEL of 10 ppm (about 11 mg/kg/day) based on a 90-day study with vinyltrimethoxysilane in monkeys is deemed an appropriate generic benchmark.

Alkoxysilanes in which the alkyl substituent is **not** a methyl group do not appear to be as toxic as methoxysilanes. The New Chemicals Program currently uses a generic benchmark NOAEL of 75 mg/kg/day, based on a 90-day inhalation study with tri(isopropenoxy)silane, for alkoxysilanes other than methoxysilanes.

Ecotoxicity - Alkoxysilanes are highly toxic to algae and moderately toxic to aquatic invertebrates. For example, the daphnid 48-hr LC_{50} for dimethyldiethoxysilane is 1.25 mg/L, and the 15-day algal $EC_{95's}$ for vinyltriethoxysilane, tetraethoxy-silane, and trifluoropropenyl(methyl)diethoxysilane are all approximately 10 µg/L.

Boundaries. Methoxy- and ethoxysilanes are presumed not to pose a hazard under any conditions if the equivalent weight is 5,000 and no more than 25% of species have molecular weights less than 1,000 and no more than 10% of species have molecular weights less than 500. For alkoxysilanes with alkyl substituents larger than propyl groups, the equivalent weight cutoff is 1,000. The degree of concern depends on the relative abundance of lower molecular weight species, but there is no molecular weight threshold above which there would be no concern.

To better define the boundaries of the category, EPA seeks testing on a limited number of alkoxysilanes that focuses on (1) the relationship between molecular weight (or alkoxysilyl equivalent weight) and inhalation toxicity and (2) the importance of increasing alkoxy chain length in limiting toxicity.

General Testing Strategy

The Agency recommends the following testing as appropriate to address health and environmental toxicity concerns for this category:

1. 90-day subchronic test in rodents by the inhalation route (40 CFR 798.2650).

2. Hydrolysis testing (40 CFR 796.3500). If $t_{1/2}$ is less than one hour, base set ecotoxicity testing (see "3," below) is conducted with the hydrolysis products only. If $t_{1/2}$ is greater than one hour, base set ecotoxicity testing is conducted with the parent material; the PMN submitter has the option of also testing with the hydrolysis products.

3. Base-set ecotoxicity testing to include fish (40 CFR 797.1400) using the static method, daphnids (40 CFR 797.1300) using the static method and algae (40 CFR 797.1050) using the static method, all nominal concentrations. Direct dilution of the test alkoxysilane and organisms is added within 10 minutes. The static-renewal method is used for fish and daphnid test, plus an additional fish test using aged stock solution.

Results of the acute ecotoxicity testing may trigger chronic fish (40 CFR 797.1600) and daphnid (40 CFR 797.1350) testing.

4. Physical-chemical or environmental fate testing including, as appropriate, melting point (40 CFR 796.1300) or boiling point (40 CFR 796.1220), water solubility (40 CFR 796.1840 or 796.1860), log K_{ow} (40 CFR 796.1550, 796.1570 or 796.1720), vapor pressure (40 CFR 796.1950), direct photolysis and indirect photolysis (40 CFR 796.3765). Need for water solubility, log K_{ow}, and photolysis testing determined by outcome of above hydrolysis testing.

September, 1988; revised June, 1994

Category: **Aluminum Compounds**

Risk Management Statement. Greatest concern is for soluble forms of aluminum (Al). If water solubility is greater than 1 part per billion (1 ppb), the Agency will prohibit releases of the PMN substance to water pending the submission of environmental toxicity testing.

Definition. This category includes inorganic salts of Al, complexes between Al and organic acids or chelates of Al by polyanionic monomers, and organoAl compounds, i.e., Al covalently-bonded with carbon. For example, some inorganic Al salts include: Al hydroxide, Al chloride, Al fluoride, Al nitrate, Al phosphate, and Al sulfate. Not included in this category are dyes complexed with Al (see dye categories addressed elsewhere within this "TSCA New Chemicals Program Chemical Categories" document).

Hazard Concerns. Soluble salts of Al are known to be highly toxic to green algae and moderately toxic to fish and aquatic invertebrates at pH values between 6.5 to 9.0 and in terms of soluble Al in mg Al/L. Toxicity information are available for Al chloride, Al sulfate, and Na aluminate. The Office of Water (USEPA, 1988, EPA440/5-86-008) cited Seipt et al. (1984, Water Air Soil Pollut. 23:81-95) who concluded that "the simple hydroxides ($Al(OH)^{2+}$ and $Al(OH)_2^{+}$) are regarded as the most dangerous forms while organically bound Al and polymeric forms are less toxic or essentially harmless." The Office of Water (USEPA, 1988) also concluded that solutions of Al in water approach chemical equilibrium rather slowly and that Al can form strong complexes with fulvic and humic acids.

The toxicity profile for soluble Al salts, listed below, is based on (1) available measured (M) toxicity data, (2) mg Al/L (ppm Al), (3) pH between 6.5 and 9.0, and (4) moderate hardness (about 150.0 mg/L as $CaCO_3$).

fish (FHM) 96-h LC50 = 35.0 M pH7.3 H220

fish (RT) 96-h LC50 = 8.6 M pH7.5 H47

fish (RT) 96-h LC50 = 7.4 M pH6.6 H47

fish (RT) 96-h LC50 = 14.6 M pH7.3 H47

mean RT 96-h LC50 = 10.0 P n3

fish (BT) 96-h LC50 = 3.6 M pH6.5 H?

mean fish 96-h LC50 = 11.0 P n3

daphnid (Cd) 48-h LC50 = 1.9 M pH7.4 H50

daphnid (Cd) 48-h LC50 = 3.7 M pH7.7 H47

mean Cd 48-h LC50 = 2.7 P n2

daphnid (Dm) 48-h LC50 = 3.9 M pH7.0 H45

daphnid (Dm) 48-h LC50 = 38.0 M pH7.1 H220

mean Dm 48-h LC50 = 12.0 P n2

mean daphnid 48-h LC50 = 5.7 P n2

OW FW Acute WQC = 1.5

green algal 96-h EC50 = 0.570 M pH7.6 H15

green algal 96-h EC50 = 0.460 M pH8.2 H15 mean algal 96-h EC50 = 0.510 P n2

fish (FHM) ChV = 3.3 M pH7.7 H220

fish (FHM) ACR = 11.0 M

daphnid (Dm) ChV = 0.742 M pH8.3 H220

daphnid (Dm) ChV = 0.320 M pH7.7 H45

mean Dm ChV = 0.490 P n2

Dm ACR = 24.0 M

daphnid (Cd) ChV = 1.9 M pH7.2 H50

Cd ACR = 1.4 M

mean daphnid ChV = 0.970 P n2

mean daphnid ACR = 5.9 M

OW FW Chronic WQC = 0.087

algal ChV = 0.100 P EC50÷4

Biological Fate

Fish (BT-eyed embryo) 30-d BCF (wb) = 50.0 M pH7.2 H242

Fish (BT-fry) 30-d BCF (wb) = 136.0 M pH7.2 H242

mean fish BCF = 93.0 P n2

The toxicity profile for soluble inorganic complexes of Al can be predicted via MW adjustment of the toxicity for Al to the toxicity of the complex.

Ca Al hydroxy phosphites [141 728-04-3]

$Ca_x\ Al_2(OH)_{2\ (x+3-y)}\ (HPO_3)_y\ mH_2O$ with x = 2 to 12, (2x+5)÷2 >y>0, and m = 0 to 12; typical composition = 31% Ca, 9.5% Al, & 8.0% P; solid with mp >250 C (dec); S = 680 mg/L; pH 11.5;

Concentration (mg/L)

Effect ---------------------------

Complex Al Notes

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fish 96-h LC50 120.0 11.0 P

fish 96-h LC50 409.0 6.0 M

daphnid 48-h LC50 60.0 5.7 P

daphnid 48-h LC50 24.0 nm M

green algal 96-h EC50 5.4 0.510 P

fish ChV 35.0 3.3 P

daphnid ChV 10.0 0.970 P

algal ChV 1.0 0.100 P

Na Al fluoride [15 096-52-3]

sodium fluoaluminate; sodium fluoride aluminum; cryolite; kryolith; M12,2673; Na_3 Al F_6; MW210; composition: 13% Al; solid with mp 1000 C; S = 610 mg/L with pH 6.2; used as an insecticide since 1929;

Concentration (mg/L)

Effect --

Complex Al Notes

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fish 96-h LC50 85.0 11.0 P

fish 96-h LC50 21.0 2.8 M

daphnid 48-h LC50 44.0 5.7 P

green algal 96-h EC50 3.9 0.510 P

fish ChV 25.0 3.3 P

daphnid ChV 7.5 0.970 P

algal ChV 0.770 0.100 P

The toxicity profile for chelates of Al with polyanionic monomers can be predicted via MW adjustment of the toxicity for Al to the toxicity of the chelate.

The toxicity profile for organoAl compounds are developed for only the hydrolysis product(s) of Al. OrganoAl compounds are unstable in air and water. MethylAl and ethylAl are pyrophoric and dodecylAl slowly hydrolyses in water.

Boundaries. The toxicity of Al compounds depends on the their water solubility, the bioavailability of Al, and their stability. The most important property determining the toxicity of Al compounds is water solubility. Water solubility cannot be predicted accurately and has to be measured. Molecular weight (MW) is only important when Al complexes are water soluble and stable. Stable complexes of Al with MWs > 1000 are not expected to be absorbed by aquatic organisms and Al is not expected to be bioavailable even if they are water soluble. Therefore, only unstable Al compounds with MWs < 1000 are expected to be toxic.

General Testing Strategy

Tier 1. Fate testing. Physical state (OPPTS 830.6303) and corresponding property, i.e., melting point-melting point range (OPPTS 830.7200) or boiling point-boiling point range (OPPTS 830.7220), water solubility (OPPTS 830.7840 or 7860), octanol/water partition coefficient (K_{ow}) (OPPTS 830.7550 or 7570), and vapor pressure (OPPTS 830.7950); and/or

Acute environmental toxicity testing. The aquatic base set of environmental toxicity tests will be recommended for aquatic exposures: fish acute toxicity, daphnid acute toxicity, and green algal toxicity. The acute toxicity tests for fish (40 CFR §797.1400 or OPPTS 850.1075) and daphnids (40 CFR §797.1300 or OPPTS 850.1010) will be done using the static method; effective concentrations will be based on 100% active ingredients (ai) and nominal concentrations; the total organic carbon (TOC) concentration of dilution water in the control must be less than 2.0 mg TOC/L; TOC must be measured in the control just prior to the start of the test; the highest treatment concentration on a nominal-basis should not exceed the aqueous solubility limit of the tested compound; solvent can not be used; and hardness of dilution water has to be less than 180.0 mg/L as $CaCO_3$.

The algal toxicity testing (40 CFR §797.1050 or OPPTS 850.5400), should be done with the static method; effective concentrations based on 100% ai and nominal concentrations; statistical analysis of effective concentrations at 24, 48, 72, and 96 hours; test medium with no more than 0.300 mg/L EDTA as a final concentration; the TOC of the test/growth medium should be less than 2.0 mg TOC/L; TOC should be measured just prior to the start of the test; the highest treatment concentration on a nominal-basis should not exceed the aqueous solubility limit of the tested compound; and solvent can not used; .

In addition fish-toxicity-mitigation testing (OPPTS 850.1085) with known amounts of humic acid (HA) added to dilution water, i.e., 20 mg HA/L and 10 mg HA/L, will be recommended.

If there is no significant risk from the AI compound after the results of tier one testing set have been integrated into the risk assessment, then no further testing will be recommended. However, if there is a significant risk, then go to Tier 2.

Tier 2. Fate testing. Aerobic biodegradation, i.e., ready biodegradation (OPPTS 835.3110) or sealed-vessel test (OPPTS 835.3120); and/or

Fish chronic toxicity testing, i.e., fish early life stage (ELS) toxicity testing (40 CFR §797.1600 or OPPTS 850.1400), with the flow-through method; effective concentrations based on 100% ai and mean measured concentrations of soluble Al; statistical analysis of effective concentrations at days 7, 14, 21, and 28; the TOC of dilution water in the control should be less than 2.0 mg TOC/L; TOC should be measured in the controls just prior to and during the test; the highest treatment concentration on a nominal-basis should not exceed the aqueous solubility limit of the tested compound; solvent can not be used; and hardness of dilution water has to be less than 180.0 mg/L as $CaCO_3$; and

Daphnid chronic toxicity testing (40 CFR §797.1330 or OPPTS 850.1300), with the flow-through method; effective concentrations based on 100% ai and mean measured concentrations of soluble Al; statistical analysis of effective concentrations at days 7, 14, and 21; the TOC of dilution water in the control should not exceed 2.0 mg TOC/L; TOC must be measured in the controls just prior to and during the test; the highest treatment concentration on a nominal-basis should not exceed the aqueous solubility limit of the tested compound; solvent can not be used; and hardness of dilution water has to be less than 180.0 mg/L as $CaCO_3$.

II. Release to Terrestrial Ecosystems: The terrestrial base set of environmental toxicity tests will be recommended for terrestrial exposures. The terrestrial base set includes: the early seeding growth test (40 CFR 797.2800 or OPPTS 850.4230), the earthworm toxicity test (40 CFR.795.150 or OPPTS 850.6200), the soil microbial community bioassay (40 CFR 797.3700 or OPPTS 850.5100), and the avian acute oral toxicity test (40 CFR 797.2175 or OPPTS 850.2100). Chronic toxicity testing for terrestrial organisms include: the plant whole life cycle test (OPPTS 850.xxxx), the plant uptake test (40 CFR 797.2850 or OPPTS 850.4800), and the avian reproduction test (OPPTS 850.2300).

Abbreviations.

ACR10 = acute-to-chronic ratio = 10;

ai = active ingredients;

BCF = bioconcentration factor;

BT = brook trout;

Cd = *Ceriodaphnia*;

ChV = Chronic value;

Dm = *Daphnia magna*;

EC = effective concentration;

FHM = fathead minnow;

FT = flow-through method;

FW = fresh water;

H = hardness in mg $CaCO_3$/L;

H? = hardness unknown;

LOEC = lowest-observed-effect concentration;

M = measured concentrations;

n# = sample size used in calculation of the mean;

nm = not measured;

NOEC = no-observed-effect concentration;

OW = Office of Water;

P = predicted;

RT = rainbow trout;

S = static method;

SAR = structure activity relationship;

SR24 = static renewal method with renewals every 24 h;

TOC = total organic carbon;

wb = whole body;

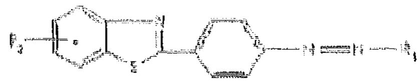
WQC = water quality criterion;

August, 1997

Category: **Aminobenzothiazole Azo Dyes** Human Health

Environmental Toxicity

Definition. Any disperse azo dye containing the substructure 2-aminobenzothiazole or 2-(p-amino)phenylbenzothiazole, or phenyl ring-substituted derivatives of the same, is considered to be a member of the category.



Hazard Concerns. There are oncogenicity/mutagenicity concerns for intact aminobenzothiazole azo dyes by analogy to dimethyl aminostyryl benzothiazole and Butter Yellow-type dyes, such as 4-ethyl-N,N-diethylaminoazobenzene. In addition, there are liver and thyroid concerns for reduction products by analogy to 2-aminothiazole, and neuro-toxicity concerns by analogy to chlorinated 2-aminobenzothiazole. Ecotoxicity concerns are generally chronic concerns only and are based on QSAR predictions for neutral organic compounds. Neutral organic compounds are an established ecotoxicity category, of which these dyes are part of the disperse dye subclass.

Boundaries. The boundaries are not strictly defined. For a typical member of the category, R_1 = N- and/or ring substituted p-aminophenyl groups, and R_2 = halogens or nitro groups.

__General Testing Strategy__

The New Chemicals Program considers the following tests to be the most appropriate for aminobenzothiazole azo dyes found to pose an unreasonable risk:

- __In vivo__ mouse micronucleus assay in bone marrow by the i.p. route (40 CFR 798.5395).

- 90-day subchronic toxicity test in rats by the oral route, with special attention to the thyroid and liver (40 CFR 798.2650).

- Fish early life stage test (40 CFR 797.1600). Chronic daphnid test (40 CFR 797.1350). Algae toxicity test (40 CFR 797.1050).

- If the mouse micronucleus assay is positive, further characterization of the potential cancer risk may be recommended: 2-year cancer bioassay by the oral route in 2 species of rodents (40 CFR 798.3260).

Potentially significant ecotoxicity risk, as well as human health risks, resulting from releases to water **ONLY**, may be addressed by environmental fate testing prior to the chronic ecotoxicity and human health testing. The results of the environmental fate testing may preclude the need for further testing.

- Jar test to determine the settling rate and extent of removal of suspended solids from solution (draft protocol available).

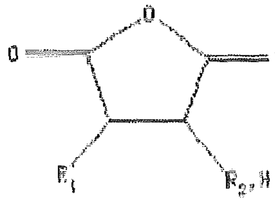
If the results of the jar test do not mitigate the health and/or ecotoxicity concerns, further characterization of the environmental fate of the dye may be recommended.

- Coupled units test (40 CFR 796.3300).

January, 1992.

Category: **Anhydrides, Carboxylic Acid** Human Health

Definition. Any molecular structure containing one or more carboxylic acid anhydride groups is considered to be a member of the category for new chemical purposes. Members of the class include new carboxylic acid anhydrides as well as new oligomers, polymers, prepolymers, or reaction products of existing carboxylic acid anhydrides. As illustrated below, a typical new chemical carboxylic acid anhydride of concern is a polymer or oligomer containing a monomer such as maleic anhydride.



Hazard Concerns. Carboxylic acid anhydrides are of concern for potential pulmonary sensitization based on data for phthalic, trimellitic, isopropylidene bis(phthalic), and sulfonyl bis(phthalic) anhydrides. Carboxylic acid anhydrides are also of concern for potential developmental or reproductive toxicity based on data for maleic, succinic, and phthalic anhydrides.

Boundaries. Structures with a carboxylic acid anhydride equivalent weight of ≥5,000 are presumed not to pose a hazard under any conditions. Typically, concerns for health effects are confined to those species with molecular weights <1,000.

The new chemical program has thus far been concerned only with those carboxylic acid anhydrides with potentially significant inhalation exposure, and has pursued developmental toxicity only for low molecular weight (<500) carboxylic acid anhydrides which are thought to have a significant potential for systemic uptake via the lung. For pulmonary sensitization, extensive systemic uptake may not be necessary for a biological response and we have therefore sought to regulate some oligomeric or polymeric carboxylic acid anhydrides only for that effect.

General Testing Strategy

The following tests are usually prescribed for carboxylic acid anhydrides found to pose a potentially unreasonable risk:

- Pulmonary sensitization by either the method of Karol (Toxicol. Appl. Pharmacol. 68:229-241, 1983), or an equivalent method.

- Oral developmental toxicity study in two species (40 CFR §798.4900).

May, 1991

Category: **Anilines** Environmental Toxicity

This category includes all anilines, both monoanilines and polyanilines. It is assumed that these compounds need to be absorbed to be toxic, therefore, compounds with MWs > 1000 will be excluded from this category. Acute toxicity for anilines which are liquids at room temperature is known to be limited by the octanol/water partition coefficient (K_{ow}). Above a log K_{ow} value of => 7.38, anilines show no effects at saturation during 96-h exposures (Veith and Broderius (1987). Anilines which are solids at room temperature may show no toxicity at saturation at lower Kow values depending on the melting point, i.e., the higher the melting point at a given K_{ow}, the greater the likelihood that no toxicity will be observed at saturation. For solids, the no effects at saturation has to be determined on a case-by-case basis. There are