

Wednesday March 6, 1991

Part VIII

Environmental Protection Agency

Twenty-Seventh Report of the Interagency Testing Committee to the Administrator; Notice



ENVIRONMENTAL PROTECTION AGENCY

[OPTS-41034; FRL 3845-3]

Twenty-Seventh Report of the Interagency Testing Committee to the Administrator; Receipt of Report and Request for Comments Regarding Priority List of Chemicals

AGENCY: Environmental Protection Agency (EPA). ACTION: Notice.

SUMMARY: The Interagency Testing Committee (ITC), established under section 4(e) of the Toxic Substances Control Act (TSCA), transmitted its Twenty-seventh Report to the Administrator of EPA on November 19, 1990. As noted in this Report, which is included with this notice, the Committee revised the Priority List by adding one chemical and four chemical groups. The Committee is designating six chemicals from the IRIS group, as well as 4vinylcyclohexene and sodium cyanide. that were previously recommended with intent-to-designate. The aldehydes chemical group is recommended with intent-to-designate. N-phenyl-1naphthylamine, two chemicals from the IRIS group, the sulfone group, and a group of substantially produced chemicals in need of subchronic tests are recommended.

The ITC has not removed any chemicals from the Priority List as a result of EPA actions.

EPA invites interested persons to submit written comments on the Report. EPA is not holding a Focus Meeting for these chemicals and will proceed immediately to rulemaking. EPA is taking this action because (1) The designated chemicals have a statutory deadline and require a response by EPA within 1 year; and (2) the intent-todesignate group is unlikely to yield consensus in a timely manner because of the inability to identify interested parties on a chemical specific basis. DATES: Written comments should be submitted by April 5, 1991. ADDRESSES: Send written submissions

bearing the document control number (OPTS-41034; FRL 3845-3) to: TSCA Public Docket Office (TS-793), Office of Toxic Substances, Environmental Protection Agency, Rm. NE G-004, 401 M St., SW., Washington, DC 20460.

The public record supporting this action, including comments, is available for public inspection in Rm. NE G-004 at the address noted above from 8 a.m. to 12 noon and 1 p.m. to 4 p.m., Monday through Friday, except legal holidays. FOR FURTHER INFORMATION CONTACT: Michael M. Stahl, Director,

Environmental Assistance Division (TS-799), Office of Toxic Substances, Environmental Protection Agency, Rm. E-543B,401 M St., SW., Washington, DC 20460, (202) 554–1404, TDD (202) 554–0551.

SUPPLEMENTARY INFORMATION: EPA has received the TSCA Interagency Testing Committee's Twenty-seventh Report to the Administrator.

I. Background

TSCA (Pub. L 94-469, 90 Stat. 2003 et seq; 15 U.S.C. 260l et seq.) authorizes the Administrator of EPA to promulgate regulations under section 4(a) requiring testing of chemicals and groups in order to develop data relevant to determining the risks that such chemicals and groups may present to health or the environment. Section 4(e) of TSCA established the Interagency Testing Committee to recommend chemicals and groups to the Administrator of EPA for priority testing consideration. Section 4(e) directs the ITC to revise the TSCA section 4(e) Priority List at least every 6 months. The ITC's most recent revisions to this List are included in the Committee's Twenty-seventh Report. The Report was received by the Administrator on November 19, 1990, and is included in this Notice. The Report adds one chemical and four groups of chemicals to the TSCA section 4(e) Priority List.

II. Written and Oral Comments and Public Meetings

EPA invites interested persons to submit detailed comments on the ITC's new recommendations. The Agency is interested in receiving information concerning additional or ongoing health and safety studies on the subject chemicals as well as information relating to the human and environmental exposure to these chemicals.

A notice will be published at a later date in the Federal Register adding most of the substances recommended in the ITC's Twenty-seventh Report to the TSCA section 8(d) Health and Safety Data Reporting Rule (40 CFR part 716), which requires the reporting of unpublished health and safety studies on the listed chemicals. The delay in publishing that notice is necessary because of the requirement to complete the economic analysis on four chemical groups. That notice will also add most of the chemicals to the TSCA section 8(a) Preliminary Assessment Information Rule (40 CFR part 712). The section 8(a) rule requires the reporting of production volume, use, exposure, and release information on the listed chemicals.

III. Status of List

The ITC's Twenty-seventh Report notes the addition of chemicals and chemical groups to the Priority List. The current List contains two designated chemicals, two designated chemical groups, three recommended with intent-to-designate chemical groups, four recommended chemicals, and five recommended chemical groups.

Authority: 15 U.S.C. 2603. Dated: February 26, 1991.

Charles M. Auer,

Director, Existing Chemical Assessment Division, Office of Toxic Substances.

Twenty-Seventh Report of the Interagency Testing Committee to the Administrator, Environmental Protection Agency

Summary

The U.S. Congress created the Interagency Testing Committee in 1976 to screen, select and recommend chemical substances and mixtures for priority health effects, chemical fate, or ecological effects testing consideration. The Committee (which consists of Members from 18 U.S. Government organizations) selects and recommends chemicals or chemical groups with testing information deficiencies because they may present an unreasonable risk of injury to health or the environment, may reasonably be anticipated to enter the environment in substantial quantities or may involve significant or substantial human exposure.

The Committee also facilitates coordination of chemical testing sponsored or required by U.S. Government organizations and enhances information exchange to promote cost-effective use of U.S. Government chemical testing resources. The Committee's statutory responsibilities are defined in section 4(e) of the Toxic Substances Control Act (TSCA) (Pub. L. 94–469, 90 Stat. 2003 et seq., 15 U.S.C. 2601 et seq.).

Section 4(e)(1)(A) of TSCA directs the Committee to recommend to the Administrator of the U.S. Environmental Protection Agency (EPA), chemicals or chemical groups to which the Administrator should give priority testing consideration. Under the authority of TSCA section 4(e)(1)(B) the EPA Administrator shall publish in the Federal Register the Committee's Priority List of chemicals or chemical groups and their associated testing recommendations. The Committee is required to designate those chemicals, from among its recommendations, to which the Administrator should respond within 12 months by either initiating rulemaking under TSCA section 4(a) or publishing the reason for not initiating rulemaking. The Congress directed the Committee to revise the TSCA section 4(e) Priority List at least every 6 months, and to transmit those revisions to the EPA Administrator.

As a result of its deliberations, the Committee is revising the TSCA section 4(e) Priority List by designating two chemicals that were previously recommended with intent-to-designate and by adding one chemical and four chemical groups. The added chemical was nominated by the Occupational Safety and Health Administration. Two chemical groups were nominated by the EPA. The Committee's computerized,

substructure-based chemical selection processes were used to identify the chemicals in the aldehyde group nominated by EPA as well as the chemicals in two chemical groups that either shared a common substructure or a common testing information deficiency. During this reporting period, the Committee considered available information on three chemicals and over thirty chemical groups. The Committee also deferred about 700 hundred chemicals from testing consideration at this time.

Chemicals or chemical groups (entries) on the Priority List are designated, recommended with intentto-designate or recommended by the Committee. Designations were created by the U.S. Congress when they drafted TSCA. Recommendations with intent-todesignate were established by the Committee in their 17th Report (50 FR 47603: November 19, 1985). Recommendations were established by the Committee in their 11th Report (47 FR 54626; December 3, 1982). Revisions to the Priority List are presented, together with the types of testing recommended, in Table 1. The footnote letters following Table 1 acknowledge the Committee's efforts to coordinate chemical testing and to comprehensively examine ongoing testing-related activities and available information previously submitted under TSCA.

TABLE 1 .- REVISIONS TO THE SECTION 4(E) PRIORITY LIST

Group	CAS No.	Chemical	Action	Date	Recommended tests
	100-40-3	4-vinylcyclohexene ^{3,4}	Designated	11/90	Chemical fate: Aqueous volatilization rate. Health effects: Pharmacokinetics and oncogenicity by Inhalation route of administration. Ecological effects: None.
	143-33-9	sodium cyanide ^{3,4,5}	Designated	11/90	Chemical fate: Soil sorption. Health effects: Under review, as cyanides. Ecological effects: Toxicity to migratory birds plant uptake and translocation.
RIS	79–10–7	acrylic acid ^{2,3}	Designated	11/90	Chemical fate: River die-away biodegradation Health effects: Reproductive effects, develop- mental toxicity, mutagenicity, neurotoxicity and inhalation encogenicity. Ecological effects: None.
RIS	98-86-2	acetophenone ³	Designated	11/90	Chemical fate: None Health effects: Oral and inhalation pharmaco kinetics, inhalation subchronic, reproductive effects, developmental toxicity, mutagenicity and neurotoxicity. Ecological effects: None.
RIS	108-95-2	phenol Laza	Designated	11/90	Chemical fate: None. Health Effects: Oral and inhalation pharmaco kinetics, inhalation subchronic, reproductive effects, and neurotoxicity. Ecological effects: None.
RIS	121-69-7	N,N-dimethylaniline 1.3	Designated	11/90	Chemical fate: Activated sludge biodegradation Health effects: Oral and inhalation pharmaco kinetics, inhalation subchronic, mutagenicity reproductive effects, developmental toxicity and neurotoxicity. Ecological effects. Algal toxicity, aquatic invertebrates acute and chronic toxicity, and fist chronic toxicity.
RIS	141-78-6	ethyl acetate	Designated	11/90	Chemical fate: None. Health effects: Screening for reproductive effects, developmental toxicity, mutaganicity and neurotoxicity. Triggering oncogenicity. Ecological effects: None.
RIS	576-26-1	2,6-dirnethylphenol	Designated	11/90	Chemical fate: Aqueous photohysis screening and river die-away blodegradation. Health effects: Screening for reproductive effects, developmental toxicity, mutagenicity and neurotoxicity. Ecological effects: Algal toxicity, aquatic invertebrate and fish chronic toxicity.
Aldehydes			Recommended with-Intent- to-designate.	11/90	Chemical fate: None. Health effects: None. Ecological effects: Algal toxicity, aquatic invertebrates acute and chronic toxicity and fish chronic toxicity.

TABLE 1.—REVISIONS TO THE SECTION 4(E) PRIORITY LIST—Continued

Group	CAS No.	Chemical	Action	Date	Recommended tests
IRIS	51-28-5	2,4-dinitrophenol ^{1,2,3}	Recommended	11/90	Chemical fate: Aqueous photolysis screening and river die-away biodegradation. Health effects: Oral and inhalation pharmacokinetics, dermal absorption, inhalation subchronic, reproductive effects, developmental toxicity, mutagenicity, and neurotoxicity. Ecological effects: Aquatic invertebrates and fish chronic toxicity.
IRIS	95-65-8	3,4-dimethylphenol	Recommended	11/90	Chemical fate: Aqueous photolysis screening and river die-away blodegradation. Health effects: Subchronic, screening for reproductive effects, developmental toxicity, mutagenicity and neurotoxicity. Ecological effects: Algal toxicity, aquatic invertebrates and fish chronic toxicity.
	90-30-2	N-phenyl-1-naphthylamine	Recommended	11/90	Chemical fate: Water solubility, octanol-water partition coefficient, vapor pressure and blo-degradation. Health effects: Oncogenicity. Ecological effects: Algal toxicity, aquatic invertebrates and fish chronic toxicity.
Sulfones			Recommended	11/90	Chemical fate: Physical and chemical properties. Health effects: None. Ecological effects. None.
Substantially produced chemicals in need of subchronic tests.			Recommended	11/90	Chemical fate: None. Health effects: Subchronic toxicity. Ecological effects. None.

Listed below are the individual chemicals for the chemical groups in Table 1. Chemicals nos. 1 through 89 are aldehydes, chemical nos. 90 through 115 are sulfones, and chemicals nos. 116 through 150 are substantially produced chemicals in need of subchronic tests.

Chemical Name	CAS No.	Notes
. 1-naphthalenecarboxaldehyde	66-77-3	
2. acetaldehyde	75-07-0 b	
l. acetaldehyde, trichioro	75-87-6	
. propanal, 2-methyl	78-84-2 b	
5. 2-propenal, 2-methyl	78-85-3	
i. benzenepropanal, 4-(1,1-dimethylethyl)amethyl	80-54-6	
. acetaldehyde, (1,3-dihydro-1,3,3-trimethyl-2H-indol-2-ylidene)	84-83-3	
benzaldehyde, 2-chloro	89-98-5	
benzaldehyde, 2-hydroxy	90-02-8	
0. benzaldehyde, 2,5-dimethory	93-02-7	
1. benzeneacetaldehyde, .amethyl	93-53-8	
2. benzaldehyde, 2,4-dihydroxy	95-01-2	
3. benzaldehyde, 2-hydroxy-5-nitro	97-51-8	
4. 2-furancarboxaldehyde	98-01-1 d	
5. 2-thiophenecarboxaldehyde	98-03-3	
6. benzaldehyde, 4-(dimethylarnino)	100-10-7	
7. 3-cyclohexene-1-carboxaldehyde	100-50-5	
8. benzaldehyde	100-52-7	
9. 2-propenal, 2-methyl-3-phenyl-	101-39-3	
20. octanal, 2-(phenylmethylene)	101-86-0	
1. benzenepropanal, .amethyl-4-(1-methylethyl)	103-95-7	
2. benzeneacetaldehyde, 4-methyl	104-09-6	
3. 2-propenal, 3-phenyl-	104-55-2	
24. benzaldehyde, 4-methyl-	104-87-0	

Superfund Amendments and Reauthorization Act (SARA) section 110.
 Emergency Planning and Community Right-to-Know Act (EPCRA) section 313.
 Clean Air Act Amendments, section 301.
 Toxic Substances Control Act (TSCA) section 8(a) Preliminary Assessment Information Rule (PAIR).
 TSCA section 8(d) Health and Safety Data Reporting Rule.

Chemical Name	CAS No.	Notes
benzaldehyde, 4-chloro	104–88–1	
6-octenal, 3,7-dimethyl		
2,6-octadienal, 3,7-dimethyl-, (Z)	106–26–3	
5-heptenal, 2,8-dimethyl-	106-72-9	
2-propenal	107-02-8 a	,b
acetaldehyde, chloro	107-20-0	
ethanedial	107-22-2	
octanal, 7-hydroxy-3,7-dimethyl	107–75–5	
undecanal, 2-methyl	110-41-8	
pentanal	110–62–3	
pentanedial		
heptanal		
decanal	112-31-2	
undecanal	112-44-7	
10-undecenal	112-45-8	
dodecanal	112-54-9	
benzaldehyde, 3,4-dimethoxy	120-14-9	
benzaldehyde, 4-(diethylamino)-		
1,3-benzodioxole-5-carboxaldehyde		
benzaldehyde, 3-ethoxy-4-hydroxy		
benzaldehyde, 4-hydroxy-3-methoxy		
heptanal, 2-(phenylmethylene)		
benzeneacetaldehyde		
hexanal, 2-ethyl-		
benzaldehyde, 4-hydroxy		
benzaldehyde, 4-methoxy		
propanal		
octanal		
nonanal		
4a(4/f)-dibenzofurancarboxaldehyde, 1,5a,6,9,9a,9b-hexahydro		
benzaldehyde, 2-methoxy-		
2,6-octadienal, 3,7-dimethyl-, (<i>E</i>)		
9-undecenal		
benzaldehyde, 4-(trifluoromethyl)-		
2-hexenal		
benzaldehyde, 2-nitro-		
butanal, 3-methyl-		
propanal, 3-hydroxy-2,2-dimethyl-		
benzaldehyde, 4-{1,1-dimethy/lethyl)-		l.e
2-pyridinecarboxaldehyde		
benzaldehyde, 4-butyl-		
2-propenal, 3-phenyl-, monopentyl deriv.		
benzaldehyde, methyl-		
3-cyclohexene-1-carboxaldehyde, 2,4,6-tr/methyl-		
2-propenal, 3-(2-methoxyphenyl)-		
1-piperidinecarboxaldehyde		
benzaldehyde, 3-bromo-		
propanal, 3-(methylthio)-		
octanal, 7-methoxy-3,7-dimethyl-		
3-cyclopentene-1-acetaldehyde, 2,2,3-trimethyl		
hexanal, 3,5,5—trimethyl-		
1,3-benzodioxole-5-carboxaldehyde, 7-methoxy		
6-octenal, 3,7-dimethyl-, (<i>S</i>)-		
octanal, 3,7-dimethyl-		
benzaldehyde 4-ethoxy-		

Chemical Name	CAS No.	Notes
2-propenal, 3- 4-(1,1-dimethylethyl)phenyl -2-methyl	13586-68-0	
benzaldehyde, 4-(diethylamino)-2-hydroxy-	17754-90-4	
hexenal, 2-ethyl	26266-68-2	
3-cyclohexene-1-carboxaldehyde, dimethyl	27939-60-2	
benzaldehyde, (dimethytamino)	28602-27-9	
3-cyclohexene-1-carboxaldehyde, 4-(4-hydroxy-4-methylpentyl)	31906-04-4	
3-cyclohexene-1-carboxaldehyde, 4-(4-methyl-3-pentenyl)	37677-14-8	
benzaldehyde, 3-phenoxy	39515-51-0	
3-cyclohexene-1-carboxaldehyde, 1-methyl-4-(4-methyl-3-pentenyl)	52475-86-2	
3-cyclohexene-1-carboxaldehyde, 1-methyl-4-(4-methylpentyl)	66327-54-6	
dimethylsulfone	67-71-0	
sulfolene	77-79-2	
sulfonyl bis-(4-chlorobenzene)	80-07-9	
4,4'-diaminodiphenyl sulfone	80-08-0	
	80-09-1	
bisphenol S		
2-amino-4-(methylsulfonyl)phenol	98-30-6	
sulfolane	126-33-0	
diphenylsulfone	127-63-9	
2,2'-sulfonyl bis-ethanol	2580-77-0	
1,1'-[Methylene bis(sulforiyl)]bisethene	3278-22-6	
D. 2-[(3-aminophenyl)sulforlyl]ethanol	5246-57-1	
1. 3-[N-ethyl-4-[[6-(methyl-sulfonyl)-2-benzothiazolyl]azo]-m-toluldino]-propionitrile	16588-67-3	
2. 6-(methylsulfonyf)-2-benzothiazolamine	17557-67-4	
3. 2-amino-4-[(2-hydroxyethyl)sulfonyl]phenol	17601-96-6	
4. 4-phenylthiomorpholine, 1,1-dioxide	17688-68-5	
5. 4-[4-[(2,8-dichloro-4-nitrophenyl)azo]phenyl]thiomorpholine, 1,1-dioxide	17741-62-7	
5. 3-(decyloxy)tetrahydrothiophene 1,1-dloxide	18760-44-6	
7. 1-(diiodomethyl)sulfonyl-4-methyl benzene	20018-09-1	
3. 1,1'-[oxybis(methylenesulfonyl)] bisethene	26750-50-5	
9. 2,2'-[oxybis(methylenesulfonyl)] bisethanol	36724-43-3	
0. 1,1'-[methylenebis(sulforyl)] bis-2-chloroethane	41123-59-5	
1. 2,2'-[methylenebis(sulforlyf)] bisethanol	41123-69-7	· ·
2. 2-[(3-nitrophenyl)sulfonyl] ethanol	41687-30-3	
3. 2-[(6-amino-2-naphthalenyl)sulfonyl] ethanol	52218-35-6	
4. 1,1'-[oxybis(methylenesulfonyl)] bis-2-chloroethane	. 53061-10-2	
5. 4-[[4-(phenylmethoxy)phanyl]sulfonyl] phenol	63134-33-8	
5. p,p'-oxybis(benzenesulforrylhydrazide)	80-51-3	
7. naphthalenedicarboxylic anhydride	81-84-5	
3. 2-ethylanthraquinone	84-51-5	
9. 7-amino-4-hydroxy-2-naphthalenesulfonic acid	87-02-5	
0. 1-naphthol	90-15-3	
1. 3-hydroxy-2-naphthoic acid	92-70-6	
2. triethylene glycol bis(2-etlrylhexanoate)	94-28-0	
3. 2-(4-morpholinyldithio)-benzothiazole	95-32-9	
4. n-butyl methacrylate	97-88-1	cd
5. 1,3-benzenedisulfonic acid	98-48-6	4,4
5. 3,4-dichloronitrobenzene	99-54-7	
7. isophthaloyl chloride	99-63-8	
3. terephthaloyl chloride	100-20-9	
9. 4 _F ethoxynitrobenzene	100-20-9	
D. acetoacetanilide	102-01-2	
I. butyric anhydride	106-31-0	
2. isobutyl acrylate	106-63-8	
3. diethylene glycol dimethyl ether	111-96-6	

Chemical Name	CAS No.	Notes .
135. bromamine acid	116-81-4	
136. 4-methyl-2-nitro-phenol	119-33-5	
137. 4-(acetylamino) benzenesulfonyl chloride	121-60-8	
138. 2,4-pentanedione	123-54-6	
139. propanoic anhydride	123-62-8	
IAD his(2-athylhand)-2-hytanadicata	142-16-5	
141. perfluorotributytamine	311-89-7	
142. perfluoro-N-hexane	355-42-0	
43. trichloromethanesulfenyl chloride	594-42-3	
144. 1,2-dichlorobutane	616-21-7	
145. 1,3-dicyanobenzene	626-17-5	
146. 3,4-dichlorobutene	760-23-6	
47 2-/2-aminoethoxyl-ethanol	929-06-6	
148. quinacridone	1047-16-1	
49. ammonium carbamate	1111-78-0	
50. hexa(methoxymethyl) melamine	3089-11-0	

Notes:

a. Superfund Amendments and Reauthorization Act (SARA) section 110. b. Emergency Planning and Community Right-to-Know Act (EPCRA) section 313.

c. Toxic Substances Control Act (TSCA) section 8(a) Preliminary Assessment Information Rule (PAIR).

d. TSCA section 8(d) Health and Safety Data Reporting Rule.

TSCA Interagency Testing Committee

Statutory Member Agencies and Their Representatives:

Council on Environmental Quality Under consideration Department of Commerce Raimundo Prat **Environmental Protection Agency** Letitia Tahan, Member Vincent Nabholz, Alternate National Cancer Institute Susan Sieber, Member (See Note 1) Thomas P. Cameron, Alternate National Institute of Environmental Health Sciences James K. Selkirk, Chairperson

National Institute for Occupational Safety and Health

Robert W. Mason, Member Rodger L. Tatken, Alternate National Science Foundation

William L. Pengelly, Member (See Note 2)

Jarvis L. Moyers, Alternate Occupational Safety and Health Administration

Loretta Schuman, Vice-Chairperson Stephen Mallinger, Alternate Liaison Agencies and Their Representatives Agency for Toxic Substances and

Disease Registry Deborah Barsotti

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Lakshmi C. Mishra Department of Agriculture Richard M. Parry, Jr. Elise A. B. Brown

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George Cushmac (See Note 3) Food and Drug Administration

Charles J. Kokoski Raju Kammula

National Library of Medicine Vera Hudson

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U.S. International Trade Commission **Edward Matusik**

James Raftery Committee Staff

John D. Walker, Ph.D., Executive Director

Norma S. L. Williams, Executive Assistant

Support Staff

Alan Carpien -- Office of the General Counsel, EPA

Notes:

- Appointed on July 25, 1990.
- Appointed on August 29, 1990.
- Appointed on May 24, 1990.
- Appointed on September 18, 1990.
- Appointed on September 18, 1990.

The Committee acknowledges and is grateful for the assistance and support Given by the staff of Syracuse Research Corp. (technical support contractor) and personnel of the EPA Office of Toxic Substances.

Chapter 1-Introduction

1.1 Background. Congress created the Interagency Testing Committee under the Toxic Substances Control Act (TSCA) to recommend to the Administrator of the U.S. Environmental Protection Agency (EPA) chemical substances and mixtures in commerce that should be given priority testing consideration. TSCA specifies that the Committee's recommendations shall be in the form of a Priority List published in the Federal Register.

At least every 6 months, the Committee revises the Priority List and transmits these revisions to the EPA Administrator. The Committee's testing recommendations are described in previous reports (Refs. 1 through 11).

1.2 Committee's previous reports. Twenty-six previous reports to the EPA Administrator have been issued by the Committee and published in the Federal Register. In these 26 reports, the Committee has recommended testing for 91 chemicals and 28 chemical groups.

1.3 Committee's activities during this reporting period. Between April 26, 1990 and September 27, 1990 the Committee processed chemicals that were nominated by Member Agencies, evaluated chemicals by using the Committee's computerized, substructure-based, chemical selection processes and examined lists of ongoing activities related to reducing testing information deficiencies for commercial chemicals.

1.3.a Nominations and selections. Member-Agency nominations for this Report include N-phenyl-1naphthylamine (Occupational Safety and Health Administration), Integrated Risk Information System (IRIS)

chemicals and aldehydes (the U.S. Environmental Protection Agency).

Nominating chemicals to the Committee offers several advantages that appear to satisfy the intentions of Congress when they created the ITC. The nominator is provided with the unique opportunity to utilize the Committee-activated networking and information exchange processes that allows the nominator to access otherwise unavailable information from Member Agencies. Committee networking is important because it allows the nominator to determine if there are unpublished studies that could satisfy the nominator's testing information deficiencies or that could provide the nominator with additional testing concerns. Information exchange is important at the Committee level because it is not limited to a single type of testing, but includes comprehensive discussions of health effects, chemical fate and ecological effects testing. It allows the nominator to save resources by analyzing only essential testing information deficiencies, while the Committee comprehensively addresses other testing information deficiencies without substantive delays in processing nominations.

Nominating chemicals to the Committee also allows the nominator to take advantage of an unusual information-collecting opportunity that only exists for Committee recommendations. For any chemical or chemical group recommended by the ITC, the EPA automatically promulgates TSCA 8(a) and 8(d) final rules. TSCA 8(a) requires that industry submit manufacturing, importation and exposure data for any chemical listed in a final section 8(a) rule. TSCA 8(d) requires that industry submit all health effects, epidemiology, medical case studies, monitoring, chemical fate and ecological effects studies for any chemical listed in a final section 8(d) rule. TSCA section 8(a) and 8(d) data are generated in 3 months through an ITC recommendation in contrast to 18 to 24 months through conventional notice and comment rulemaking. The resulting TSCA section 8 data are analyzed and a report is generated for the nominator that indicates whether any of the data submissions are likely to satisfy the nominator's testing information deficiencies.

Chemical group selections for this Report include sulfones and substantially produced chemicals in need of subchronic tests. Sulfones and substantially produced chemicals in need of subchronic tests were identified by using the Committee's computerized, substructure-based, chemical selection processes. The substantially produced chemicals in need of subchronic tests selection exemplifies a feature of these processes that is being utilized for the first time, i.e., the ability of the processes to identify a group of chemicals that have a common testing information deficiency. This costeffective feature should allow EPA to add those identified chemicals that satisfy the TSCA section 4 statutory requirements [and for which TSCA section 8 information does not reduce the need to consider subchronic toxicity testing) to a subchronic toxicity listing rule and should provide others (e.g., NTP, OECD, etc.) with the option of selecting any of the remaining chemicals for testing.

The Committee uses their computerized processes to enhance their ability to cost-effectively screen chemicals for exposure potential or potential to persist and cause adverse health or ecological effects by: (1) Identifying chemical groups with identical substructures and similar adverse effects potentials or chemical fate characteristics, (2) identifying chemical groups with similar uses or common testing information deficiencies and (3) recommending chemical groups, with insufficient test data, for health effects, chemical fate, or ecological effects testing. The Committee continues to recommend groups of structurally- or use-related chemicals or groups with common testing information deficiencies for screening tests and to review the TSCA section 8(a) and 8(d) information that is submitted in response to recommendations. The Committee believes recommending groups of structurally- or use-related chemicals or groups of chemicals with common testing information deficiencies for screening tests and reviewing TSCA section 8(a) and 8(d) information before making subsequent testing recommendations is a cost-effective approach to satisfying chemical testing information deficiencies because it promotes a comprehensive analysis of chemicals that may produce similar effects or that may involve similar exposures. The Committee processes external nominations of structurally- or use-related chemical groups or groups with common testing information deficiencies and encourages external nominators to take advantage of the Committee's unique networking and information exchange processes and accelerated TSCA 8(a) and 8(d) information-collecting authority.

Processing and recommending Member-Agency and other nominations and computer-facilitated chemical group selections enhances information exchange that promotes cost-effective use of U.S. Government chemical testing resources, encourages harmonization of methods for chemical testing, and facilitates coordination of testing being sponsored or required by U.S. Government organizations.

1.3.b Comprehensive information processing. During this reporting period, several For Your Information (FYI). TSCA section 8(d) and 8(e) documents were reviewed. These documents are stored on microfiche in the TSCA Public Docket Office, Office of Toxic Substances, Environmental Protection Agency, Room G-004 NE Mall, 401 M St., SW., Washington, DC 20460. These microfiched documents are also available from the National Technical information Service, 5285 Port Royal Road, Springfield, Virginia 22161 (1-800-336-4700), and from Chemical Information Systems, Inc., 7215 York Road, Baltimore, Maryland 21212 (1-800-CIS-USER). The Committee referenced several of these documents in Chapter 2 of this report and readers are referred to the above addresses to obtain further information. Interested parties can also obtain, from the EPA address, copies of publicly-available reports, letters and published references supporting recommendations of chemicals in this report.

The Committee continues to comprehensively search available domestic and international lists of ongoing activities related to reducing testing information deficiencies on chemicals under review. Efforts to conduct these searches identified chemicals listed in other statutes, e.g., chemicals listed in Title III of the 1990 amendments of the Clean Air Act. The Committee has recommended over 50 chemicals listed in this statute, including 5 Iris chemicals for inhalation testing (acrylic acid, acetophenone, phenol, 2,4dinitrophenol and N,N-dimethylaniline). The Committee continues to review information on chemicals listed in this and other relevant statutes. Efforts to conduct searches also identified chemicals for which TSCA informationgathering activities are ongoing (see Table 1 footnotes). The Committee makes the results of these searches publicly available by referencing TSCA submissions in Reports to the EPA Administrator or making tables and references of these submissions available in the public dockets supporting a Report to the EPA Administrator.

During this reporting period, the Committee considered available

information on 3 chemicals and over 30 chemical groups. Chemical groups currently under consideration include alkenes, alkylamines, alkylnitros, alkylsulfonates, alkynes, anhydrides, aromatic dianhydrides, aromatic sulfhydryls, aromatic sulfonates, aryl ethers, benzothiazoles, carbamates, dialkylamines, ethanolamines, epoxides, ethylhexyl derivatives, glycol ethers, haloalkyl ethers, heterocyclics, hinderd phenols, hydrazines, inorganics, isophthalic acids, isothiocyanates, nitriles, phenylenediamines, phosphates, phosphoniums, pyrrolidinones, siloxanes, sulfenamides, thiocarbamates, thiol esters, thios, triazines, etc. The Committee designated two chemicals that were recommended with intent-to-designate in the 25th and 26th, Reports. One chemical and four chemical groups were selected for addition to the section 4(e) Priority List. Review of the remaining chemicals and chemical groups is ongoing.

1.3.c Information dissemination. To emphasize the Committee's efforts to

promote public understanding of the ITC's functions and purposes, the Committee is listing for the first time some of the Committee-related activities that occurred during this reporting period. On June 20, 1990 the Committee's Executive Director testified before the House Subcommittee on Environment, Energy and Natural Resources. On June 29, 1990, during an information exchange symposium, the Committee's Chairperson and Executive Director presented chemical selection procedures used by the National Toxicology Program (NTP) and the ITC. On July 2 and September 7, 1990, the Executive Director briefed the Synthetic Organic Chemical Manufactures Association and the Chemical Manufactures Association, respectively, on ITC activities. On September 20, 1990, the Executive Director described the ongoing efforts to evaluate the ITC's substructure-based computerized chemical selection processes at an international workshop convened in the Netherlands.

1.3.d Deferrals. To promote public understanding of the total number of chemicals that the Committee processes, the Committee is listing for the first time about 700 chemicals in 4 chemical groups that are being deferred from further consideration at this time because the chemicals were not reported to the EPA or the U.S. International Trade Commission as being recently produced. Four IRIS chemicals (ammonium sulfamate, CFC-113, HMX and hydrogen sulfide) are also being deferred; the rationales for which for which are described in section 2.2.c. of this Report. Deferred and other chemicals are recycled through the Committee's computerized processes to identify chemicals whose production volumes have substantially changed. On the following list of deferrals, chemicals no 1 through 429 are aldehydes, chemicals no 430 through 525 are brominated flame retardants, chemicals no 526 through 605 are isocyanates and chemicals 606 through 686 are sulfones.

	Chemical Name	CAS No.
1.	4-pyridinecarboxaldehyde, 3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-	54-47-7
2.	propanal, 2,3-dihydroxy-, (±)-	56-82-6
3.	4-pyridinecarboxaldehyde, 3-hydroxy-5-{hydroxymethyl}-2-methyl-, hydrochloride	65-22-5
١.	hexanal	66-25-1
5.	2-furancarboxaldehyde, 5-(hydroxymethyl)-	67-47-0
3.	acetaldehyde, trifluoro-	75-90-1
7.	propanal, 2-oxo-	78-98-8
3.	acetaldehyde, dichloro-	79-02-7
).	1/-pyrrole-3-carboxaldehyde, 2.5-dimethyl-1-phenyl-	83-18-1
0.	benzaldehyde, 2,6-dichloro-	83-38-5
11.	benzaldehyde, 3,4,5-trimethoxy-	86-81-7
12.	2-butenoic acid, 2,3-dichloro-4-oxo-, (2)-	87-56-9
13.	3-cyclohexene-1-carboxaldehyde, 6-methyl-	89-04-1
14.	benzaldehyde, 3,5-dici-loro-2-hydroxy-	90-60-8
15.	benzaldehyde, 4-[(2-chloroethyl)ethylamino]-2-methyl-	92-10-4
16.	benzalderlyde, 4-(12-Unit-Oethyl)erlynda (110)-2-methyl-benzalderlyde, 4-(14-thylamhor)-2-methyl-benzalderlyde, 4-(14-t	92-14-8
17.	benzaldehyde, 4-[(2-chloroethyl)methylamino]-	94-31-5
18.	ostzatostyce, 4-(2-Carocetry)metrylamino1- butanal, 2-methyl-	96-17-3
19.		97-96-1
20.	butanal, 2-ethyl-	99-61-6
21.	benzaldehyde, 3-nitro-	99-72-9
	benzeneacetaldehyde, a, 4-dimethyl	100-83-4
22.		104-53-0
23. 24.	benzenepropanal	105-88-4
	undecanal, 2,6,10-trimethyl	
25.	butanal, 3-hydroxy-	107-89-1
26.	acetaidehyde, tribromo	115-17-3
27.	1, 3-cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-	116-26-7
28.	retinal	116-31-4
29.	benzaldehyde, 4-ethoxy-3-methoxy-	120-25-2
30.	benzaldehyde, 4-(1-methylethyl)-	122-03-2
31.	pentanal, 2-methyl	123-15-9
32.	2-butenal, (E)	123-73-8
33.	tetradecanal	124-25-4
34.	benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3
35.	9-undecenal, 2,6,10-trimethyl-	141-13-9
36.	7-octenal, 3,7-dimethyl-	141-26-4
7.	2, 4-hexadisnal, (<i>E, E</i>)-	142-83-6
8.	benzaldehyde, 2-hydroxy-3-methoxy-	148-53-8
39.	benzaldehyde, 2-chloro-3-fluoro-	387-45-1
Ю.	2-cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl-	432-24-6
11.	1-cyclohexene-1-carboxaidehyde, 2,6,6-trimethyl-	432-25-7
2.	benzaldehyde, 3-(trifluoromethyl)	454-89-7
13.	benzaldehyde, 3-fluoro-	456-48-4
14.	benzaldehyde, 4-fluoro-	459-57-4
15.	2-cyclohexene-1-acetaldehyde, 2,6,6-trimethyl-	472-64-0
16.	1-cyclohexene-1-acetalclehyde, 2,6,6-trimethyl	472-66-2
47.	retinal, 13-cis-	472-86-6

	Chemical Name
•	benzaldehyde, 2,4,6-trimethyl-
	1H-indole-3-carboxald∈hyde
	benzaldehyde, 3-ethox;-2-hydroxy-
	hexanal, 2-ethyl-3-hydroxy-
	2-butenal, 2-methyl-, (£)-
	3-thiophenecarboxalds/nyde
	3-pyridinecerboxalidny/9
	2, 6,10-dodecatrienal, 3,7,11-trimethyl-, (<i>E,E</i>)
	retinal, 9-cis
	banzaldehyde, 4-nitro-
	berzaldehyde, 4-mino-
	2.6-nonadienal, (E.Z)-
	bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde, 6,6-dimethyl-
	benzaldehyde, 3-methoxy-
	benzaklehyde, 2,4,6-trk-itro-
	benzaldehyde, 4-(dipropytamino)
	benzaldehyde, 2-othoxy
	benzaldehyde, 2-hydroxy-5-methyl-
	2-furancarboxaldehyde, 5-methyl-
	benzaldehyde, 3-methyl-
	benzaldehyde, 3-hydroxy-4-methoxy-
	1, 4-benzenedicarboxaklehyde
	2-portenal, 2-methyl-
	2-proprial 2
	hexadecanal hexadecanal
	propanal, 2,2-dimethyl-
	benzaldehyde, 5-chloro-2-hydroxy-
	butanedial
	9-anthracenecarboxaldehyde
	1, 2-benzenedicarboxakiehyde
	2-hexenal, 2-ethyl-
	benzaldehyde, 2-hydroxy-4-methoxy-
	1-naphhalenecarboxaldehyde, 2-hydroxy-
	2-pentenal
	2, 4-pentadienal 2-propenal, 2-methyl-3-[4-(1-methylethyl)phenyl]-
	4-pyridinecarboxaldehyde
	benzaldehyde, 2,4-dichloro-
	2-propenal, 3-(2-furaryf)-2-methyl-
	berzaldehyde, 4-(acetyloxy)-
	benzaldehyde, 4-(acetyloxy)-3-methoxy-
	propanal, 2-chloro-2-methyl-
	1H-pyrrole-2-carboxaldehyde
	benzeneacetaldehyde, 4-methoxy-a-oxo-
	B'-apo- eta , psi-carotenal
	pentanal, 4-methyl-
	2-pyridinecarboxaldehyde, 6-methyl-
	benzaldehyde, 4-bromo
	Genzalenyod, 2, 3-dinyoloxy- 1, 3-benzodoxole-5-propinal, a,-methyl-
	propanal, phenyl-
	hexenal
	benzeneacetaldehyde, ar-(1-methylethyl)-
	undecenal
	benzaldehyde, 2-chloro-4-(dimethylarnino)-
	benzaldehyde, 3-amino
	2-propenal, 3-(4-nitrophenyl)-
	1H-Indole-3-carboxaldehyde, 1-methyl-2-phenyl-
	benzaldehyde, 5-bromo-2-hydroxy
	2-propenat, 3-(4-methoxyphenyl)
	4-pentenal
	benzaldehyde, 2,3,4-trimetrioxy-
	1-cyclohexene-1-carboxaldutryde, 4-(1-methylethenyl)
	acetaldehyde, phenoxy-
	propanal, 3-hydroxy-
	benzaldehyde, 2,3,4-trihydruxy-
	benzaldehyde, 4-hydroxy-3, 5-dimethyl-
	6-nonenal, (Z)-
	2, 4-decadienal
	2-octenal (C)
	6-octenal, 3,7-dimetriyl-, (r)-
	benzaldehyde, 2-hydroxy-3,5-dinitro-
	2-nonenal
	2-heptenal
	benzaldehyde, 4-erthoxy-3-hydroxy-
	2-octenal, (E)

	Chemical Name	CAS No.
10.	2-nonenal, 2-pentyl-	3021-89
	2-butenal, 2-methyl-4-(2,6.3-trimethyl-1-cyclohexen-1-yl)-	3155-71
	benzaldehyde, 4 (methylthio)	3446-88
3.	2-pentenal, 8-methyl-	3592-19
١.	propanal, 8-hydroxy-2,2-bis(hydroxymethyt)-	3618-32
	2-decenal	3913-71
	1,4-piperazinedicarboxaldehyde	4164-38
	benzaldehyde, 4-(diphenylumino)-	4181-05
	2-benzofuranoarboxaldehyde	4265-16
	2,4-heptadienel, (E,E)- benzenacetaldehyde, 4-(1-methydethyl)-	4313-03
	benzáldehyde, 4-(phenyimethoxy)-	4395-98 4397-53
	berzenacetaldehyde, a-einylidene	4411-8
	3-hexenal	4440-6
	benzakiehyde, 2,4,5-trimetilioxy-	4460-8
	4-hexenal (2)-	4634-8
	benzaldehyde, 4-ethyl-	4748-7
	2-dodecenel	4626-6
	2,6,9,11-dodecatetraenal, £,6,10-trimethyl-	4955-3
	benzeneacetaldehyde, a-(2-phenylethylidene)-	5031-8
	benzaldehyde, 2-hydroxy-8-nitro-	5274-7
	2-pentenal, 4-methyl-	5862-5
	berzenepropanal, 4-methyl-	5406-1
	1/f-indole-3-carboxaldehydu, 2-methyl-	5416-8
	benzaldehyde, 4-hydroxy-9-iodo-5-methoxy-	5438-3
	bicycle[2,2,1]hept-5-ene-2-carboxaldehyde	5453-8
	benzelidehyde, 4 - hydpory	5738-
		5736-
	benzaldehyde, 4-(pentyloxy)	5736-1 5736-1
	Self-acception (*Trexpoxy)	5910-
	2, 4-nonadienal, (E,E)	5910-
	2-propenal, 3-[4-(dimethylsinino)phenyi]-	6203-
	benzaldehyde, 2,4-dihydroxy-3-methyl-	6248-2
	berzaldehyde, 3,4-dichloro-	6287-
	berzaldehyde, 2,3-dichloro	6334-
	propanal, 3-(diethylamino)-2,2-dimethyl-	6343-
	benzaldehyde, 2-chloro-5-nitro-	6361-
	Z-propenal, 2-methyl-9-[2-(1-methylethyl)phenyl]-	6502-
	4-hexenal, 5-methyl-2-(1-methylethenyl)-, (-1)-	6544-
	benzaldehyde, 2-bromo	6630-
	undecanal, 2-ethylidene-	6720-
	2-hexenal, (E)	6726-2
	4-heptenal, (Z)	6728-
	2, 4-nonadienal.	6750-0
	3-hexenal, (2)	6769-4 6853-4
	2-propenal, 3-(1,3-benzodioxol-5-yl)-2-methyl-	6974~
	9,10-anthracenedicarboxaldehyde	7044-9
	2-thiophenecarboxaldehyde, 5-chloro-	7283-
	hexanal, 2-(phenylmethylene)-	7492-
	acetaldehyde, [(3,7-dimethy-6-octenyl)oxy}-	7492-
	3-cyclohexene-1-carboxalde(ryde, 4-methyl-	7580-
	1-piperazinecarboxaldehyde	7755-
	2-tridecenal	7774-
	octanal, 2-methyl-	7786-2
	benzeneacetaldehyde, 2-me/hyl-	10186-
	berzaldehyde, 3,5-dichloro-	10209-
	1-naphthaleneacetaidehyde, 5,6,7,8-tetrahydro-	10484-
	tridecanal	
	cyclohexanecarboxaldehyde, 2,2,6-trimethyl	13/66
	2-thiophenecarboxaldehyde, 5-methyl-	
	2-perrional, 2-metryl-, (E).	
	1/f-Indole-3-carboxaldehyde, 1-methoxy-2-phenyl-	14960-
	propanal, 3-(dimethylamino)-2,2-dimethyl-	
	propanal, 2-methyl-2-(methylithio)-	
	butanal, 3-(methyithio)-	18630-5
	2,6-nonadierral, (E,E)-	
	2.6,9,11-dodecatetraenal, 2,6,10-trimethyl-, (<i>E,E,E</i>)-	
	3-cyclohexene-1-carboxaldel:yde, 2-(1-methytallyl)	
	benzenepropanal, 4-(1,1-dimethylethyl)	
	propanal, 3-hydroxy-2-(hydroxymethyl)-2-methyl-	
	2-heptenel, (£)	
	2-nonenal, (E)	
	decanal, 2-methyl	
	Z-butenal, Z-ethyl- Donanal, Z	
	nonanal, 2-benzylidene	
	2-octenal, (2)	

	Chemical Name .	CAS No.
212.	7-decenal, (Z)	21661-97-2
213.		21662-09-9
214.		21662-13-5
215.		21662-15-7
216.		21662-16-8
218.	benzaldehyde, 4-(2-hydroxyethoxy)-	
219.		
220.		22414-68-2
	decanal, 2-methylen-s-	
222.		
223.	acetaldehyde, (methylthio)	
225.		24083-13-4
226.		
227.		24254-01-1
228.		
229.		25016-02-8
230. 231.		
232.		
233.		
234.	acetaldehyde, (3,3-dinethylcyclohexylidene)-, (Z)	
235.	acetaldehyde, (3,3-dimethylcyclohexylidene)-, (E)	26532-25-2
236.	benzeneacetaldehyde, α-(2-methylpropylidene)-	
237.		
238. 239.	2-pentenal, 2-ethyl-4-methyl	28419-86-5
240.	botania, 2-pretymentymentymeny- benzaldehyde, 4-propyl-	
241.	Indole-3-carboxaldehyde, 1,2-diphenyl-	
242.	3-cyclohexene-1-acetaldehyde, α, 4-dimethyl-	29548-14-9
243.	2,4-octadienal, (<i>E,E</i>)-	30361-28-5
244.	-1, (-1)	30361-29-6
245.	4-decenal	30390-50-2
246.		30551-17-8
247. 248.		30772-79-3 30897-75-7
249.	bicyclo[3.1.1]hept-2-ene-2-acetaldehyde, 6,6-dimethyl- benzaldehyde, dichloro-	31155-09-6
250.		31704-80-0
	o-Tolualdehyde, 4-[ethyl(2-hydroxy-3-phenoxypropyl)amino]-, carbanilate (ester).	32089-69-3
252.	3-butenal, 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	32791-31-4
253.	4,9-decadienal, 2,5,9-Irimethyl	32803-39-7
254. 255.		33985-71-6
256.		34291-99-1 34687-42-8
257.	6-octenal, 3-ethyl-3,7-tilmethyl-	34687-43-9
258.		34880-43-8
259.	2-hexenal, 5-methyl-2-(1-methylethyl)-	35158-25-9
260.	11-Tetradecenal, (Z)	35237-64-0
261.	benzaldehyde, 3-(1,1,2,2-letrafluoroethoxy)-	35295-35-3
262. 263.	benzaldehyde, 4-{1,1,2,2-tetrafluoroethoxy}-	35295-36-4
	benzaldehyde, 4-[bis[2-(benzoyloxy)ethyl]amino]-2,5-dimethoxy	35473-23-5 35746-21-5
265.		36208-33-0
266.	bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 4-methyl-1-(1-methylethyl)-, (1a,2a,4β)-	36208-34-1
267.	bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 1-methyl-4-(1-methylethyl)-, (1a,2\(\beta\),4\(\beta\)	36208-35-2
268.	bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 4-methyl-1-(1-methylethyl)-, (1α,2β,4β)	36208-59-0
269.	2-thiophenecarboxaldeinyde, 5-ethyl-	36880-33-8
270.	dodecanal, 2-methyl	37596-36-4 37677-09-1
272.	3-cyclohexene-1-carboxaldehyde, 4-[2-[3,3-dimethyloxiranyl)ethyl]	
273.	2-propenal, 3-bicyclo[2.2.1]hept-5-en-2-yl-2-methyl-	38284-42-3
274.	3-cyclohexene-1-carboxaldehyde, 2,4-dimethyl-6-propyl-	39067-36-2
	bicyclo[2.2.1]hept-5-ene-2-carboxaldehyde, 3-propyl-	39067-39-5
276.	8-nonenal	39770-04-2
276. 277.	9-decenal	39770-05-3
276. 277. 278.	9-decenal	39770-05-3 40364-80-5
276. 277. 278. 279.	9-decenal	39770-05-3
276. 277. 278. 279. 280. 281.	9-decenal	39770-05-3 40364-80-5 41448-29-7
276. 277. 278. 279. 280. 281. 282.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-55-1
276. 277. 278. 279. 280. 281. 282. 283.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-55-1 42507-56-2
276. 277. 278. 279. 280. 281. 282. 283. 284.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-55-1 42507-56-2 42507-57-3
276. 277. 278. 279. 280. 281. 282. 283. 284. 285.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-56-1 42507-56-2 42507-58-4
276. 277. 278. 279. 280. 281. 282. 283. 284. 285. 286.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-55-1 42507-56-2 42507-57-3 42507-58-4 42906-19-4
276. 277. 278. 279. 280. 281. 282. 283. 284. 285. 286. 287.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-56-1 42507-56-2 42507-58-4
276. 277. 278. 279. 280. 281. 282. 283. 284. 285. 286. 287. 288. 289.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-55-1 42507-56-2 42507-57-3 42507-58-4 42906-19-4 49576-57-0
276. 277. 278. 279. 280. 281. 282. 283. 284. 285. 286. 287. 288. 289.	9-decenal	39770-05-3 40384-80-5 41448-29-7 41767-05-9 41847-88-5 42507-55-1 42507-56-2 42507-56-3 42906-19-4 4995-19-4 99763-66-8 49763-68-1 50262-48-1
275. 276. 277. 278. 279. 280. 281. 282. 283. 284. 285. 286. 287. 288. 290. 291.	9-decenal	39770-05-3 40364-80-5 41448-29-7 41767-05-9 41847-88-5 42507-55-1 42507-55-3 42507-57-3 42507-58-4 42906-19-4 49576-57-0 49763-68-8 49763-68-8

_	Chemical Name .	CAS No
94.	3-cyclohexene-1-carboxal:dehyde, 1-methyl-3-(4-methyl-3-pentenyl)-	52474-6
15.	3-cydlohexene-1-oarboxal dehyde, 3-(4-methyl-3-pentenyl)-	
6.	benzaldehyde, 3-(ohleremethyl)-4-methoxy-	
7. B.	cyclohexeneoarbexaldehysle, 2,6,6-trimethyl- 2-propenal, 2-bremo-2-mithoxy-	
9.	c-propries, control-officially a solution of the control of the co	
).	9-tetradecenel (2)-	
	11-hexadeoenal, (Z)	
	benzeldehyde, ethyl-	
	5,9 undecadional, 2,6,10-trimethyl	
	3-cyolohexene-1-carboxeldehyde, 5-(3-hydroxy-3-methylbutyl)-3-methyl- 2,44etradecadional	
	cyclohexenecarbexeldehyrie, (4-methyl-3-pentenyl)-	
	B-octenal, 7-methyl-3-methylene	
	acetafdehyde, 1-ethyl-1, 3-dihydro-3,3-dimethyl-5-{phenylsulfonyl}-2H-indol-2-ylidene-	55203-
	3,6-ectadienal, 3,7-dimethyl-	
	4-hemnal, 2-ethenyl-2,5-dimethyl-	
	8-hevadecenal, (Z)	
	2.5-ectadional, (E.E.)	
	7-heistdeoenal (2)-	
	4-leoxazoleoarbexaldehydii, 2,5-dihydro-2-methyl-5-oxo-3-phenyl-	
	benzeneacetaldehyde, «-{2-furanylmethylene}-	57568-
	4-hexenal, 5-methyl-2-(1-methylethyl)-	58191-
	2-naphthalenecarboxaldehyde, 2-ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-	58243-
	8-undecenal benzaldehyde, 2,4,6-triprogroxy-	58470
	2.6-decadional, 3.7.9-time:hyl-	
	7-nonenal, 4,8-dimethyl-	58772-
	2,3b-methano-2bH-cyclopenta 1,3 cyclopropa 1,2 benzene-4-carboxaldehyde, octahydro-7,7,8,8-tetramethyl-	59056-
	propanal, 2-bromo-3,3-dimethoxy-	
	4,7-methano-1/H-indene-6-; arboxaldehyde, 3e,4,5,6,7,7e-hexahydro-, (3ea,4a,6a,7a,7aa)	
	4,7-methano-1/-indehen-5-roxxaldehryda, 3a,4,5,6,7,7a-hexahydro-, (3aa,4a,5a,7a,7aa)-	
	2-pentenal, 5-(methytthio)-2-((methythio)methyl)	
	2.4.9-decatrienal, 2.5.9-trimethyl-	
	6-hexadecenal, 14-methyl- (Z)-	
	2-nenenal, (Z)-	60784-
	2,44/idecadienal	60998-
	4-Nexonal, 5-methyl-2-(1-methylathylidene)-, dihydro deriv.	61792-
	2H-2,4a-methanonaphthalene-8-carboxaldehyde, 1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-, (2S)- heptanal, 6-methoxy-2,6-dimethyl-	
	tH, 5/-benzo[ij]quinolizine-9-carboxaldehyde, 2,3,6,7-tetrahydro-8-hydroxy-	
	benzaldehyde, 2-hydroxy-5-nonyl-	
	2-tetradeconal	
	decanal, 2-ethylidene-	
	benzaldehyde, 4-Lbis[2-(benzoyloxy)ethyl]amino]	
	4-decenal, (E)	65405-
	acetaldehyde, [(3,7-dimethyl-2,6-octadienyl)oxy]-, (E)-	65405-
	cyclohexenebutanal, c,2,2,6-tetramethyl-	05405-
	2-oydlohexene-1-carboxaldehyde, 4-(4-methyl-3-pentenyl)-1-(2-propenyl)-	
	bensenepropanal, 4-cyclopentyl-α-methyl	66867-
	3-cyclohexene-1-carboxaldehyde, 3,5,8-trimethyl-	67860
	bicyolo[2.2.2]octane-2-carb::xaldehyde, 6-(1-methylethyl)- 3-cyclohexene-1-carboxaldehyde, 1-methyl-4-(4-methyl-4-penteryl)-	
	Sastanal 2-hydroxy-3-methyl-	
	2-prepenal, 3-{2.2-dimethyl-ti-methylenecyclohexyl)-2-methyl-	67801-
	2-propenal, 2-methyl-3-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	67801-
	ectames, 2-(2-furany/methylene)	
	2-mg/hthaleneacetaidehyde, 5,6,7,8-tetrahydro- heptenal, 2-(2-turanylmethylene)-	
	3-oproloxeno-1-carboxaldenyde, 3,6-dimethyl-	
	bensaldehyde, 2,4,5-triethox/-	
	bicyclo[2,2,2]oct-5-ene-2-carboxaldehyde, 6-methyl-8-(1-methylethyl)-	67845-
	soetaldehyde, (4-methylphenoxy)-	
	acetaldehyde, [4-{1, 1-dimethylethyl)-2-methylphenoxy]- bioyclo[2,2,2]oct-5-ene-2-carboxaldehyde, 1-methyl-4-(1-methylethyl)	
	bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 1-methyl-1-(1-methylethyl)	
	2-cyclohexene-1-carboxaldelyde, 6-[1-(1-methylethyl)-2-propenyl]-	
	propanal, 2-methyl-2-(methyldithio)-	67952-
	3-cyclohexene-1-carboxaldelyde, 3, 5-dimethyl-	68039-
	3-cyclohexene-1-carboxaldeliyde, 2, 4-dimethyl-	68039-
	havenal, 3, 3, 5-trimethyl-	
	benzeneacetaldehyde, 4-athyl-	
	S-electroatic taber you, 2, 4-time try-	
	-postanal, 3-ethoxy-4-methyl-	68084-
	oyolohexenecarboxaldehyde, dimethyl-	68084-
	aostaldehyde, (3-hexenyloxy)-, (Z)-	
	3-cyclohexene-1-carboxaldehyde, 3,5-dimethyl-6-propyl-	

	Chemical Name	CAS No.
76.	3-cyclohexene-1-carpoxaldehyde, 1-methyl-2-(1-methylethenyl)-	68140-59
77.		68140-60
78.	nonanal, 5-ethyl-2-methyl-	
79.	3-dodecenal, (Z)	
80.	acetaldehyde, [(3,7-dimethyl-2,8-octadienyl)oxy]	
B1.	benzeneacetaldehyde, ar, α-diethyl	
82.	bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 5(or 6)-methyl-7(or 8)-(1-methylethyl)	
83	blcyclo[2.2.2]oct-5-ene-2-carboxaldehyde, 3,5(or 3,6)-dimethyl-7(or 8)-(1-methylethyl)	
84.	hexanal, 2,3,5,5-letramethyl-	
85 86	acetaldehyde, (4-methoxyphenoxy)	
87.	betzaladnyoz (2-4-us) rinednyouy)- butanai, 3-(heptyloxy)-2-oxo-	
88.	2-butenal, 2-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	
39.	3-cyclohexene-1-carloxaldehyde, dimethyl-	
90.	2-naphthalenecarboxaldehyde, octahydro-8,8-dimethyl-	
1.	2-naphthalenecarboxaldehyde, octahydro-5,5-dimethyl-	68738-96
2.	acetaldehyde, [2,6-bis(1,1-dimethylethyl)-4-methylphenoxy]	
3.	benzeneacetaldehyde, 3,4-dimethyl-	
34.	4,9-decadienal, 5,9-cimethyl-	
5.	3-cyclohexene-1-carioxaldehyde, 4-(4-hydroxy-3,4-dimethylpentyl)	
96. 97.	acetaldehyde, (2-furanytthio)	
8.	2-naphthalenecarbo aldehyde, 1,23,45,6,7,8-octahydro-8,8-dimethyl-	
9.	2-hrancarboxaldehvide, tetrahvide, tetrahvide-5-oxo- (F)-	
0.	4.9-decadienal, 4.8-dimethyl-	
1.		
2.	dodecanal, 11(or 12)-methyl-	
3.	benzaldehyde, 4-[(2,3-dihydroxypropyl)ethylamino]-2-methyl-, sulfate (1:1) (salt)	71673-10
4.	1,5-cyclododecadienecarboxaldehyde, trimethyl-	
5.	3-cyclohexene-1-cartioxaldehyde, 1,2,4(or 1,3,5)-trimethyl-	
6.	acetaldehyde, (2,6-dimethylphenoxy)-	
7.	benzaldehyde, 4-(acetyloxy)-3-ethoxy-	
8.	2-hexenal, 4(or 6)-methyl-2-propyl-	
9.	heptanal, 3,5,5-trimethyl- 5-octenal, 2,6-dimethyl-	
1.	cinnamaldehyde, still bottoms	72860_3
2.	acetalderlyde, (decyloxy)-	72894_0
3.	10-undecenal, 2-ethylidene-	
4.	2,12-tridecadienal	
5.	benzeneacetaldehyde, 3-methyl	
6.	acetaldehyde, [(3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-inden-6-yl)oxy]-	
7.	3-cyclohexene-1-cart:oxaldehyde, 5-(2-hydroxy-2-methylpropylidene)	
8. 9.	4,9-decadienal, 2,4,8-trimethyl- acetaldehyde, [(3a,4,5,6,7,7a-hexahydro-4,7-methano-1 <i>H</i> -inden-5-yl)oxy]-	
0.	2-cyclohexene-1-acetaldehyde, a, 2-dimethyl-5-(1-methylethenyl)-	
1.	undecanal, 2-methyt-2-(2-propenyl)	72928-3
2.	acetaldehyde, [4-(1,1-dimethylethyl)phenoxy]-	72928-50
3.	3-cyclohexene-1-carboxaldehyde, 2-(2-hydroxy-2-methylpropylidene)-	
1.	2-cyclohexene-1-acetaldehyde, 2-methyl-5-(1-methylethenyl)-	
5.	2-butenal, 2,3-dimethyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)	
5.	3-butenal, 2,3-dimethyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	
	4,7-methano-1/Hindene-2-carboxaldehyde, octahydro-5-methoxy	
3.	1/F-Indenecarboxaldehyde, 2,3,3a,4,5,6- hexahydro-1,3,3-trimethyl-	
).	biphenyl, polybromo- bromophenol (br1-br2, br5)	
	carbamate, bis(dibromopropyl)	
2	phosphile, bis(2,3-dibromoproyr)-	
1.	biphenyl, polybromo- (br8-br10)	
١.	phosphite,	No CAS
	toluene, tetrabromochloro	No CAS
ì.	brominated terphenylis	
	carbamate, dibromopropyl-	
).	phosphite, allyl bis(2,3-dibromopropy)-	
	phosphoryl chloride, bis(dibromopropyl)- 1-propanol, 2,3-dibromo-, phosphate (3:1)	126-7
	phenol, pentabromo	608-7
2	prominated terphenyls	623-2
	brominated terphenyls	626-1
	oxetane, 3,3-bis(bromomethyl)-	2402-8
	oxirane, bromoethyl	3132-6
	brominated terphenyls	3365-0
	brominated terphenyls	3365-0
	benzene, pentaborno (2-propenyloxy)	3555-1
	brominated terphenyls	4266-9
).	brominated terphenyls	4456-4 6386-7
	1,2-benzenedicarboxylic acid, bis(2,3-dibromopropyl) ester	7415-8
3.	1,2-centerieucerooxylic acid, bis(2,3-doromopropy)) ester brominated terphenyls	
1.	phosphonium, 1.2-ethanediylbis[tris(2-cyanoethyl)]-, dibromide	
5.	oxirane, (2-bromoethyl)-	13287-4
8.	1,1'-biphenyl, 2,2,3,3',4,4',5,5',6,6'-decabromo-	13654-09

	Chemical Name .	CAS N
58.	fumaric acid, bis(pentabromophenyl) ester	15108-
9.	4,7-methano-1/H-indene, 1,2-dibromo-4,5,6,7,8,8-hexachloro-2,3,3a,4,7,7a-hexahydro-	18300-
	1,2-benzenedicarboxytic acid, 3,4,5,6-tetrabromo-, dipotassium salt	
	brominated terphenyls ethanol, 2-(2,4,6-tribromochenoxy)-	
	furnario, 2-(2)	
	phenol, tribromo-	
	ethene, dibromo	25429-
	1-1111	
	benzene, tribromo(2-propenyloxy)-	
	1,1'-biphenyl, nonabromo- 1,1'-biphenyl, ar, ar, ar, ar', ar', ar', ar'-octabromo-	
	romated terphenyls.	
	phenol, 4,4'-(1-methylethylidene)bis 2,6-dibromo-, diacetate	33798-
	toluene, 2-chloro, tetrabrono-	
	phenol, 4,4'-sutfonylbis(2,6-dibromo)	
	brominated terphenyls	51211-
	1-propanol, 2,3-dibromo, carbamate.	
	brominated terphenyls	
	brominated terphenyls	
	phenol, 2,3,6-tertabromo-5-methyl-	
	ethanol, 2-(pentabromophenoxy)	60593-
	carbamic acld, bis(2,3-dibromopropyl)-, ethyl ester	
	2.4.8,10-tetraoxa-3,9-diphaspiro[5.5]undecane, 3,9-bis[3-bromo-2,2-bis(bromomethyl)propoxy]-, 3,9-dioxide	
	brominated terphenyls	
	prosperior and execution of the proper place o	
	diphenoxyethane, decabrorno	
	phenol, 2,4,6-tribromo-, carbonate (2:1)	
	phenol, pentabromo, aluminum salt	
	1,2-benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, magnesium salt (1:1)	
	2-Butenedioic acid (Z)-, bis(pentabromophenyl) ester	
	benzene, pentabromo[2-(tetrabromochlorophenoxy)ethoxy]-	
	benzene, 1,3,5-tribromo-2-(2-bromoethoxy)-	
	benzene, brominated chlorinated	
	hexanedioic acid, bis[3-bromo-2-(bromomethyl)-2-(hydroxymethyl)propyl] ester	
	brominated terphenyls	
	rominated terphenyis	
	brominated terphenyls	73206-
	brominated terphenyls	
	brominated terphenyls	
	brominated terphenyls	
	Prominated terphenyls.	
	brominated terphenyls	89961-
	brominated terphenyls	
	brominated temphenyls	
	brominated terphenyis	89961-
	brominated terphenyls	95918-
	brominated terphenyls	
	brominated terphenyls	
	ordinated terphenyis.	
	brominated terphenyls.	
	brominated terphenyls	108802-
	brominated terphenyls.	
	Naphthalene, 1-isocyanato	139-
		621-
	benzene, 1-isocyanato-2-meihoxy-	700-
	sulfuryl chloride Isocyanate.	1189-
	propane, 2-isocyanato-2-methyl-	1609-
	propane, 2-socyanato-	1795-
		1942-
	ethane, 1-chloro-2-lsocyanato	1943-
	hexane, 1-socyanato	2525-
	benzene, 1,1'-methylenebis(2-isocyanato)	2536-
	cyclohexane, 1,4-diisocyanato-	2556-
	benzonktrile, 4-isothiocyanato	2719- 3019-

_	Chemical Name	CAS No.
40.	Naphthalene, 1,5-diisocyaneto	3173-72
	benzene, 1-chloro-2-socyanatio-	3320-83
	benzene, 1-isocyanato-2-nitro-	3320-86
	benzene, 1-isocyenato-3-nitro-	3320-87
4.	berzene, 1,3-bis(ii ocyanatomethyl)	3634-83
5. 6.	berzane, 1,1'-oxytie(4-ieocyanato)-	4128-73
-	dodecane, 1-isocyanato	5392-82
8.	bergere, 1-ethory-2-leocyanato-	5395-7
S.	benzene, 1-lsocyanato-4-methoxy-	
O.	ethanamine, 2-iso:yanato-W-(2-isocyanatoethyl)-W-nitro-	
1.	cyclohexane, 1,4-bis(isocyanatomethyl)-	
2	formamide, M-ethenyl-	
3. 4.	benzene, 4-leocyanato-1-methyl-2-nitro	
5.	seem of the second of the seco	
6.	acotic acid, isocyaniato, butyl ester	
7.	sitene, chloro(3-iscovanatopropyl)dimethyl-	
8.	1,3-diazetidine-2, 4-dione, 1,3-bis[4-[(4-isocyanatophenyl)methyl]-	17589-2
9.	benzenesulfonic acid, 4-ieothiocyanato-, sodium salt	
3.	benzene, 1-isocyaneto-3-methoxy-	
t.	sporyanic acid, (2,4-dioxo-1,3-uretidinediyl)bls[methylene(3,5,5-trimethyl-3,1-cyclohexylene)] ester	
).).	silane, triethoxy(3-licocyanatopropy)-	
i.	carbamic acid, (3-i-i-ocyanatomethylphenyl)-, 1,2,3-propanetriyl ester	
	1,3-diazetidin-2-one, 1,3-bis[4-[(4-isocyanstophenyl)methyl]phenyl]-4-[[4-[(4-isocyanstophenyl)methyl]phenyl]imino]-	
	berzene, 1-ethoxy-1-isocyanato-	
	1,5-naphthalenedisultonic acid, 3-isothiocyanato-, disodium salt	
	cyclohexana, 1,3-bis(leocyanatomethyl)	38661-7
k,	berzene, 2-isocyanato-1,4-dimethyl-	
i.	benzonitrile, 4-isocyanato	
	benzoic acid, 2-(formytamino)-, methyl ester	41270-8
	cyclohexana, bis(isrcyanatomethyl)— berganesulfools and 5 (confidence) 0.12 (4 locthicoments 2 adderboudtethoud 1 disetting ont	
	benzenesulfonic acid, 5-(acetylamino)-2-[2-(4-leothiocyaneto-2-sulfophenyl)ethenyl]-, disodium salt	5455A-3
	carbamic acid, (3-isocyanatomethylphenyl). 2-ethylhexyl ester	
	ures, N.Nbis [(5-isocyanato-1,3,3-trimethylcyclohaxyl)methyl}-	
	carbamic acid, (3-is-ocyanatomethylphenyl)-, 2-ethylhexyl ester	
	carbamic acid, (3-is-ocyanatomethylphenyl)-, oxydi-2,-ethenediyl ester	60732-5
į,	sptro[isobenzofuran-1(3H), 9'T3H]xanthen]-3-one, 3',6'-dihydroxy-5-isothlocyanato-, hydrochloride	
	carbemic acid, 4-[(-isocyanatocyclohexyl)methyl cyclohexyl]-, oxydi-1,2-ethanediyl ester	
	Imidodicarbonic diarnide, 2,2"-(methylenebis(2-chloro-4,1-phenylene)]bis[N,M-bis(3-isocyanatomethylphenyl)]	
	carbamic acid, (3-isncyanatomethylphenyl)-, 1-methyl-1,3-propanediyl ester	
	1,3, 5-triazine-2,4,6(1H,3H, 5H)-trione, 1,3,5-tria((5-isocyanato-1,3,3-trimethylcyclohexyl)methyl)-	
	berzenamine, M.M-methanetetraylbis[3-isocyanato-2,4,6-trie(1-methylethyl)]]	
	carbamic acid, (3-is:rcyanatomethylphenyl)-, 1,2-ethanediyl ester	68092-7
	carbamic acid, (3-is-cyanatomethylphenyl)-, oxybis(1-methyl-2,1-ethanediyl) ester	68092-7
	carbamic acid, (3-is::cyanatomethylphenyl)-, [[(diethoxyphosphinyl)methyl]imino]di-2,1-ethanediyl ester	
	hexanoic acid, [2-e/hyt-2-[[[[[5-isocyanato-1(or 5)-(methoxycarbonyl)pentyl]amino]carbonyl]oxy]methyl]-1,3-propenediyl]	
	carbamic acid, (3-la: cyanatomethylphenyl)-, 1-methyl-1,3-propanediyl ester	
	1,3-diazetidine-2,4-dione, 1,3-bis(4-isocyanato-3-methylphenyl)- carbamic acid, (5-isocyanato-2-methylphenyl)-, 2-ethylphenyl ester	
	carbanic acid, [15-icoyanato-1,3-trimethylcyclohaxyl/methyl-], 2-ethyl-2-[[[[[5-isocyanato-1,3,3-trimethylcyclohaxyl/methyl-]]	
	carbamic acid, (5-isocyanato-1,3,3-trimethylcyclohexyl)methyl), oxyd-2,1-ethanediyl ester	68975-8
	hexanoic acid, 2,6-diisocyanato-, 2-isocyanatoethyl ester	69878-1
	undecane, 1,6,11-trisocyanato-	70198-2
	wrea, N-[[(aminophenyl)methyl]phenyl]-N-(3-isocyanatomethylphenyl)-	71106-5
	ures, N-(3-isocyanatomethylphenyl)-N-[[[4-[[(3-isocyanatomethylphenyl)amino]carbonyl]amino]phenyl]methyl]phenyl]	71130-7
	carbamic chloride, ethyl(5-isocyanato-2-methylphenyl)- carbamic acid, [4-[(4-isocyanatophenyl)methyl]phenyl}-, oxydi-2,1-ethanediyl ester	71832-3
	carbernic acid. [(5-is-ocyanato-1,3,3-trimethyloyclohexyl)methyl]-, 2-butoxyethyl ester	72152-8
	benzene, 2-isocyanalo-4-[(4-isocyanatophenyl)methyl]-1-methyl-	75790-8
	benzene, 1-isocyana:/o-2-[(4-isocyanatophenyi)thio]-	75790-8
	benzene, 1-chloro-4 (phenyfsulfonyi)-	80-0
	bertzenamine, 2-(methylsulfornyl)-4-nitro-	96-7
	benzene, 1-chloro-4-(methylsulfonyl)-2-nitro-	97-0 96-5
	benzene, 1-chloro-4-(methylsulfonyl)- 1,4-oxathiane, 4,4-dixxide	107-6
	benzene, 1,1'-sulfonythis(4-fluoro-3-nitro)-	312-3
	benzene, i,i'-suitonyibis(4-fluoro)	383-2
	methane, bis[(trifluoromethyl)sulfonyl]-	428-7
	propane, 1,1'-sulfony/bis-	596-0
	butane, 1,1'-sulfonythis-	598-0
	benzenamine, 3,3'-sulfonyibis-	599-6
	berzene, 1,1'-sulfony/bis(4-methyl)-	599-6
	berzene, 1-methyl-4-(phenytsulfonyi)- thiophene, tetrahydro-3-methyl-, 1,1-dioxide	640-5 872-9
	thiophene, 2.5-dihydro-3-methyl-, 1,1-dioxide berzene, 1,1'-sulfony/bis(3-nitro)-	1193-1 1228-5

	Chemical Name	CAS No.
622.	sulfone, 4-chioro-2-nitrophenyl methyl	2163-97-
623.		2182-69-6
624.	methane, sulfonylbis(trichloro)-	3064-70-1
625.		3737-41-4
626.		5184-75-4
627.		5397-34-
628.	3-thiophenamine, tetrahydro-, 1,1-dioxide	6338-70-
629.	1-propanamine, 2-[2-[[4-[3-(4-chlorophenyl)-4,5-dihydro-1 <i>H</i> -pyrazol-1-yl]phenyl]sulfonyl]ethoxy]- <i>N</i> , <i>N</i> -dimethyl	6608-82-
630.	ethanol, 2-[(3-amino-4-methoxyphenyl)suifonyl]-	7425-81-
631.		10215-25-
632.	benzene, 1,1'-sulfonylbis(2,4,6-trinitro)	10580-80-
633.		
534.		13244-35-
635.		
536.		
B37.		
638.		
639.	thiophene, 3,4-dibromotetrahydro-, 1,1-dioxide	
840.	phenol, 2,2"-sulfonylbis[4-(1,1,3,3-tetramethylbutyl)]-	
641.		
642.		
643.		
644.		
645. 646.		
647.	propionitrile, 3-[N-(2-hydroxyethyl)-p-[16-(methylsulfonyl)-2-benzothiazolyl]azo]anilino]-	
648.	,	
649.		
650.		
651.		29124-54-
652.		30203-11-
653.	benzothiazole, 2-[(tribrorriomethy)]sulfonyl]-	31274-42-
654.		
655.	ethanamine, 2-[2-[[4-[3-(4,5-dichloro-2-methylphenyl]-4,5-dihlydro-1//-pyrazol-1-yl]phenyl]sulfonyl]ethoxy]-W,M-dimethyl	
656.	benzene, 1,2-dichloro-4-(inethylsulfonyl)-	
657.		
658.		39635-79-
659.		40456-28-
660.		
661.		
662.		
663.	benzenamine, 4,4'-[[(4-methylphenyl)sulfonyl]methylene]bis(N,N'-dimethyl)-	49630-05-
664.	benzenamine, 2,2'-[sulforylbis(4,1-phenyleneoxy)]bis-	52338-52-
665.	ethanol, 2-[(4-methoxy-3-nitrophenyl)sulfonyl]-	52398-83-
666.	acetonitrile, (dodecytsulfcnyl)-	52821-30-
667.	thiophene, 3-bromo-2,3-dihydro-, 1,1-dioxide	53336-42-
668.	3H-indole, 2,3,3-trimethyl-5-(phenylsulfonyl)	55203-59-
669.		55203-60-
670.	1H-benzimidazolium, 2-(6-methoxy-2-benzofuranyl)-1,3-dimethyl-5-(methylsulfonyl)-	55911-28-
671.	benzene, 1,1'-sulfonyibis[4-(1-methylethyl)]-	57913-35-
672.		60345-53-
573.	1(2H)-quinolineethanol, 6-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-3,4-dihydro-2,2,4,7-tetramethyl-	63134-03-
374.	3-pyridinecarbonitrile, 5-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-4-methyl-2,6-bis[[3-(2-phenoxyethoxy)propyl]amino]	63281-10-
375.		
576.		
77.		
78.		65243-01-
379.	, -,	
80.	benzenesulfonic acid, 3-[[4-[ethyl(phenylmethyl)amino]phenyl]azo]-4-[(4-methylphenyl)sulfonyl]-	
81.	benzenamine, 4-[(1-ethyl-1/H-indol-3-yl)[(4-methylphenyl)sulfonyl]methyl]-N,N-dimethyl	
682. 683.	benzenamine, 5-chloro-2-[(4-methylphenyl)sulfonyl]-	
	1/Fyprazol-5-amine, 3-methyl-4-[[4-(methylsulfonyi)-2-nitrophenyi]azo]-1-phenyi-	
684.	3H-pyrazol-3-imine, 2,4-dihydro-5-methyl-4-[[4-(methylsulfonyl)-2-nitrophenyl]azo]-2-phenyl	70528-91-
685.	hydrazine, [4-(phenylsulfonyl)phenyl]-	70714-83-

1.3.e Removals. No chemicals were removed from the Priority List as a result of EPA responses to Committee recommendations.

1.4 The TSCA section 4(e) Priority
List. Section 4(e)(1)(B) of TSCA directs
the Committee to: """ make such
revisions in the [priority] list as it
determines to be necessary and ""
transmit them to the Administrator
together with the Committee's reasons

for the revisions." Under this authority, the Committee is revising the Priority List by designating two chemicals (4-vinylcyclohexane and sodium cyanide) that were previously recommended with intent-to-designate and adding one chemical (N-phenyl-1-naphthylamine) and four chemical groups (IRIS chemicals, aldehydes, sulfones and substantially produced chemicals in

need of subchronic tests). These revisions are listed in Table 1 above.

The Priority List (Table 2) includes designated, recommended with intent-to-designate and recommended chemicals and chemical groups. Individual chemicals in Priority List chemical groups are listed in Table 1 or the paragraph immediately following Table 1 of this and previous Reports with appropriate notes that minimize

ambiguities related to TSCA section 8(a)

and 8(d) reporting requirements. Table 2

containing the section 4(e) priority list follows:

TABLE 2.—THE SECTION 4(E) PRIORITY LIST

Entry	Action	Date
Brominated flame retardants	designated	November 1989
4-vinylcyclohexane	designated	November 1990
sodium cyanide	designated	November 1990
IRIS chemicals	designated	November 1990
chloroalkyl phosphates		November 1988
isocyanates	recommended with intent-to-designate	May 1990
aldehydes	recommended with Intent-to-designate	November 1990
imidazolium quaternary ammonium compounds	1	May 1988
ethoxylated quaternary ammonium compounds	recommended	May 1988
butyraldehyde	recommended	November 1988
brominated flame retardants	recommended	November 1989
brominated flame retardants.	recommended	May 1990
alkyi phosphates	recommended	May 1990
IRIS chemicals	recommended	November 1990
N-phenyl-1-naphthylamine	recommended	November 1990
sulfones	,	November 1990
substantially produced chemicals in need of subchronic tests	recommended	November 1990

References

(1) Sixteenth Report of the TSCA
Interagency Testing Committee to the
Administrator, Environmental Protection
Agency. TSCA Interagency Testing
Committee, May 21, 1985, 50 FR 20930–20939.
Includes references to Reports 1 through 15
and an annotated list of removals.

(2) Seventeenth Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, November 19, 1985, 50 FR 47603– 47612.

(3) Eighteenth Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, May 19, 1986, 51 FR 18368–18375.

(4) Nineteenth Report of the TSCA

(4) Nineteenth Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, November 14, 1986, 51 FR 41417– 41432.

(5) Twentieth Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, May 20, 1987, 52 FR 19020–19026.

(6) Twenty-first Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, November 20, 1987, 52 FR 44830– 44837.

(7) Twenty-second Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, May 20, 1988, 53 FR 18196-18210.

(8) Twenty-third Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, November 16, 1988, 53 FR 46262– 46278.

(9) Twenty-fourth Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, July 27, 1989, 54 FR 31248-31249

Committee, July 27, 1989, 54 FR 31248-31249.
(10) Twenty-fifth Report of the TSCA
Interagency Testing Committee to the
Administrator, Environmental Protection
Agency. TSCA Interagency Testing
Committee, December 12, 1989, 54 FR 5111451130.

(11) Twenty-sixth Report of the TSCA Interagency Testing Committee to the Administrator, Environmental Protection Agency. TSCA Interagency Testing Committee, June 5, 1990, 55 FR 23050-23062.

Chapter 2—Recommendations of the Committee

2.1 Chemicals recommended for priority consideration by the EPA Administrator. As provided by section 4(e)(1)(B) of TSCA, the Committee is revising the Priority List by designating two chemicals that were previously recommended with intent-to-designate and adding one chemical and four chemical groups (see Table 1). The recommendation of these chemicals is made after considering the factors identified in section 4(e)(1)(A) and other relevant information, such as the chemical testing information deficiencies of Member Agencies.

2.2 Designated chemicals—2.2.a 4-Vinylcyclohexane. 4-Vinylcyclohexane was designated because there were no TSCA section 8(d) submissions that satisfied the National Institute for Occupational Safety and Health nominated testing information deficiencies. The rationale for the original recommendation with intent-to-designate appeared in the Committee's 25th Report (54 FR 51114, December 12, 1989).

2.2.b Sodium cyanide. Sodium cyanide was designated and the testing recommendations changed because discussions among the Department of Interior, the EPA and industry identified additional testing information deficiencies and because there was a general understanding that there were no TSCA section 8(d) submissions that were likely to satisfy the testing information deficiencies nominated by the Department of Interior. The rationale for the original recommendation with intent-to-designate appeared in the Committee's 26th Report (55 FR 23050, June 5, 1990).

2.2.c. IRIS chemicals. At the request of EPA, the Committee reviewed a subset of chemicals that are listed on the Agency's Integrated Risk Information System (IRIS). IRIS is an electronic database, prepared and maintained by EPA, that contains health risk and EPA regulatory information on chemical substances. IRIS was developed for EPA staff in response to a growing demand for consistent risk information on chemical substances for use in decisionmaking and regulatory

activities. Although IRIS was designed for EPA staff, it is also accessible to state and local environmental health agencies, private citizens, libraries and organizations through Dialcom, Inc.'s electronic mail telecommunications system. For more information contact IRIS User Support in EPA's Environmental Criteria and Assessment Office, Cincinnati, Ohio (513/569-7254 or FTS 684-7254).

The chemicals that EPA nominated to the Committee for health effects testing information deficiencies are those chemicals for which the Agency has determined that there is a lack of confidence in the available health effects data. The EPA believes that the development of reliable health effects data will increase the confidence in the data and reduce the uncertainties in the assessment of risk. EPA nominated the IRIS chemicals to the Committee to recommend testing that would provide reliable data.

The Committee-activated comprehensive networking and information exchange processes were used to facilitate communication and coordination of chemical testing as intended by Congress and suggested by industry. The Committee considered unpublished studies in Member Agency's files, and past, present and future Member Agency activities. The Committee discussed studies conducted by NTP and EPA's Health Effects Research Laboratory and Environmental Research Laboratories, studies sponsored by NIOSH, studies used by OSHA and CPSC, studies submitted under TSCA as well as studies in FDA's files. The Committee learned about ongoing international activities, about ATSDR's data research needs, about EPA's Toxics Release Inventory (TRI) information, about Health Hazard Evaluations and Hazard Evaluation and Technical Assistance Reports, walkthrough surveys, etc., conducted by NIOSH, uses considered by the FDA. activities under other statutes, and so on. As part of the Committee's efforts to comprehensively consider testing information deficiencies, the Committee reviewed available information on physical/chemical properties and persistence as well as ecological effects and identified a number of chemical fate and aquatic toxicity testing information deficiencies. EPA's Neurobehavioral Toxicology Branch also reviewed these chemicals for potential neurotoxicology concerns and the Committee identified neurotoxicity testing deficiencies.

EPA nominated several IRIS chemicals to the ITC to take advantage of (1) The Committee's comprehensive

networking and information exchange capabilities that conserve resources and promote cost-effective testing required or sponsored by U.S. Government organizations and (2) the opportunity to obtain recent production and exposure information and unpublished health and safety studies that are automatically required under TSCA section 8(a) and 8(d), respectively, for any Committee recommendation. For 13 IRIS chemicals, the Committee has comprehensively assessed available health effects, chemical fate and ecological effects information. As a result of these assessments, the Committee is recommending 8 chemicals for testing (see Table 1), returning 2 chemicals to the EPA because the Committee's review identified health effects data that appear to be sufficient to reduce the uncertainty associated with risk assessments (vanadium pentoxide, CAS 1314-62-1 and hydrogen sulfide, CAS 7783-06-4), returning 2 chemicals for which there are uncertainties related to testing under TSCA (HMX, CAS 2691-41-0 and ammonium sulfamate, CAS 7773-06-0), and returning 1 chemical for which domestic production is being substantially reduced (CFC-113, CAS 76-13-1). The Committee identified algal toxicity and aquatic invertebrate acute and chronic toxicity testing deficiencies for vanadium pentoxide, but is not recommending testing at this time because, in a future Report it plans to recommend such testing for an inorganic chemical group. The EPA requested that the Committee designate 6 of the 8 IRIS chemicals. Five of the IRIS chemicals that were listed in Title III of the 1990 amendments of the Clean Air Act (acetophenone, acrylic acid, N,Ndimethylaniline, 2,4-dinitrophenol and phenol) were recommended for inhalation testing to reduce the uncertainty associated with risk assessments that need to be developed for these chemicals. The Committee is continuing to review information on numerous IRIS chemicals, including several that are listed in the Clean Air Act.

Summary of recommended studies. Recommended studies are summarized in Table 1 above.

Acrylic Acid

Physical and Chemical Information

CAS Number: 79–10–7
Synonyms and Trade Names: Acroleic acid, 2-propenoic acid.
Empirical Formula: C₃H₄O₂
Molecular Weight: 72.1
Physical State at 25° C: Liquid Description of Chemical: Corrosive liquid, acrid odor and fumes (Ref. 164, Windholz et al., 1983)

Melting Point: 13.5 (Ref. 96, Lide, 1990) Boiling Point: 141.6 (Ref. 34, Daubert and Danner, 1985)

Vapor Pressure: 4.00 mm Hg @ 25° C (Ref. 34, Daubert and Danner, 1985) Specific Gravity: 1.0621 (Ref. 164, Windholz et al., 1983)

Log Octanol/Water Partition Coefficient: 0.161 (Ref. 128, PCGEMS, 1987) Water Solubility at 25° C: miscible (Ref. 130, Perry and Green, 1984)

Log K_{oc}: 1.5 (Ref. 100, Lyman et al., 1982) Henry's Constant: 1.17 × 10⁻⁷ atm m³ mole⁻¹ (Ref. 75, Hine and Mookerjee, 1975)

Rationale for Recommendations

A. Exposure Information-Production/use/disposal/exposure/ release. In 1988, 1,068,834,000 lbs of acrylic acid were produced at 4 different U.S. facilities (Ref. 159, U.S. ITC, 1989). Acrylic acid has the following uses: surface coatings-25 percent; polyacrylic acid and salts (including superabsorbent polymers, detergents, water treatment and dispersants)-20 percent; textiles and nonwovens-13 percent; exports-12 percent; adhesives and sealants-9 percent; leather and polishes-4 percent; paper coating-3 percent; miscellaneous acid and ester uses (including specialty acrylates)-8 percent (Ref. 29, CMR, 1986).

B. Evidence for exposure—Human exposure. The National Occupational Exposure Survey (NOES) indicates that 56,512 workers (14,643 female) are potentially exposed to acrylic acid; 82 percent of this exposure is from the use of trade name products containing this compound (Ref. 120, NIOSH, 1990). Potential exposure to acrylic acid was associated with 22 different industrial classifications. OSHA's Permissible Exposure Limit (PEL) of 10 ppm 8-hour Time Weighted Average (TWA) and a skin notation are based on irritation by analogy to acetic acid (54 FR 2614-2621, January 19, 1989). OSHA concluded that these were necessary to protect workers from nasal and eye irritation, but NIOSH believed the limit should be lower based on recent studies demonstrating nasal mucosa degeneration, pulmonary function changes and skin absorption (54 FR 2621).

Environmental exposure. In a survey of 172 product/process effluents at 40 different petrochemical manufacturing sites, 26 percent of the samples contained acrylic acid at concentrations greater than 0.5 ppm (Ref. 165, Wise and Fahrenthold, 1981). According to the TRI, 832,056 lbs of acrylic acid were released to the atmosphere in 1967, while 16,126 and 6,153 lbs were released to water and land, respectively (Ref. 153, TRI, 1990). For 1988, TRI indicates that

798,567 lbs were released to air, 15,950 lbs were released to land, and 16,396 lbs were released to water (Ref. 153, TRI, 1990).

I. Chemical Fate Information

In the atmosphere, acrylic acid is expected to undergo rapid oxidation with gas phase hydroxyl radicals and ozone (Ref. 8, Atkinson, 1987; Ref. 9, Atkinson and Carter, 1984). In water, acrylic acid is not expected to significantly volatilize to the atmosphere, nor is it expected to adsorb to sediment or suspended organic matter (Ref. 100, Lyman et al., 1982). Limited screening studies suggest that acrylic acid will biodegrade under aerobic conditions (Ref. 19, BIOLOG, 1990; Ref. 127, Pahren and Bloodgood, 1961). Avialable persistence data are probably inadequate to predict the biodegradation rate of acrylic acid in the environment, because the data were not generated using test systems that simulated in situ biodegradation. The Committee recommends chemical fate testing because there are insufficient data to reasonably determine or predict the persistence of acrylic acid and because there are potentially substantial environmental releases.

II. Health Effects Information

Acrylic acid was rapidly absorbed, metabolized and excreted following oral or inhalation exposure (Ref. 88, Kutzman et al., 1982).

Effects identified in a 3-month drinking water study in groups of 15 male and 15 female Fischer F-344 rats given drinking water that provided doses of 83, 250 or 750 mg acrylic acid per kg per day included decreased food and water intake, reduced body weights, and alterations in organ weights (Ref. 39, DePass et al., 1983). Reduced weight gain, lethargy and nasal irritation were observed in the high dose in groups of 4-8 Alderley Park rats of both sexes exposed by inhalation to 80 or 300 ppm acrylic acid, 6 hours per day, 5 days per week for 4 weeks (Ref. 57, Gage, 1970). More recent inhalation studies in groups of 5 male and 5 female rats and mice exposed to 25 to 223 ppm acrylic acid, 6 hours per day, 5 days per week for 2 weeks (Ref. 112, Miller et al., 1979) and in groups of 15 male and female F-344 rats and B6C3F1 mice exposed to 5 to 75 ppm acrylic acid, 6 hours per day, 5 days per week for 13 weeks (Ref. 113, Miller et al., 1979; Ref. 114, Miller et al., 1981) identified mice as more sensitive than rats to the effects of inhalation exposure (nasal irritation and degeneration of the olfactory epithelium).

The fetuses of Sprague-Dawley rats given 24, 4.8 or 8.0 mg per kg intraperitoneal injections of acrylic acid on days 5, 10 and 15 of gestation had a dose-related decrease in body weights and an increase in the incidence of gross and skeletal malformations (Ref. 140, Singh et al., 1972). There is probably insufficient information on the effects of treatment to characterize the developmental toxicity of acrylic acid.

Maternal effects (nasal irritation and reduced rate of body weight gain) but no fetal effects were observed in the 2 highest dose groups of Sprague-Dawley rats exposed to 40, 120 or 360 ppm acrylic acid by inhalation on gestation days 6 to 15 (Ref. 87, Klimisch and Hellwig, 1989). Decreased fertility in females, decreased numbers of live pups per litter, decreased offspring body weight, and a decreased percentage of pups weaned were observed in a onegeneration reproduction study in groups of 10 male and 20 female rats that were provided acrylic acid in the drinking water at doses of 83, 250 or 750 mg per kg per day (Ref. 39, DePass et al., 1983). A 2-generation study may be necessary to characterize the reproductive effects of acrylic acid.

Acrylic acid was negative in the reverse mutation test in Salmonella (Ref. 97, Lijinsky and Andrews, 1980; Ref. 13, BASF, 1989), did inhibit incorporation of thymidine into DNA and uracil into RNA in S. aureus and E. coli (Ref. 60, Glombitza and Heysen, 1971) and was positive for mutagenicity and clastogenicity in L5178Y mouse lymphoma cells (Ref. 115, Moore et al., 1988). Acrylic acid was positive for chromosomal aberrations in an in vitro test in Chinese hamster ovary cells (Ref. 106, Microbiological Associates, 1986), but did not induce chromosomal aberrations in the bone marrow cells of rats treated by gavage for up to 5 days (Ref. 107, Microbiological Associates, 1986). In vivo testing may be necessary to characterize the mutagenicity of acrylic acid.

Acrylic acid was negative in 1 skin painting study in 40 male C3H/Hej mice treated with 1 percent acrylic acid in acetone thrice weekly for life (Ref. 40, DePass et al., 1984), but was weakly positive as a complete carcinogen and as a promoter in a study in which 30 female ICR/HA mice were treated with 4 mg acrylic acid in acetone thrice weekly for 1.5 years (Ref. 32, Cote et al., 1986). IARC (Ref. 79, IARC, 1987) assigned acrylic acid to Group 3; not classifiable as to its carcinogenicity to humans. The National Cancer Institute (NCI) reviewed a draft chronic study conducted by the Basic Acrylic Monomer Manufacturers Association and supports the EPA nomination and Committee recommendation for

inhalation oncogenicity testing.

Available data are probably insufficient to characterize the oncogenic potential of acrylic acid because they were not developed using an appropriate route of administration.

The Committee recognizes that NIOSH has Health Hazard Evaluations, Hazard Evaluation and Technical Assistance reports and walk-through survey reports for acrylics that are available from NTIS and the Committee is placing a list of these documents in the public docket. A table containing a list of FYI studies submitted to EPA is also contained in the public docket. The Committee recommends health effects testing because there are potentially substantial exposures, because there are insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty associated with risk assessments for acrylic acid.

III. Ecological Effects Information

The Committee recognizes that acute LC₆₀ values are available for fresh water fish, that growth of blue-green and green algae is inhibited at 0.15 and 18 mg/L acrylic acid, respectively and that protozoan growth is inhibited at acrylic acid concentrations ranging from 0.9 to 20 mg/L (Ref. 4, AQUIRE, 1990). The Committee is not recommending ecological effects testing at this time.

Acetophenone

Physical and Chemical Information

CAS Number: 98-86-2
Synonyms and Trade Names:
Phenylmethylketone, hypnone, acetylbenzene
Empirical Formula: C₆H₈O
Molecular Weight: 120.2
Physical State at 25° C: Liquid
Description of Chemical: Colorless liquid
with sweet, pungent, odor and taste (Ref. 136,
Sax and Lewis, 1987)
Melting Point: 19.8° C (Ref. 134, Riddick
et al., 1988)

Boiling Point: 202° C (Ref. 134, Riddick et al., 1986)
Vapor Pressure: 0.397 mm Hg @ 25° C

Vapor Pressure: 0.397 mm Hg @ 25* C (Ref. 163, Weber et al., 1981) Specific Gravity: 1.033 (Ref. 164, Windholz et al., 1983) Log Octanol/Water Partition Coefficient:

Log Octanol/Water Partition Coefficient:
1.58 (Ref. 68, Hansch and Leo, 1981)
Water Solubility at 25° C: 6,130 mg/L
(Ref. 69, Hasset et al., 1980)

Log Koc: 1.65 (Ref. 69, Hasset et al., 1980) Henry's Constant: 1.09 × 10.6 atm m³ mole. (Ref. 100, Lyman et al., 1982)

Rationale for Recommendations

A. Exposure Information—
Production/use/disposal/exposure/
release. Acetophenone is produced in substantial volumes; actual production volumes are CBI. Acetophenone is used

in fragrances and flavorings, and as a solvent, chemical intermediate for pharmaceuticals and resins, polymerization catalyst, and as a photoinitiator (Ref. 27, Chemcyclopedia, 1989; Ref. 136, Sax and Lewis, 1987).

B. Evidence for exposure—Human exposure. The NOES survey indicates that 39,880 workers (17,664 female) were potentially exposed to acetophenone in 18 different industrial applications (Ref. 120, NIOSH, 1990). Of these workers, 97 percent were potentially exposed during the use of trade name products containing acetophenone. Acetophenone has been detected in U.S. drinking water supplies. In a survey of 10 U.S. cities between 1969 and 1972, acetophenone was found in Philadelphia's drinking water, on 7 different occasions, at a concentration of approximately 1.0 µg/L (Ref. 84, Keith et al., 1976; Ref. 149, Suffet et al., 1980). Acetophenone was also detected in drinking water samples of Britain during 1977-79 (Ref. 53, Fielding et al., 1981).

Environmental exposure. Acetophenone was detected in 131 samples obtained from 28 industries and POTWs at a maximum concentration of 16 ppm (Ref. 138, Shackelford et al., 1983). Of 204 sites monitored in 14 heavily industrialized river basins in the U.S., acetophenone was detected in 3 of them at a concentration of 1 to 3 ppb (Ref. 51, Ewing et al., 1977). The STORET database indicates that acetophenone has been found in 1 surface water sample monitored during the 1980's (Ref. 148, STORET, 1990). Acetophenone was detected in both surface and deep water samples from the Baltic Sea, 1979-80, and thought to arise from the photooxidation of fuel oil components, suggesting that acetophenone is likely to be present in water polluted by fossil fuels (Ref. 46, Ehrhardt et al., 1982; Ref. 45, Ehrhardt, 1987). In a compilation of air monitoring data collected between 1970 and 1987. the median concentration of acetophenone in urban and source dominated sites was 0.041 and 0.094 ppb, respectively (Ref. 139, Shah and Heyerdahl, 1988).

1. Chemical Fate Information

In the atmosphere, acetophenone is expected to slowly degrade by the gas phase oxidation with photochemically produced hydroxy radicals (Ref. 8, Atkinson, 1987). Its fate in water will depend on photolytic degradation (Ref. 44, Draper and Crosby, 1983; Ref. 90, Lande et al., 1976), volatilization to the atmosphere (Ref. 102, Mackay et al., 1982), and biodegradation (Ref. 18, BIODEG, 1990; Ref. 99, Ludzack and Ettinger, 1963). The available data

indicate that acetophenone will not significantly adsorb to soil (Ref. 157, U.S. EPA, 1987). The Committee is not recommending chemical fate testing at this time.

II. Health Effects Information

Available pharmacokinetic data were limited to in vitro (Ref. 55, Fraser et al., 1967; Ref. 92, Leibman, 1971; Ref. 90, Lande et al., 1976) and in vivo (Ref. 151, Thierfelder and Daiber, 1923; Ref. 152, Thierfelder and Klenk, 1924; Ref. 141, Smith et al., 1954; Ref. 85, Kiese and Lenk, 1974) metabolism studies using rabbits, rats, humans and dogs. Quantitative data regarding absorption, distribution, or excretion may be necessary to characterize the oral and inhalation pharmacokinetics of acetophenone.

Subchronic studies failed to identify adverse effects in groups of 5 male and 5 female albino rats fed diets containing acetophenone at levels of 0.003, 0.05, 0.125 or 0.2 percent for 30 days (Ref. 142, Smyth, 1946) or in groups of 10 male and 10 female Osborne-Mendel rats fed diets containing 1,000, 2,500 or 10,000 ppm acetophenone for 17 weeks (Ref. 66, Hagan et al., 1967). An inhalation study reported a specific pattern of degeneration of the olfactory bulb in groups of 4 Wistar rats continuously exposed to acetophenone vapors for 1 week to 3 months (Ref. 132, Pinching and Doving, 1974). Other parameters of toxicity were not evaluated in this study. Although respiratory irritation was indicated in a number of studies. there are probably insufficient data to characterize the subchronic inhalation toxicity of acetophenone.

Reproductive toxicity data were limited to a study that reported no effects on length of gestation or postnatal development in the offspring of rats exposed dermally at 0.48 mg/kg on days 10 to 15 of gestation (Ref. 89, Lagno and Bakhtizina, 1969). A 2—generation study may be necessary to characterize the reproductive effects of acetophenone.

Acetophenone was negative for mutagenicity in 3 strains of Salmonella (Ref. 47, Elliger et al., 1984). Additional testing in non-bacterial systems may be necessary to characaterize the mutagenicity of acetophenone.

Anger and Johnson (Ref. 3, 1985) suggested that acetophenone could be neurotoxic. Data were not located regarding the oncogenicity of acetophenone.

The Committee recognizes that NIOSH has a Hazerd Evaluations and Technical Assistance report for acetophenone that is available from NTIS and the Committee is placing the reference for this report in the public docket. The Committee recommends health effects testing because there are potentially substantial exposures, because there are insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty associated with risk assessments for acetophenone.

III. Ecological Effects Information

The Committee recognizes that acetophenone is acutely toxic to fathead minnows; the LC₆₀ values ranged from 155 to 162 mg/L (Ref. 4, AQUIRE, 1990). The Committee is not recommending ecological effects testing at this time.

Phenol

Physical and Chemical Information

CAS Number: 108-95-2 Synonyms and Trade Names: Carbolic acid, hydroxybenzene, phenylic acid, benzophenol.

Empirical Formula: C₆H₆O Molecular Weight: 94.1 Physical State at 25° C: Solid Description of Chemical: Colorless, acicular crystals or white, crystalline mass (Ref. 164, Windholz et al., 1983) Melting Point: 43° C (Ref. 70, Hawley,

Boiling Point: 182° C (Ref. 70, Hawley, 1981)

Vapor Pressure: 0.35 mm Hg @ 25° C (Ref. 81, Jones, 1960) Specific Gravity: 1.071 (Ref. 164, Windholz et al., 1983) Log Octanol/Water Partition Coefficient:

1.46 (Ref. 68, Hansch and Leo, 1981) Water Solubility at 25° C: 93,000 mg/L (Ref. 23, Callahan et al., 1979) Log K :: 1.20 (Ref. 22, Boyd, 1982)

Log K_{oc}: 1.20 (Ref. 22, Boyd, 1982) Henry's Constant: 3.33 × 10⁻⁷ atm m³ mole ¹ (Ref. 56, Gaffney et al., 1987) pK_a: 9.994 (Ref. 137, Serjeant and Dempsey, 1979)

Rationale for Recommendations

A. Exposure Information-Production/use/disposal/exposure/ release. In 1988, 7 U.S. facilities produced 3,561,734,000 pounds of phenol (Ref. 159, U.S. ITC, 1989) and 13 facilities were listed as manufacturing this compound in 1989 (Ref. 145, SRI, 1989). Phenol has the following uses: phenolic resins-38 percent; synthesis of bisphenol A-23 percent; synthesis of caprolactam—17 percent; synthesis of alkylphenols—4 percent; synthesis of aniline-3 percent; miscellaneous uses-5 percent; exports—6 percent (Ref. 30, CMR, 1987). The miscellaneous uses of phenol include the synthesis of adipic acid, salicylic acid, phenolphthalein. pentachlorophenol, acetophetidine, picric acid, and pharmaceuticals, as a selective solvent for refining lubricating

oils, germicidal paints, laboratory reagent, dyes and indicators, slimicide, biocide, and as a general disinfectant (Ref. 138, Sax and Lewis, 1987). Many products containing phenol are utilized by consumers. The Committee is concerned with the potential for exposure to phenol because of its very high production volume, potential for release, and presence in commercial and consumer products.

B. Evidence for exposure—Human exposure. Phenol is used in a variety of commercial applications, many of which can lead to worker exposure. The NOES conducted during 1981-1983 by NIOSH estimated that 341,516 workers (108,851 female) were potentially exposed to phenol in 35 different industrial categories (Ref. 120, NIOSH, 1990). In a compilation of air monitoring data collected between 1970 and 1987, the mean concentration of phenol in suburban and urban areas was reported as 0.015 and 6.883 ppb, respectively (Ref. 139, Shah and Heyerdahl, 1988). The concentration of phenol in the air of Portland, OR, during 7 rain events in 1984 was 56 to 105 ppt, while the concentration of phenol in the rain ranged from 75 to 1,200 ppt (Ref. 93, Leuenberger et al., 1985). From 1977 to 1979, phenol was detected in 36 percent of drinking water supplies in England, which were drawn from groundwater, river water, and reservoirs (Ref. 53, Fielding et al., 1981). It has also been detected in U.S. drinking water supplies (Ref. 49, EPA, 1980; Ref. 119, Nicola et al., 1987). Phenol is used in numerous consumer products indicating a potential for exposure to the general population.

Environmental exposure. Phenol was detected in 738 samples obtained from 33 industries and publicly owned treatment works (POTWs) at a maximum concentration range of 7.5 ppb to 530 ppm (Ref. 138, Shackelford et al., 1983). Data from the STORET database indicates that phenol was found in 42.1 percent of industrial effluent samples obtained from 1980-83, at a median concentration of 10 ppb (Ref. 146, Staples et al., 1985). The STORET database also indicates that phenol was found in 13 percent of ambient surface water samples, and 9 percent of sediment samples (Ref. 146, Staples et al., 1985), and also in groundwater samples (Ref. 148, STORET, 1990). Phenol was detected in 4 percent of 86 samples obtained during the National Urban Runoff Program of 1982, at concentrations ranging from 3 to 10 ppb (Ref. 31, Cole et al., 1984). According to the TRI for 1987, 8,100,731 lbs of phenol were released to the air, 402,579 pounds

were released to water, and 1,098,624 lbs were released to land (Ref. 153, TRI, 1990). For 1988, TRI indicates that 10,155,101 lbs were released to air, 262,127 lbs were released to water, and 2,162,250 lbs were released to land (Ref. 153, TRI, 1990).

I. Chemical Fate Information

In the atmosphere, phenol will undergo rapid oxidation during the daytime by the reaction with photochemically produced hydroxyl radicals and at night with nitrate radicals (Ref. 8, Atkinson, 1987). Phenol is not expected to significantly volatilize from water to the atmosphere; however, it is likely to undergo rapid biodegradation under both aerobic and anaerobic conditions (Ref. 18, BIODEG, 1990). Biodegradation of phenol is well documented in the literature; it is often the benchmark for determining the rate of biodegradation of other organic compounds. Phenol may also undergo oxidation by alkoxy radicals in sunlit waters containing humic materials (Ref. 108, Mill and Mabey, 1984). Phenol is unlikely to adsorb to soil (Ref. 78, Howard et al., 1989), although in soils with substantial metal or clay content, phenol may be strongly adsorbed in a pH dependent process (Ref. 7, Artiola-Fortuny and Fuller, 1982). The Committee is not recommending chemical fate testing at this time.

II. Health Effects Information

Phenol was readily absorbed through the gastrointestinal tract, lungs, and skin (Ref. 37, Deichmann and Keplinger, 1981) and was widely distributed in rats and rabbits (Ref. 35, Deichmann, 1944; Ref. 95, Liao and Oehme, 1981). At lethal oral doses (0.5 g/kg in rabbits), it was eliminated by oxidation to CO2 and urinary excretion as free or conjugated phenol (Ref. 37, Deichmann and Keplinger, 1981). At low (0.01 to 50 mg/ kg) doses in several species treated by oral, intravenous or intramuscular administration, elimination was largely by urinary excretion of free and conjugated phenol; the proportion of free and conjugated phenol varied with species (Ref. 37, Deichmann and Keplinger, 1981; Ref. 24, Capel et al., 1972; Ref. 104, Mehta et al., 1978; Ref. 111, Miller et al., 1976; Ref. 82, Kao et al., 1979). Quantitative data regarding absorption, distribution, or excretion may be necessary to characterize the oral and inhalation pharmacokinetics of phenol.

Subchronic exposure of 17 humans to drinking water containing phenol (10 to 40 mg per person per day) resulted in a burning sensation in the mouth, sores in the mouth, and diarrhea (Ref. 11, Baker

et al., 1978). Groups of 10 male and 10 female F344 rats and B6C3F1 mice given phenol in drinking water at levels of 100, 300, 1,000, 3,000, or 10,000 ppm for 90 days exhibited decreased water consumption and weight gain at the high dose, but no histopathological effects (Ref. 116, NCI, 1980). Gavage treatment of rats with 50 or 100 mg/kg, 5 days per week for 6 months resulted in slight (unspecified) liver and kidney effects (Ref. 43, Dow Chemical Co., 1945). Decreased weight gain at the 2 highest doses was the only effect observed in rats given drinking water containing phenol at 800, 1200, 1,600, 2,000 or 14,000 ppm for 12 months (Ref. 36, Deichmann and Oesper, 1940). In a 2-year study, groups of 50 male and female B6C3F1 mice and F344 rats given drinking water containing 2,500 or 5,000 ppm phenol exhibited reduced water consumption and body weight gain but no clear evidence of compound-related histopathological alteration (Ref. 116, NCI, 1980).

In subchronic inhalation studies, increased mortality and CNS signs were reported in 12 guinea pigs and histological lesions were reported in the heart, liver, and kidneys of guinea pigs and 6 rabbits exposed to 100 to 200 mg/ m³ phenol for 7 hours per daý, 5 days per week for 6 to 13 weeks; effects were not observed in 25 rats similarly exposed for 11 weeks (Ref. 35, Deichmann et al., 1944). Slightly reduced body weight gain, but no other evidence of toxicity, was observed in 50 rats and 10 monkeys, whereas increased stress test endurance was observed in 100 mice exposed by inhalation to 19 mg/m3 phenol for 8 hours per day, 5 days per week for 90 days (Ref. 135, Sandage, 1961). A 15-day study associated behavioral effects with continuous inhalation exposure of rats to 100 mg/m3 phenol (Ref. 33, Dalin and Kristoffersson, 1974). There are probably insufficient data to characterize the subchronic inhalation toxicity of phenol, because existing studies were not sufficiently comprehensive in scope to identify effects on the respiratory tract and thresholds for inhalation exposure.

Anger and Johnson (Ref. 3, 1985) suggested that phenol could be neurotoxic.

A standard developmental toxicity gavage study reported reduced fetal body weight in the high dose in groups of 20 to 22 CD rats treated with 30, 60 or 120 mg per kg per day on gestation days 6 to 15 and maternal mortality, decreased body weight and CNS effects and reduced fetal body weight and increased incidence of cleft palate at the high dose in CD mice treated with 70,

140 or 280 mg per kg per day on days 6 to 15 gestation (Ref. 121, NTP, 1983). Maternal weight loss at the highest dose, but no effects on fetuses or offspring were reported in a developmental toxicity screening test with a single 100, 333, 667 or 1,000 mg/kg gavage dose given to groups of 12 to 13 Sprague-Dawley rats on day 11 of gestation (Ref. 83, Kavlock, 1990).

A multi-generation drinking water study identified adverse effects on offspring growth and survival, but failed to adequately evaluate effects on reproductive function and postnatal survival in rats given drinking water containing 100 to 12,000 ppm phenol (Ref. 73, Heller and Pursell, 1938). A study designed to adequately evaluate effects on reproductive function and postnatal survival may be necessary to characterize the reproductive effects of phenol.

The Committee recognizes that NIOSH has a Hazard Evaluations and Technical Assistance Report, walkthrough surveys, etc. for phenol that are available from NTIS and the Committee is placing a list of these documents in the public docket. A table containing a list of TSCA section 8(d) studies submitted to the EPA is also contained in the public docket for the 27th ITC Report. ATSDR published their priority toxicity data needs for phenol (55 FR 11566, March 28, 1990) and supports the **EPA** nomination and Committee recommendation for health effects testing. The Committee recommends health effects testing because there are potentially substantial exposures, because there are insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty

III. Ecological Effects Information

associated with risk assessments for

The ecological effects of phenol have recently been reviewed by Walker (Ref. 160, Walker, 1988). The Committee is not recommending ecological effects testing at this time.

N,N-Dimethylaniline

phenol.

al., 1986)

Physical and Chemical Information

CAS Number: 121-69-7
Synonyms and Trade Names:
Dimethylphenylamine, "N-dimethylbenzeneamine, xylidene
Empirical Formula: C₆H₁₁N
Molecular Weight: 121.2
Physical State at 25° C: Liquid
Description of Chemical: Yellowish to
brownish oily liquid (Ref. 136, Sax and Lewis, 1987)
Melting Point: 2.4° C (Ref. 134, Riddick et

Boiling Point: 194° C (Ref. 134, Riddick et al., 1986)

Vapor Pressure: 0.518 mm Hg @ 25° C (Ref. 163, Weber et al., 1981)

Specific Gravity: 0.956 (Ref. 138, Sax and Lewis, 1987)

Log Octanol/Water Partition Coefficient: 2.31 (Ref. 68, Hansch and Leo, 1981) Water Solubility at 25° C: 1,450 mg/L (Ref. 26, Chao et al., 1983)

Log K_{oc} : 1.90 (Ref. 100, Lyman et al., 1982) Henry's Constant: 5.68 \times 10 ⁵atm m³ mole ¹ (Ref. 100, Lyman et al., 1982) p K_a : 5.15 (Ref. 26, Chao et al., 1983)

Rationale for Recommendations

A. Exposure Information—
Production/use/disposal/exposure/
release. In 1979, domestic production of N,N-dimethylaniline was 13.7 million pounds (Ref. 158, U.S. ITC, 1980).
Information on current production volumes is CBI, but production is substantial. N,N-Dimethylaniline is used in dyes, as a synthetic intermediate for vanillin, pharmaceuticals, and other compounds, solvent, stabilizer, and polymerization catalyst (Ref. 91, Lawrence and Marshall, 1985; Ref. 136, Sax and Lewis, 1987).

B. Evidence for exposure—Human exposure. The NOES survey estimated that 28,048 workers (7395 females) were potentially exposed to N,N-dimethylaniline in 9 different industrial classifications (Ref. 120, NIOSH, 1990). Of these workers, 39 percent were potentially exposed during the use of trade name products containing this compound.

Environmental exposure. N,Ndimethylaniline was detected in 8 samples obtained from 3 industries and POTWs at a maximum concentration of 3.1 ppm (Ref. 138, Shackelford et al., 1983). According to TRI, 129,829 lbs of N,N-dimethylaniline were released to the air, 17,613 pounds were released to water, and 250 lbs were released to land in 1987 (Ref. 153, TRI, 1990). For 1988, TRI indicates that 98,905 lbs were released to air, 250 lbs were released to land, and 19,967 lbs were released to water (Ref. 153, TRI, 1990). N,N-Dimethylaniline was detected in soil samples obtained near the bank of the Buffalo River, NY, 1979 at concentrations of 10 to 40 ppm (Ref. 118, Nelson and Hites, 1980). N.N-Dimethylaniline was found in the Rhine River, Germany, in 1984 (Ref. 144, Sontheimer et al., 1985) and in the Wall River, Netherlands, in 1974 at a maximum concentration of 3.6 ppb (Ref. 105, Meijers and Vanderleer, 1976). N,N-Dimethylaniline was qualitatively detected in water from Lake Ontario, but not Lake Erie (Ref. 64, Great Lakes Water Quality Board, 1983).

I. Chemical Fate Information

N,N-dimethylaniline is expected to undergo rapid atmospheric oxidation by reaction with photochemically produced hydroxyl radicals, ozone, and with nitrate radicals at night (Ref. 8, Atkinson et al., 1987). In water, N.Ndimethylaniline is expected to degrade by its reaction with singlet oxygen (Ref. 65, Haag and Hoigne, 1985), and alkoxy radicals (Ref. 108, Mill et al., 1980) in sunlit waters. Biological processes are also likely to remove N,Ndimethylaniline from the aquatic compartment (Ref. 18, BIODEG, 1990; Ref. 117, Niemi et al., 1987), but there are uncertainties associated with its fate in wastewater treatment facilities. It is not expected to volatilize from water to the atmosphere nor is it likely to adsorb to soil (Ref. 100, Lyman et al., 1982). Available persistence data are probably inadequate to predict the activated sludge biodegradation of N.Ndimethylaniline, because data were not generated using test systems that simulated in situ wastewater treatment. The Committee recommends chemical fate testing because there are insufficient data to reasonably determine or predict the persistence of N,N-dimethylaniline and because there are potentially substantial environmental releases.

II. Health Effects Information

Data related to the pharmacokinetics of N.N-dimethylaniline were limited to several in vitro metabolism studies with rat and rabbit microsomal enzymes (Ref. 6, Arrhenius, 1968; Ref. 72, Heinze et al., 1970; Ref. 155, Uehleke et al., 1971; Ref. 17. Bickel et al., 1971; Ref. 166, Ziegler and Gold, 1971; Ref. 42, Devereux and Fouts, 1974; Ref. 133, Rane, 1974; Ref. 76, Hlavica and Kehl, 1974; Ref. 77, Hlavica and Kehl, 1976; Ref. 16, Beije and Arrhenius, 1978; Ref. 63, Gorrod et al., 1979; Ref. 62, Gorrod and Gooderham, 1981; Ref. 124, Ohmiya and Mehendale, 1983; Ref. 125, Olsson et al., 1983; Ref. 67, Hamill and Cooper, 1984; Ref. 123, Odenbro and Arrhenius, 1984; Ref. 126, Olsson et al., 1984; Ref. 42, Devereux et al., 1985) and in vivo metabolism studies in rats, rabbits and dogs (Ref. 74, Hildebrandt, 1907; Ref. 48, Elson et al., 1946; Ref. 86, Kiese and Renner, 1974). Quantitative data regarding absorption, distribution, or excretion may be necessary to characterize the oral and inhalation pharmacokinetics of N,Ndimethylaniline.

A 13-week gavage study (that included comprehensive histopathological examination) in groups of 10 male and 10 female F344/N

rats and B6C3F1 mice treated with 31.25, 62.5, 125, 250 or 500 mg/kg for 5 days per week identified the erythrocyte and the spleen as the most sensitive target organs in both species; however, a NOAEL was not reported (Ref. 1, Abdo et al., 1984; Ref. 122, NTP, 1989). Compound-related clinical signs included lethargy in rats and mice and cyanosis in rats. The only inhalation study available was a brief abstract that reported altered muscle chronaxie and evidence of hemolytic anemia in the high dose group of rats continuously exposed for 100 days to 0.04 or 0.3 mg/ m3 (Ref. 103, Markosyan, 1969). There are probably insufficient data to characaterize the subchronic inhalation toxicity of N,N-dimethylaniline, because existing studies were not available in sufficient detail to identify effects on the respiratory tract and thresholds for inhalation exposure.

Anger and Johnson (Ref. 3, 1985) suggested that N,N-dimethylaniline could be neurotoxic.

A 2-year chronic toxicity-oncogenicity gavage study in groups of 50 male and 50 female F344/N rats treated with 3 or 30 mg/kg, 5 days per week and similarly sized groups of B6C3F1 mice treated with 15 or 30 mg/kg, 5 days per week identified the rat as more sensitive than the mouse to the noncarcinogenic effects of N,N-dimethylaniline on the erythrocyte and spleen (Ref. 122, NTP, 1989). This study also reported some evidence of carcinogenicity in male rats (sarcomas and osteosarcomas of the spleen) and equivocal evidence of carcinogenicity in female mice (squamous cell papillomas of the forestomach).

Mutagenicity data were limited to negative results for reverse mutation in four strains of Salmonella and positive results for forward mutation in mouse lymphoma L5178Y cells and for sister chromatid exchange and chromosomal aberrations in Chinese hamster ovary cells (Ref. 122, NTP, 1989). In vivo testing may be necessary to characterize the mutagenicity of N,N-dimethylaniline.

Data regarding reproductive and developmental toxicity were limited to a study in 50 CD-1 albino mice treated with N,N-dimethylaniline in corn oil at 365 mg per kg per day on gestation days 7 to 14; maternal mortality, but no effects on body weight or viability of the neonatal offspring were reported (Ref. 131, Piccirillo et al., 1983). A 2-generation study designed to adequately evaluate effects on body weight or viability of the neonatal offspring may be necessary to characterize the reproductive effects of N,N-dimethylaniline.

The Committee recognizes that OSHA has recently reconsidered the PEL for occupational exposure (54 FR 2654). The Committee recognizes that NIOSH has Health Hazard Evaluations and other reports for N,N-dimethylaniline that are available from NTIS and the Committee is placing a list of these documents in the public docket. The Committee recommends health effects testing because there are potentially substantial exposures, because there are insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty associated with risk assessments for N,N-dimethylaniline.

III. Ecological Effects Information

Algal toxicity data are limited to an algal bioassay (Ref. 15, Batterton et al., 1978) and a study of energy metabolism enzymes in marine algae (Ref. 5, Armstrong et al., 1981). Acute aquatic toxicity studies are available for a ciliated protozoan and several species of fish (Ref. 4, AQUIRE, 1990). The committee reviewed available algal and acute aquatic invertebrate toxicity data and believes these data are insufficient because no EC60 values were reported. The Committee recommends ecological effects testing because there are insufficient data to reasonably determine or predict the ecological effects of N,N-dimethylaniline and because there are potentially substantial environmental releases.

Ethyl Acetate

Physical and Chemical Information

CAS Number: 141-78-6
Synonyms and Trade Names: Acetic
ether, acetic ester, vinegar naphtha.
Empirical Formula: C₄H₅O₂
Molecular Weight: 88.1
Physical State at 25° C: Liquid
Description of Chemical: Clear, volatile,
flammable liquid; characteristic fruity odor
pleasant taste when diluted (Ref. 164,
Windholz et al., 1983).
Melting Point: -83.6° C (Ref. 96, Lide,

1990)
Boiling Point: 77.1 (Ref. 96, Lide, 1990)
Vapor Pressure: 94.5 mm Hg @ 25° C
(Ref. 2, Ambrose et al., 1981)
Specific Gravity: 0.898 (Ref. 164,

Windholz et al., 1983)

Windholz et al., 1983)
Log Octanol/Water Partition Coefficient:
0.73 (Ref. 68, Hansch and Leo, 1981)
Water Solubility at 25° C: 80,000 mg/L
(Ref. 12, Banerjee, 1984)

Log K_{oc}: 0.94 (Ref. 100, Lyman et al., 1962) Henry's Constant: 1.38 × 10⁻⁴ atm m³ mole ¹ (Ref. 20, Bocek, 1976)

Rationale for Recommendations

A. Exposure Information— Production/use/disposal/exposure/ release. In 1988, 254.2 million pounds of ethyl acetate are produced in the United States (Ref. 159, U.S. ITC, 1989). Ethyl acetate has the following uses: coatings—41 percent; exports—36 percent; solvent—13 percent; plastics—8 percent; chemical synthesis—2 percent (Ref. 29, CMR, 1986). Many of its solvent uses include consumer products.

B. Evidence for exposure—Human exposure. The NOES survey estimated that 419,180 workers (99,059 female) were potentially exposed to ethyl acetate (Ref. 120, NIOSH, 1990). Of these workers, 87 percent were potentially exposed during the use of trade name products containing this compound. Potential exposure to ethyl acetate was associated with 34 different industrial classifications (Ref. 120, NIOSH, 1990). In addition, ethyl acetate is used as a solvent in numerous consumer applications. OSHA's PEL = 400 ppm 8hour TWA; the Committee learned that Sweden may reduce their PEL to 150 ppm, but is unaware of the basis for this potential reduction.

Environmental exposure. Ethyl acetate was detected in 68 samples obtained from 17 industries and POTWs at a maximum concentration of 7.7 ppm (Ref. 138, Shackelford et al., 1983). Of 204 sites monitored in 14 heavily industrialized river basins in the U.S., ethyl acetate was detected at a concentration of 1 ppb (Ref. 51, Ewing et al., 1977). In a compilation of air monitoring data collected between 1970 and 1987, the median concentration of ethyl acetate in urban sites was 0.733 ppb (Ref. 139, Shah and Heyerdahl, 1988). Ethyl acetate was also detected in industrialized and urban sites in Virginia and West Virginia at concentrations ranging from <0.012 to 1.9 ppb (Ref. 50, Erickson and Pellizzari, 1978). The STORET database indicates that ethyl acetate has also been detected in groundwater (Ref. 148, STORET, 1990).

I. Chemical Fate Information

In the atmosphere, ethyl acetate appears to be susceptible to removal by oxidative processes (Ref. 8, Atkinson, 1987; Ref. 28 CHEMFATE, 1990). The available data indicates that ethyl acetate's fate in water will be dominated by both rapid volatilization to the atmosphere (Ref. 100, Lyman et al., 1982) and rapid biodegradation (Ref. 18, BIODEG, 1990). Biodegradation is also likely to be a significant fate process in soil (Ref. 18, BIODEG, 1990). Ethyl acetate should not significantly adsorb to soil (Ref. 100, Lyman et al., 1982). The Committee is not recommending chemical fate testing at this time.

II. Health Effects Information

Ethyl acetate was readily absorbed following oral or inhalation administration to rabbits and rats, respectively, and was rapidly hydrolysed to ethanol and acetic acid (Ref. 150, Tambo, 1973; Ref. 58, Gallaher and Loomis, 1975). In a comprehensive 90-day gavage study in groups of 30 male and 30 female Sprague-Dawley rats treated with ethyl acetate in corn oil at doses of 300, 900 or 3,600 mg per kg per day, toxic effects resulting in reduced food intake and body weight, and altered organ weights were reported in high dose males; increased salivation, breathing changes and lethargy were also observed in high-dose groups (Ref. 156, U.S. EPA, 1986). Adverse effects on body weights, blood counts and urinalysis were not reported in a study in which 3 guinea pigs were intermittently exposed by inhalation to 7,206 mg ethyl acetate vapors/m³ for about 11 weeks (Ref. 143, Smyth and Smyth, 1928).

Data were not located regarding the developmental effects or reproductive

toxicity of ethyl acetate.

Ethyl acetate was negative for induction of reverse mutation in Salmonella when tested with (but not without) metabolic activation (Ref. 80, Ishidate et al., 1984). Positive results were observed for mitotic aneuploidy but negative results were observed for point mutations and recombination in yeast (Ref. 167, Zimmerman et al., 1985). In mammalian test systems, a positive response was reported for chromosomal aberrations in Chinese hamster fibroblasts in vitro (Ref. 80, Ishidate et al., 1984) and a negative response was reported for micronucleus formation in Chinese hamsters (Ref. 14, Basler, 1986). In vivo gene mutation testing may be necessary to characterize the mutagenicity of N.N-dimethylaniline.

Ethyl acetate was not a complete carcinogen when applied dermally (0.2 mL, 45 times during 23 weeks) to 8 female CD-1 mice (Ref. 98, Lindenfelser et al., 1974). Ethyl acetate at doses of 3.6 or 18 g/kg by intraperitoneal injection 3 times per week for a total of 24 injections was negative in the Strain A mouse lung tumor assay (Ref. 147, Stoner et al., 1973). The mice were sacrificed 24 weeks after the first dose.

The Committee recognizes that NIOSH has Hazard Evaluation and Technical Assistance reports, etc. for ethyl acetate that are available from NTIS and the Committee is placing these documents in the public docket. The Committee recommends screening health effects testing and triggering oncogenicity testing because there are

potentially substantial exposures, because there are insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty associated with risk assessments for ethyl acetate.

III. Ecological Effects Information

The Committee recognizes that acute LC₅₀ values are available for 14 invertebrate species, 3 species of freshwater fish, freshwater algae, a salamander, and a toad. These data indicate that ethyl acetate is acutely toxic to aquatic fauna at concentrations ranging from 9 to < 1,000 mg/L (Ref. 4, AQUIRE, 1990). The Committee is not recommending ecological effects testing at this time.

2,6-Dimethylphenol

Physical and Chemical Information

CAS Number: 576-26-1

Synonyms and Trade Names: 2,6-Xylenol Empirical Formula: CeH10O Molecular Weight: 122.2 Physical State at 25° C: Solid Description of Chemical: White crystalline solid (Ref. 96, Lide, 1990) Melting Point: 49° C (Ref. 96, Lide, 1990) Boiling Point: 212° C (Ref. 96, Lide, 1990) Vapor Pressure: 0.15 mm Hg @ 20° C (Ref. 163, Weber et al., 1981) Log Octanol/Water Partition Coefficient: 2.36 (Ref. 68, Hansch and Leo, 1981) Water Solubility at 25° C: 96,000 mg/L (Ref. 162, Wasik et al., 1981) Log K_{oc} : 1.45 (Ref. 100, Lyman et al., 1982) Henry's Constant: 7.5×10^{-7} atm m³ mole 1 (Ref. 100, Lyman et al., 1982) 10.59 (Ref. 129, Pearce and Simkins,

Rationale for Recommendations

A. Exposure Information-Production/use/disposal/exposure/ release. In 1977, between 2 and 20 million pounds of 2.6-dimethylphenol were produced at 6 different facilities in the United States (Ref. 154, TSCAPP, 1990). There were 2 facilities that manufactured 2,8-dimethylphenol in the U.S. in 1989 (Ref. 145, SRI, 1989). Information on current production volumes is CBI, but production is substantial. It is used primarily in the production of poly(phenylene oxide) resins (Ref. 52, Fiege, 1987). 2,6-Dimethylphenol is also used in the manufacture of tetramethylbisphenol A, 2,6-dimethylaniline, bis(4-hydroxy-2,5dimethylphenyl)methane, dyes, pharmaceuticals and fragrances, and as a mixture with other xylenols, in disinfectants, solvents, pharmaceuticals, insecticides, fungicides, plasticizers, rubber chemicals, lubricant and gasoline additives, and wetting agents (Ref. 136, Sax and Lewis, 1987).

B. Evidence for exposure-Human exposure. 2,6-Dimethylphenol is used in a variety of commercial applications, many of which can lead to worker exposure. The NOES survey estimated that 1,941 workers (179 females) were potentially exposed to 2,6-dimethylphenol. Of these workers, 95 percent were potentially exposed during the use of trade name products containing this compound.

Environmental exposure. 2,6-Dimethylphenol was detected in 64 samples obtained from 33 industries and POTWs at a maximum concentration of 2,895 ppm (Ref. 138, Shackelford et al., 1983). In a compilation of air monitoring data collected between 1970 and 1987, the mean concentration of 2,6dimethylphenol in source dominated areas was reported as 0.080 ppb (Ref. 139, Shah and Heyerdahl, 1988). The mean concentration of 2.6dimethylphenol in the air of Portland, OR, during 7 rain events in 1984 was 2.2 ppt, while the concentration of 2,6dimethylphenol in the rain ranged from 84 to 280 ng/L (Ref. 93, Leuenberger et al., 1985). 2,6-Dimethylphenol was detected in shale oil wastewater in the range 0.75 to 1.7 μ g/L (Ref. 71, Hawthorne and Sievers, 1984) and at 12 mg/L in the wastewater from the gasification of coal (Ref. 59, Giabbi et al., 1985). It was detected in groundwater samples from a wood preserving facility in Florida at a concentration of 0.90 mg/L, while the concentration of 2,6-dimethylphenol 330 m from the site was 0.29 mg/L (Ref. 61, Goerlitz et al., 1985).

I. Chemical Fate Information

Atmospheric degradation by photochemically produced hydroxyl radicals should rapidly remove 2,6dimethylphenol in sunlight (Ref. 10, Atkinson, 1987); degradation at night should be more rapid in urban areas through the reaction with nitrate radicals (Ref. 25, Carter, 1981). Rain washout is expected to be an effective method of atmospheric removal for 2,6dimethylphenol (Ref. 93, Leuenberger et al, 1985). Limited data are available on the fate of 2,6-dimethylphenol in water. Volatilization from water is not expected to be a significant removal process based on the Henry's Law constant (Ref. 100, Lyman et al, 1982). In humic waters, reaction with alkyl peroxy radicals should occur (Ref. 110, Mill, 1982); however, no chemical specific data are available. Screening studies suggests that 2,6-dimethylphenol biodegrades fast under aerobic conditions after acclimation (Ref. 18, BIODEG, 1990); however, data are

limited and no studies of the degradation of 2,6-dimethylphenol in environmental samples are available. Under anaerobic conditions, one screening study indicates that 2.6dimethylphenol is not expected to biodegrade (Ref. 18, BIODEG, 1990). Aqueous photolysis rate estimates and biodegradation data are probably inadequate to determine photolysis and biodegradation rates of 2,6dimethylphenol in the environment, because the estimates and data were not generated using test systems that simulate in situ processes. The Committee recommends chemical fate testing because there are insufficient data to reasonably determine or predict the persistence of 2,6-dimethylphenol and because there are potentially substantial environmental releases.

II. Health Effects Information

In 2 reports of an 8-month rat gavage study, histopathological changes in the liver, spleen and kidneys and changes in body weight, blood pressure and levels of protein sulfhydryl groups in blood serum and internal organs were observed in 53 male rats treated with 6 mg per kg per day (Ref. 160, Veldre and Janes, 1979 and Ref. 101, Maazik, 1968). Effects were not seen in rats dosed with 0.6 mg per kg per day. Increased relative liver and spleen weights, decreased body weight gain and marked atrophy and parenchymatous dystrophy of liver cells were observed in 10 male albino rats treated by gavage with 29.5 mg per kg per day for 10 weeks (Ref. 101, Maazik, 19687).

Data on the developmental toxicity or reproductive effects of 2.6dimethylphenol were not located.

Oncogenicity data were limited to a dermal study that identified 2.6dimethylphenol as a weak promoter in the two-stage mouse skin assay (Ref. 21, Boutwell and Bosch, 1959). In this study, 30 female Sutter mice were treated with an initial 75 µg application of dimethylbenzanthracene followed by 25 μL of 20 percent 2,6-dimethylphenol in benzene for 15 weeks. The mice were sacrificed at 23 weeks. In a second part of this study, 25 µL of 10 percent 2,6dimethylphenol was applied twice weekly for 20 weeks to mice that had not been initiated with dimethylbenzanthracene and the mice were maintained for an additional 8 weeks. There were "minimal effects" indicating carcinogenicity

Mutagenicity testing of 2,6dimethylphenol was limited to a single study in which the compound was negative with and without metabolic activation in the reverse mutation test in 4 strains of Salmonella (Ref. 54, Florin et al., 1980). Additional testing in nonbacterial systems may be necessary to characterize the mutagenicity of 2,6dimethylphenol.

The Committee recommends screening health effects testing because there are potentially substantial exposures, because there are insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty associated with risk assessments for 2,6dimethylphenol.

III. Ecological Effects Information

Acute aquatic toxicity studies are available for green algae, duckweed, daphnids, sea urchins, fathead minnows and Atlantic cod, and one chronic study is available for the fathead minnow (Ref. 4, AQUIRE, 1990). Available algal toxicity data are probably insufficient because no EC60 values were reported. Available fish chronic toxicity data are probably insufficient because they do not provide information on the effects of 2,6-dimethylphenol to sensitive fish life stages. The Committee recommends additional ecological effects testing because there are insufficient data to reasonably determine or predict the ecological effects of 2,6-dimethylphenol and because there are substantially potential environmental releases.

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2.3 Recommended with intent-todesignate chemicals-2.3.a Aldehydes. The aldehyde group was nominated to the Committee by EPA for aquatic toxicity testing. The Committee's computerized substructure-based selection processes were used to identify individual chemicals in the aldehyde group. Two aldehydes, crotonaldehyde (CAS # 4170-30-3) and butyraldehyde (CAS # 123-72-8) were previously recommended in the 22nd and 23rd reports, respectively. Two aldehydes, isobutyraldehyde (CAS # 78-84-2) and propanal [CAS # 123-38-6] are among the 53 chemicals in the Organization for Economic Cooperation and Development's (OECD) Screening Information Data Sets (SIDS) phase one voluntary testing program. Submission of reliable data or data development through the voluntary OECD SIDS program could change the Committee's testing recommendations for these two aldehydes. Two of the recommended aldehydes, acetaldehyde (CAS 75-07-0) and propanal were listed among the chemicals in Title III of the 1990 amendments of the Clean Air Act that the Committee is continuing to review. The Committee's recommendation of aldehydes is consistent with its comprehensive approach to processing Member Agency chemical groups and identifying substructure-based chemical groups in need of testing. Other chemical-group based actions include groups such as brominated flame retardants recommended in the 25th report and alkyl phosphates and isocyanates recommended in the 26th report.

The TSCA Inventory names are used in the paragraph following Table 1. These names are used to facilitate comparison with the names in the TSCA section 8(a) and 8(d) rules that EPA will prepare for chemicals recommended in this Report. Since common names of aldehydes are used in this chapter, the CAS number is listed in parentheses following the first use of a common name to facilitate identification of chemicals listed in the paragraph following Table 1.

Summary of recommended studies.
Testing recommendations for the aldehydes listed in the paragraph following Table 1 are summarized in Table 1.

Physical and Chemical Information

The physical and chemical properties of the very large volume aldehydes listed in the paragraph following Table 1 are well described in the literature. The Committee, however, was unable to identify the physical and chemicals properties of environmental and health significance for all members of this group.

Rationale for Recommendation

A. Exposure Information—
Production/use/disposal/exposure/
release. The Committee believes that
the aldehydes listed in the paragraph
following Table 1 are commercially
available, and that many are produced
in substantial quantities. For example,
acetaldehyde, isobutyraldehyde, and
propanal have current domestic
production capacities exceeding 300
million pounds (Ref. 22, SRI, 1990).
Actual production volumes of the other
aldehydes are CBI.

Aldehydes are used primarily as synthetic intermediates, yet aldehydes are also used in significant quantities in applications that are expected to result in both human and environmental exposure. Aldehydes are used in the production of alcohols, carboxylic acids, agricultural chemicals, pharmaceuticals, disinfectants, dyes, detergents, food additives, catalysts for crosslinking polymers, and fragrance chemicals (Ref. 5, Falbe et al., 1985; Ref. 21, Sherman, 1978). Acetaldehyde, propanal, and acrolein (CAS 107-02-8) have particular importance in commercial applications.

Many members of the aldehydes listed in the paragraph following Table 1 are used in fragrances and flavors. For example, α-pentylcinnamaldehyde (CAS 122-40-7) is a popular perfume in soaps, the Co.C13 saturated alkyl aldehydes are used as fragrances and toning agents (Ref. 5, Falbe et al., 1985), and 4methylphenylacetaldehyde (CAS 99-72-9), vanillin (CAS 121-33-5), and piperonal (CAS 120-57-0) are used in flavors (Ref. 5, Falbe et al., 1985; Ref. 19, Sax and Lewis, 1987). Piperonal is used in suntan and mosquito repellents and citronellal (CAS 106-23-0) is used in insect repellents (Ref. 19, Sax and Lewis, 1987). The Committee, therefore, is concerned with the potential for release and exposure resulting from the high production volumes and numerous uses of the various members of this group.

B. Evidence for exposure—Human exposure. There is an extensive data base relating aldehydes to human exposure. For example, acetaldehyde, isobutyraldehyde, propanal, furfural (CAS 98-01-1), and benzaldehyde have been found in U.S. drinking water

supplies (Ref. 2, Coleman et al., 1976; Ref. 9, Keith et al., 1976; Ref. 11, Krasner et al., 1989; Ref. 10, Kool et al., 1982; Ref. 12, Lucas, 1984). Benzaldehyde, nonanal, and dodecanal have been found in breath, personal air, or tap water samples (Ref. 26, Wallace et al., 1984). Acetaldehyde, isobutyraldehyde, butyraldehyde, methylbutyraldehyde (CAS 590–86–3), valeraldehyde (CAS 110–62–3), furfural, heptanal, benzaldehyde, octanal, decanal, undecanal, and dodecanal have been identified in samples of human mothers' milk (Ref. 18, Pellizzari et al., 1982).

The NOES conducted during 1981-83 by NIOSH reported that 14,054 workers were potentially exposed to acetaldehyde; 28 to trichloroacetaldehyde (CAS 75-87-6); 4113 to isobutyraldehyde; 22,173 to 4-(1,1-dimethylethyl)-a-methylbenzenepropanal (CAS 80-54-6); 2,187 to 1,3,3-trimethyl-2-(formylmethylene)indoline (CAS 84-83-3); 4,598 to salicylaldehyde (CAS 90-02-8); 34 to 2,5-dimethoxybenzaldehyde (CAS 93-02-7); 1,557 to αmethylbenzeneacetaldehyde (93-53-8); 134,158 to furfural; 17,271 to 4-(dimethylamino)benzaldehyde (CAS 100-10-7); 30,517 to benzaldehyde; 23,972 to 2-(phenylmethylene)-octanal (CAS 101-86-0); 44,721 to α -methyl-4-(1methylethyl)benzenepropanal (CAS 103-95-7); 62,450 to 3-phenyl-2-propenal (CAS 104-55-2); 12,494 to p-tolualdehyde (CAS 104-87-0); 6,573 to pchlorobenzaldehyde (CAS 104-88-1); 2,162 to citronellal; 1,300 to acrolein; 42,978 to ethanedial; 10,938 to 7hydroxy-3,7-dimethyloctanal (CAS 107-75-5); 1,863 to 2-methylundecanal (CAS 110-41-8); 1,557 to pentanal; 350,626 to pentanedial; 21,760 to heptanal; 20,732 to decanal; 1,557 to undecanal; 1,650 to 10undecenal; 7,056 to dodecanal; 72 to veratraldehyde (CAS 120-14-9); 1,450 to 4-(diethylamino)benzaldehyde (CAS 120-21-8); 15,846 to piperonal; 18,034 to 3-ethoxy-4-hydroxybenzaldehyde (CAS 121-32-4); 65,750 to vanillin; 14,182 to 2-(phenylmethylene)heptanal (CAS 122-40-7); 868 to phenylacetaldehyde (CAS 122-78-1); 43,899 to p-anisaldehyde (CAS 123-11-5); 2,087 to propanal; 12,959 to octanal; 7,149 to nonanal; 3,433 to hexahydrodibenzofurancarboxaldehyde (CAS 126-15-5); 5,331 to 2nitrobenzaldehyde (CAS 552-89-6); 1,557 to a-pentylcinnamaldehyde; and 28 to methylbenzaldehyde (CAS 1334-78-7) (Ref. 17, NIOSH, 1989).

Environmental Exposure. According to the TRI, 9,486,569 pounds of acetaldehyde were released to the environment in 1988 (Ref. 24, TRI, 1990). Corresponding releases for other members of the aldehydes group listed in TRI are as follows: propanal: 1,048,296 pounds; isobutyraldehyde: 791,996 pounds and acrolein: 103,068 pounds (Ref. 24, TRI, 1990). A compilation of published and unpublished data on the atmospheric concentration of volatile organic compounds determined between 1970 to 1987 found that acetaldehyde, benzaldehyde, 2-propenal, propanal, and methylbenzaldehyde have been detected in remote, rural, suburban, urban, source dominated, indoor, or workplace air samples (Ref. 20, Shah

and Heyerdahl, 1988).

Members of the aldehyde group have been detected in various environmental samples. For example, acetaldehyde, ethanedial, acrolein, propanal, benzaldehyde, and valeraldehyde have been detected in rain and/or fog samples (Ref. 7, Grosjean and Wright, 1983; Ref. 13, Mazurek and Simoneit, 1986; Ref. 23, Steinberg and Kaplan, 1984). Isobutyraldehyde, furfural, and benzaldehyde were detected in surface water samples obtained from 204 sites in the United States near heavily industrialized areas (Ref. 4, Ewing et al., 1977). Isobutyraldehyde and propanal were listed as frequently detected organics in the U.S. National Organics Reconnaissance Survey of surface waters (Ref. 6, Fielding and Packham, 1977). Acetaldehyde, propanal, ethanedial, heptanal, octanal, nonanal, decanal, undecanal, and dodecanal have been detected in seawater samples (Ref. 8, Gschwend et al., 1982; Ref. 15, Mopper and Stahovic, 1986); although acetaldehyde, propanal, and ethanedial may arise from natural as well as industrial sources (Ref. 15, Mopper and Stahovic, 1986). Isobutyraldehyde has been detected in the Delaware River (Ref. 3, DeWalle and Chian, 1978), and benzaldehyde has been detected in samples from freshwater lakes (Ref. 14, McFall et al., 1985). Benzaldehyde and 4-(dimethylamino)benzaldehyde have been detected in soil samples taken near the Buffalo River (Ref. 16; Nelson and Hites, 1980).

I. Chemical Fate Information

Chemical fate testing for the aldehydes is not recommended at this time.

II. Health Effects Information

Health effects testing for the aldehydes is not recommended at this time.

III. Ecological Effects Information

Structure-activity relationships (SAR) are frequently used to predict the toxic potential of untested chemicals when assessing their potential for adverse

ecological effects (Ref. 1, Auer et al. 1990). The Committee previously used SAR to identify the toxic potential of 2,6-di-tert-butylphenol in the 17th report. SARs used as part of the Committee's computerized, substructure-based chemical selection processes suggested that aldehydes could be toxic to birds, fish and mammals (Ref. 25, Walker and Brink, 1989). SARs have suggested that aldehydes could have excess toxicity (Ref. 1, Auer et al. 1990). Chemicals that could have excess toxicity are those that could be more toxic than would be predicted for neutral organics based on a narcotic mode of action. The Committee is concerned that SARs for aldehydes are only available to predict acute toxicity to fish. The Committee recommends ecological effects testing because there are potentially substantial environmental releases and because there are insufficient data to reasonably determine or predict the ecological effects of aldehydes that are submitted to the EPA as new chemicals.

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2.4 Recommended chemicals—2.4.a IRIS Chemicals—Summary of recommended studies. Recommended studies are summarized in Table 1.

2,4-Dinitrophenol

Physical and Chemical Information

CAS Number: 51–28–5
Synonyms and Trade Names: 1-hydroxy2.4-dinitrobenzene (or 2.4-DNP)
Empirical Formula: C₆H₆N₂O₅
Molecular Weight: 184
Physical State at 25° C: Solid
Description of Chemical: Light yellow
crystals (Ref. 62, Windholz et al., 1983
Melting Point: 113° C (Ref. 62, Windholz
et al., 1983)

Boiling Point: Sublimes (Ref. 34, Lide,

1990)

Vapor Pressure: 5.1 × 10⁻³ mm Hg @ 20³ C (Ref. 47, Schwarzenbach et al., 1988) Specific Gravity: 1.683 (Ref. 34, Lide, 1990) Log Octanol/Water Partition Coefficient: 1.54 (Ref. 25, Hansch and Leo. 1981)

1.54 (Ref. 25, Hansch and Leo, 1981)
Water Solubility at 20° C: 2,787 mg/L (Ref.
47, Schwarzenbach et al., 1988)
Log K_{oc}: 1.75 (Ref. 36, Lyman et al., 1982)
Henry's Constant: 4.43 × 10⁻⁷ atm m³
mole' (Ref. 36, Lyman et al., 1982)
pK_a: 4.09 (Ref. 23, Gordon and Ford, 1972)

Rationale for Recommendations

A. Exposure Information-Production/use/disposal/exposure/ release. The production volume of 2,4dinitrophenol is CBI, but current production is substantial. 2,4-Dinitrophenol is used in the synthesis of dyes, picric acid, picaramic acid, wood preservatives, diaminophenol dihydrochloride (a photographic developer), explosives, insecticides, and as a pH indicator (Ref. 46, Sax and Lewis, 1987; Ref. 62, Windholz et al., 1983). 2,4-Dinitrophenol may also be formed in the atmosphere by the reaction of nitrate radicals with phenol or other aromatic compounds.

B. Evidence for exposure—Human exposure. Few data were located.
ATSDR believes that 2,4-dinitrophenol may have been present in eight superfund sites. Eckel et al. (Ref. 16,

1986) reported an average concentration of 1,312 + 2,519 ppm 2,4-dinitrophenol for four hazardous waste dumpsite samples. The substantial production volume and uses in a variety of applications suggest significant occupational exposure potential.

Environmental exposure. 2,4-Dinitrophenol was detected in 21 samples obtained from 8 industries and POTWs at a maximum concentration of 10.2 ppm (Ref. 49, Shackelford et al., 1983). The STORET database indicates that 2,4-dinitrophenol was found in 2 percent of industrial effluent samples monitored between 1980 and 1983, and 0.4 percent of the ambient water samples (Ref. 52, Staples et al., 1985). According to TRI, the total release of 2,4-dinitrophenol to the air in 1987 was 32,600 lbs, while 86,500 lbs and 750 lbs were released to water and land, respectively (Ref. 55, TRI, 1990). For 1988, TRI indicates that 20,085 lbs were released to air, 98,692 lbs were released to water, and 257 lbs were released to land (Ref. 55, TRI, 1990).

I. Chemical Fate Information

2,4-Dinitrophenol is expected to rapidly degrade in the atmosphere through oxidative reactions with photochemically produced hydroxyl radicals and through the night-time reaction with nitrate radicals (Ref. 3, Atkinson 1987, Ref. 4, Atkinson et al., 1984, Ref. 5, Atkinson et al., 1987). Limited data are available on the fate of 2,4-dinitrophenol in water. Based on the Henry's Law constant, volatilization is not expected to be a significant process (Ref. 36, Lyman et al., 1982). Screening studies suggest that 2,4-dinitrophenol degrades fast under aerobic conditions after acclimation (Ref. 7, BIODEG 1990); however, data are limited. Under anaerobic conditions in flooded soils, loss is rapid and appears to be via reduction to the corresponding amine (Ref. 7, BIODEG, 1990; Ref. 29, Khoping and Wiegel, 1987). It is not clear, however, whether biodegradation or abiotic degradation is occurring or whether degradation proceeds beyond loss of the parent compound. The Committee recommends chemical fate testing because there are insufficient data to reasonably determine or predict the persistence of 2,4-dinitrophenol and because there are potentially substantial environmental releases.

II. Health Effects Information

Pharmacokinetic studies for 2,4dinitrophenol included an intraperitoneal study in rabbits and ducklings that indicated that uptake from the peritoneal cavity was very rapid (peak serum levels were obtained in rabbits within 5 minutes of treatment) (Ref. 20, Gehring and Buerge, 1969). Pharmacokinetic studies also included in vitro (Ref. 42, Parker, 1952; Ref. 17, Eiseman et al., 1974) and in vivo (Ref. 43, Perkins, 1919; Ref. 61, Williams, 1959; Ref. 48, Senczuk et al., 1971) metabolism studies that indicated that reduction and conjugation are the major biotransformation pathways.

A review of the therapeutic use of 2,4-dinitrophenol to correct obesity in humans reported over 100 cases of cataract formation at the lower range of the recommended therapeutic dose, 2 mg per kg per day (Ref. 26, Horner, 1942). The study did not identify a NOAEL for this effect. A 6-month study in male rats fed diets containing 0.01, 0.02, 0.05 or 0.2 percent 2,4-dinitrophenol identified a threshold for weight loss in rats, but cataracts were not reported even at doses sufficient to cause severe emaciation or death (Ref. 51, Spencer et al., 1948).

Data regarding reproductive and developmental effects were limited. Female rats treated by gavage twice daily with 20 mg/kg, from 8 days before mating through lactation, delivered more stillborn per litter and more litters with higher neonatal mortality than controls (Ref. 63, Wulff et al., 1935). Pregnant mice treated by gavage (25.5 or 38.3 mg/kg) or intraperitoneal injection (7.7 or 13.6 mg/kg) during a portion of gestation were hyperexcitable and hyperthermic; embryotoxicity (not specified) was also observed (Ref. 21, Gibson, 1973).

2,4-Dinitrophenol induced mutations in E. coli (Ref. 15, Demerec et al., 1951) but not in Salmonella (Ref. 14, Deflora, 1981) and produced chromatid breaks in bone marrow cells of mice treated by intraperitoneal injection. Oncogenicity data were limited to dermal studies in which 2,4-dinitrophenol was not a complete carcinogen (Ref. 51, Spencer et al., 1948) or a tumor promoter (Ref. 8, Boutwell and Bosch, 1959; Ref. 53, Stenback and Garcia, 1975).

NIOSH supported the EPA nomination and recommended dermal absorption testing. The Committee recommends health effects testing because there are insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty associated with risk assessments for 2,4-dinitrophenol.

III. Ecological Effects Information

The toxicity of 2,4-dinitrophenol has been tested in five species of algae (Ref. 27, Huang and Gloyna, 1967; Ref. 13, Dedonder and Van Sumere, 1971; Ref. 57, U.S. EPA, 1978; Ref. 10, Bringmann and Kuhn, 1978; Ref. 2, AQUIRE, 1990)

and in duckweed (Ref. 50, Simon and Blackman, 1953; Ref. 2, AQUIRE, 1990). Acute toxicity has been tested in invertebrates (Ref. 6, Bernstein, 1955; Ref. 30, Kojima, 1960; Ref. 31, Kopperman et al., 1974; Ref. 9, Bringmann and Kuhn, 1977; Ref. 57, U.S. EPA, 1978; Ref. 2, AQUIRE, 1990), fish (Ref. 44, Phipps et al., n.d.; Ref. 64, Zitko et al., 1976; Ref. 57, U.S. EPA, 1978; Ref. 2, AQUIRE, 1990) and bullfrogs (Ref. 33, Lewis and Frieden, 1959). An acute oral toxicity test in birds has been reported (Ref. 45, RTECS, 1990). The Committee recommends ecological effects testing because there are insufficient data to reasonably determine or predict the ecological effects of 2,4-dinitrophenol and because there are potentially substantial environmental releases.

3,4-Dimethylphenol

Physical and Chemical Information

CAS Number: 95–65–8
Synonyms and Trade Names: 3,4-Xylenol Empirical Formula: C₀H₁₀O
Molecular Weight: 122.2
Physical State at 25° C: Solid
Description of Chemical: White crystalline solid (Ref. 34, Lide, 1990)
Melting Point: 67° C (Ref. 34, Lide, 1990)
Boiling Point: 225 (Ref. 34, Lide, 1990)
Vapor Pressure: 0.075 mm Hg @ 20° C (Ref. 60, Weber et al., 1981)
Specific Gravity: 0.9830 (Ref. 34, Lide, 1990)
Log Octanol/Water Partition Coefficient: 2.23 (Ref. 25, Hansch and Leo, 1981)
Water Solubility at 25° C: 50,000 mg/L

Log K_{oc} : 1.06 (Ref. 38, Lyman et al., 1982) Henry's Constant: 7.56×10^{-7} atm m³ mole' (Ref. 36, Lyman et al., 1982) pK_a: 8.42 (Ref. 39, Miller and Faust, 1973)

Rationale for Recommendations

(Ref. 18, Fiege and Bayer, 1987)

A. Exposure Information—
Production/use/disposal/exposure/
release. In 1977, between .21 to 2.1
million pounds of 3,4-dimethylphenol
were produced in the United States (Ref.
56, TSCAPP, 1990). Information on
current production volumes is CBI, but
production is substantial. 3,4Dimethylphenol, as a mixture with other
xylenols, is used in disinfectants,
solvents, pharmaceuticals, insecticides
and fungicides, plasticizers, rubber
chemicals, additives to lubricants and
gasoline, and dyestuffs (Ref. 46, Sax and
Lewis, 1987).

B. Evidence for exposure—Human exposure. The NOES survey estimated that 93 workers (56 females) were potentially exposed to trade name products containing 3,4-dimethylphenol (Ref. 41, NIOSH, 1990). 3,4-Dimethylphenol has been qualitatively identified in the drinking water supplies of Cincinnati, OH (Ref. 35, Lucas, 1984).

The mean concentration of 3,4dimethylphenol in the air of Portland, OR during 7 rain events in 1984 was 2.2 ppt, while the concentration of 3,4dimethylphenol in the rain ranged from 54 to 190 ng/L (Ref. 32, Leuenberger et al., 1985). It was detected in groundwater samples from a wood preserving facility in Florida at a concentration of 2.4 mg/L, while the concentration of 3,4-dimethylphenol 330 m from the site was 0.85 mg/L (Ref. 22, Goerlitz et al., 1985). 3,4-Dimethylphenol also was detected in underground wells near a coal gasification site (Ref. 54, Stuermer et al., 1982).

Environmental exposure. 3,4-Dimethylphenol was detected in 10 samples obtained from 8 industries and POTWs at a maximum concentration of 3 ppm (Ref. 49, Shackelford et al., 1983). The concentration of 3,4-dimethylphenol in the raw effluent from a paper mill was 0.0457 mg/L (Ref. 28, Keith, 1976). It was detected in Los Angeles county effluent during 1980-81 at a concentration of 20 µg/L (Ref. 24, Gossett et al., 1983). 3,4-Dimethylphenol was also found in refinery effluent in Australia at 0.02 mg/L (Ref. 11, Cardwell et al., 1986). 3,4-Dimethylphenol was qualitatively detected in samples taken from the Saint Lawrence River (Ref. 59, Visser et al., 1977). It was also identified in the leachate of a sanitary landfill in Barcelona, Spain (Ref. 1, Albaiges et al., 1986).

I. Chemical Fate Information

Atmospheric degradation by photochemically produced hydroxyl radicals should be a rapid removal process for 3,4-dimethylphenol in sunlight (Ref. 3, Atkinson, 1987); degradation at night should be more rapid in urban areas through the reaction with nitrate radicals (Ref. 12, Carter, 1981). Also, rain washout is expected to be an effective method of atmospheric removal for 3,4dimethylphenol (Ref. 32, Leuenberger et al., 1985). Limited data are available on the fate of 3,4-dimethylphenol in water. Volatilization from water is not expected to be a significant removal process based on the Henry's Law constant (Ref. 36, Lyman et al, 1982). In humic waters, reaction with alkyl peroxy radicals should occur (Ref. 38, Mill, 1982); however, no chemical specific data are available. Screening studies suggests that 3,4-dimethylphenol biodegrades fast under aerobic conditions without acclimation (Ref. 7, BIODEG, 1990); however, data are somewhat limited and no studies of the degradation of 3,4-dimethylphenol in environmental water samples are available. One grab sample study at

high concentration (500 ppm) in soil suggests that 3,4-dimethylphenol biodegrades in soil; however, the data do not adequately predict the biodegradation of 3,4-dimethylphenol at low concentrations. Under anaerobic conditions, one screening study indicates that 3,4-dimethylphenol is not expected to biodegrade (Ref. 7, BIODEG, 1990). The Committee recommends chemical fate testing because there are insufficient data to reasonably determine or predict the persistence of 3,4-dimethylphenol and because there are potentially substantial environmental releases.

II. Health Effects Information

Data related to the pharmacokinetics of 3,4-dimethylphenol were limited to a single study in male Wistar rats that reported recovery of 93.5 percent of the radioactivity in the urine within 24 hours of giving a single oral 35 mg/kg dose (Ref. 40, Miyamoto et al., 1969).

In two reports of an 8-month rat gavage study, histopathological changes in the liver, spleen and kidneys and changes in body weight and blood pressure were observed in 53 male rats treated with 1.4 or 14 mg per kg per day (Ref. 58, Veldre and Janes, 1979 and Ref. 37, Maazik, 1968). Increased relative liver and spleen weights, decreased body weight gain and marked atrophy and parenchymatous dystrophy of liver cells were observed in 10 male albino rats treated by gavage with 72.5 mg per kg per day for 10 weeks (Ref. 37, Maazik, 1968).

Data on the developmental toxicity or reproductive effects of 3,4dimethylphenol were not located. Oncogenicity data were limited to a dermal study that identified 3,4dimethylphenol as a complete carcinogen and a tumor promoter in a mouse skin assay (Ref. 8, Boutwell and Bosch, 1959). In the promotion study groups of 30 female Sutter mice were treated with an initial application of 75 ug dimethylbenzanthracene followed by 25 µL of 20 percent 3,4-dimethylphenol in benzene twice weekly for 15 weeks. The mice were sacrificed at 23 weeks. In the complete carcinogen study 25 µL of 10 percent 3,4-dimethylphenol was applied twice weekly for 20 weeks and the mice were sacrificed at 28 weeks. Mutagenicity testing of 3,4dimethylphenol was limited to a single study in which the compound was negative with and without metabolic activation in the reverse mutation test in 4 strains of Salmonella (Ref. 19, Florin et

The Committee recommends health effects testing because there are

insufficient data to reasonably determine or predict health effects and because these data are needed to reduce the uncertainty associated with risk assessments for 3,4-dimethylphenol.

III. Ecological Effects Information

Some acute aquatic toxicity data are available for green algae, sea urchins, sand shrimp and fathead minnows (Ref. 2, AQUIRE, 1990). No algal EC60 data were available. The Committee recommends ecological effects testing because there are insufficient data to reasonably determine or predict the ecological effects of 3,4-dimethylphenol.

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2.4.b N-Phenyl-1-napthylamine. N-phenyl-1-naphthylamine was nominated to the Committee by OSHA as an ongoing effort to identify chemicals for which Permissable Exposure Limits may be proposed.

Summary of recommended studies.
Recommended studies are summarized in Table 1.

N-Phenyl-1-napthylamine

Physical and Chemical Information

CAS Number: 90–30–2 Synonyms and Trade Names: Vulkanox PAN

Empirical Formula: C₁₆H₁₃N Molecular Weight: 219.29 Physical State at 25° C: Solid Melting Point: 60–62° C (Ref. 1, Aldrich, 988)

Boiling Point: 335° C (Ref. 16, Sax and Lewis, 1987)

Water Solubility @ 25° C: ≈10 mg/L (Ref. 4, Greenhouse, 1978) Log Octanol/Water Partition Coefficient:

4.8 (Estimated, Ref. 11, Lyman et al., 1982) Log Koc: 3.7 (Estimated, Ref. 11, Lyman et al., 1982)

Rationale for Recommendation

A. Exposure Information-Production/use/disposal/exposure/ release. N-Phenyl-1-naphthylamine is used as an antioxidant in rubber, silicone oils, paraffinic oils for lubrication, anti-rust oils, paint, and plastics, and in the manufacture of dyes and other organic chemicals (Ref. 9, Kirk-Othmer, 1981, Ref. 12, Meylan et al., 1976, Ref. 10, Kirk-Othmer, 1981, Ref. 8, Kirk-Othmer, 1967, Ref. 16, Sax and Lewis, 1987, Ref. 6, Jarvholm and Lavenius, 1981, Ref. 18, Sikka et al., 1981). While actual production volumes are CBI, N-phenyl-1-naphthylamine is produced in substantial quantities.

B. Evidence for exposure—Human exposure. The NOES conducted during 1981–83 by NIOSH estimated that 96,478 workers (8,274 females) were potentially exposed to N-phenyl-1-naphthylamine, almost exclusively through trade name products (Ref. 13, NIOSH, 1990).

Environmental exposure. N-Phenyl-1naphthylamine has been detected (but not quantified) in the wastewater of a chemical specialty plant as well as in the river water and sediment receiving the wastewater (Ref. 7, Jungclaus et al., 1978). In a wastewater survey conducted by the Effluent Guidelines Division of EPA, over 4,000 wastewater samples from industrial facilities and publicly owned treatment works were surveyed (Ref. 17, Shackelford et al., 1983). This survey found N-phenyl-1-naphthylamine in one sample from the non-ferrous metals industry at a concentration of 8.46 ppb.

I. Chemical Fate Information

N-phenyl-1-naphthylamine has been tested for biodegradation in a number of screening studies as well as in soil and freshwater grab samples (Ref. 15, Rosenberg, 1983, Ref. 18, Sikka et al., 1981). In screening studies using sewage sludge as the inoculum and N-phenyl-1naphthylamine at 2 mg/L, the time to 50 percent disappearance was approximately 4.2 days. Autoclaved sewage showed less than 20 percent removal after 18 days. In lake water dosed with 2 mg/L N-phenyl-1naphthylamine, no degradation was observed in the first 5 days, but approximately 50 percent disappearance was observed after 10 days. No further degradation was seen at day 18. In soil exposed to N-phenyl-1-naphthylamine at 1.54 mg/kg, 17 percent of N-phenyl-1naphthylamine was mineralized to CO2 after 11 days. Sterile samples of water and soil showed almost no degradation. When exposed to sunlight, distilled water solutions of N-phenyl-1naphthylamine had a half-life of 5.7 days. The Committee recommends chemical fate testing because there are insufficient data to reasonably determine or predict the persistence of N-phenyl-1-naphthylamine.

II. Health Effects Information

Pharmacokinetics studies in rats indicate that N-phenyl-1-naphthylamine is rapidly absorbed and distributed widely following gavage administration (Ref. 18, Sikka et al., 1981). The urine and the feces are the primary routes of excretion with 35 and 60 percent, respectively, of the dose eliminated by each route after 72 hours. In vitro metabolism with rat liver microsomes produced the mono- and dihydroxy derivatives as well as other metabolites (Ref. 18, Sikka et al., 1981).

Negative results have been reported in a reverse mutation assay in bacteria, a forward mutation assay in cultured mammalian cells, a dominant lethal assay in rodents, and unscheduled DNA synthesis in cultured cells (Ref. 2, Brusick and Matheson, 1977). NTP also reported negative results in bacterial reverse mutation assays and in a chromosomal aberration assay in cultured mammalian cells, but reported positive results in a sister chromatid

exchange assay in cultured cells (Ref. 14, NTP, 1990).

In an oncogenicity study, groups of 23 to 25 male mice were administered purified N-phenyl-1-naphthylamine by subcutaneous injection 3 times per week for 9 weeks (Ref. 19, Wang et al., 1984). The mice were observed after the administration of N-phenyl-1naphthylamine; after the 10th month of observation a statistically significant higher incidence of total malignant tumors, lung carcinomas, and hemangiosarcomas was recorded. Technical grade N-phenyl-1naphthylamine produced similar effects. Although the tumor incidence was increased, the response was not clearly dose related. In a second experiment, using a different strain of mice, unilateral nephrectomy appeared to enhance the development of renal hemangiosarcomas. In a study with insufficient detail to allow for the evaluation of the data, dogs that were orally administered N-phenyl-1naphthylamine for 3.5 years had no observed increase in the incidence of bladder tumors (Ref. 3, Du Pont, 1945).

In Sweden, a cohort of 20 men and 78 women who were exposed to N-phenyl-1-naphthylamine in an anti-rust oil used for packing bearings were studied (Ref. 6, Jarvholm and Lavenius, 1981). The oil contained 50 percent white spirits, 16.5 percent each of mineral oil, lanolin, and zinc naphthenate, and 0.5 percent Nphenyl-1-naphthylamine, while the paper used as packing material for the bearings contained sodium nitrite. The authors note the potential for forming the nitrosamine of N-phenyl-1naphthylamine. The workers were exposed any time between 1954 to 1957 and followed until 1976. When compared to national gender- and agespecific cancer rates, there was an increased rate of morbidity and mortality from cancer in women. There was no site specific increase in incidence of cancer, with tumors of the colon, breast, uterus, ovary, bladder, brain, and thyroid reported, along with a reticulosarcoma. This study provides inconclusive evidence that N-phenyl-1naphthylamine is carcinogenic in humans, because of the small group size, the lack of increase in site-specific cancers, and confounders from exposure to multiple chemicals.

The Committee recommends health effects testing because there are insufficient data to reasonably determine or predict the health effects of N-phenyl-1-naphthylamine and because there are potentially substantial human exposures.

III. Ecological Effects Information

A 48-hour EC50 of 2.1 mg/L was reported for larval Xenopus laevis (South African clawed toad) (Ref. 5, Greenhouse, 1977). Concentrations of ≧ 5 mg/L caused 100 percent mortality in larval Rana pipiens (Leopard frog) after 48-hour's exposure (Ref. 4, Greenhouse, 1976). N-Phenyl-1-naphthylamine caused teratogenic effects in both Xenopus laevis and Rana pipiens (Ref. 5, Greenhouse, 1977, Ref. 4, Greenhouse, 1976). A 48-hour and 21-day staticrenewal test in Daphnia yielded LC60 values of 0.68 mg/L and 0.06 mg/L, respectively (Ref. 18, Sikka et al., 1981). The no observed effect concentration was 0.13-0.36 and 0.02 mg/L for 48-hour and 21-day exposure, respectively, but reproductive effects were not examined. The 8-day LC₀₀ values for bluegill and rainbow trout exposed to N-phenyl-1naphthylamine under flow-through conditions were 0.48 and 0.30 mg/L, respectively. No observable effect concentrations under the same conditions were 0.24 and 0.11 mg/L for bluegill and rainbow trout, respectively. The Committee recommends ecological effects testing because there are insufficient data to reasonably determine or predict the ecological effects of N-phenyl-1-naphthylamine.

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2.4.c. Sulfones—summary of recommended Studies. Testing recommendations for the sulfones listed in the paragraph following Table 1 are summarized in Table 1.

Sulfones

Physical and Chemical Information

Except for the melting point of bis(4-chlorophenyl)sulfone (146° C; Ref. 1, Aldrich, 1988), the log octanol/water partition coefficient (0.97; Ref. 5, Hansch and Leo, 1981) and pK_a (2.41; Ref. 10, Perrin, 1965) of 4,4'-diaminodiphenyl sulfone, the log octanol/water partition coefficient (-0.77; Ref. 5, Hansch and Leo, 1981), melting point (27° C; Ref. 1, Aldrich, 1988), boiling point (285° C; Ref. 1, Aldrich, 1988), vapor pressure (7.70 × 10°3 mm Hg; Ref. 3, Daubert and Danner,

1989) and water solubility (3.79 \times 105 mg/L; Ref. 2, Brown et al., 1975) of sulfolane, melting point (65–66° C; Ref. 1, Aldrich, 1988) of sulfolane, and melting point of bisphenol S (246° C; Ref. 1, Aldrich, 1988), the Committee has no information on measured physical/chemical properties of the sulfones listed in the paragraph following Table 1.

Rationale for Recommendation

A. Exposure Information—
Production/use/disposal/exposure/
release. The Committee believes that
the sulfones listed in the paragraph
following Table 1 are commercially
available, and that many are produced
in substantial quantities; actual volumes
are CBI. In 1977, many of the chemicals
were produced in quantities of 0.1 to 20
million lbs per year (Ref. 11, TSCAPP,
1990).

Sulfolane is used primarily as a solvent for the extraction of benzene, toluene, and xylene from aliphatic hydrocarbon mixtures. It is also used for the removal of acidic gases from natural gas and other gas streams, and it has extensive application as a specialty solvent (Ref. 8, MacGregor and Orle, 1983). Sulfolene is used as a specialty solvent in petroleum relining and in the manufacture of sulfolane (Ref. 8, MacGregor and Orle, 1983). The unique thermal stability and properties of the sulfones are utilized in the manufacture of specialty products. For example, bis(4-chlorophenyl)sulfone is used in the manufacture of engineering thermoplastics (Ref. 8, MacGregor and Orle, 1983).

B. Evidence for exposure-Human exposure. Sulfolane, diphenylsulfone, dimethylsulfone, and bis{4-chlorophenyl}sulfone have been detected (no quantitative data available) in U.S. drinking water supplies (Ref. 7, Lucas, 1984; Ref. 6, Kool et al., 1982). The NOES conducted during 1981–83 by NIOSH estimates that 6,461 workers were potentially exposed to sulfolane and 1,510 were potentially exposed to sulfolene (Ref. 9, NIOSH, 1989).

I. Chemical Fate Information

Except for data on the slow biodegradation of bis(4-chlorophenyl)sulfone in soil (Ref. 4, Guenzi and Beard, 1981), the Committee has no experimental chemical fate information on the sulfones listed in the paragraph following Table 1. Chemical fate testing is recommended because data are insufficient to reasonably determine or predict the physical/chemical properties of sulfones.

II. Health Effects Information

No health effects testing is recommended at this time. NTP's Board of Scientific Counselor's decision to defer a testing recommendation for bis(4-chlorophenyl)sulfone (referred to as p.p'-dichlorodiphenylsulfone by NTP) is consistent with the Committee's efforts to facilitate coordination of testing required or sponsored by U.S. Government organizations. The decision is also consistent with the Committee's procedures of reviewing production and exposure data (submitted under TSCA section 8(a)) as well as unpublished health and safety studies (submitted under TSCA section 8(d)) that are recommended for testing before designating subsequent health effects, chemical fate or ecological effects testing. These TSCA section 8 data and studies are automatically required for any ITC recommendation.

III. Ecological Effects Information

No ecological effects testing is recommended at this time.

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2.4.d. Substantially produced chemicals in need of subchronic tests-Introduction. On May 17, 1989, a list of 166 substantially produced, commercial chemicals were discussed by the Committee because they were coded for exposure and adverse effects potentials in the ITC's computerized, substructurebased chemical selection system. This computerized system allows the Committee to cost-effectively screen chemicals by identifying chemical groups with exposure potentials or with adverse effects potentials and chemicals that have common testing information deficiencies, e.g. subchronic toxicity, fish chronic toxicity, biodegradation, physical/chemical properties, etc. For chemicals produced in substantial quantities and for which there may be potential occupational exposure or environmental release or for which there may be potential adverse effects concerns and for which there appear to be basic testing information deficiencies, there should be a minimum amount of data to identify potentially problematic chemicals, e.g., a minimum amount of chemical fate, bioconcentration, bioaccumulation or ecological effects data should be available for potentially problematic chemicals (Ref. 4, Walker, 1990). The concept of obtaining minimum data to identify potentially problematic chemicals is consistent with the OECD's approach to voluntarily obtaining SIDS for high production volume chemicals.

In addition to using their system to identify chemical groups of concern, the Committee uses their computerized system and associated processes to implement Member Agency testing nominations. EPA and other Member Agencies have taken advantage of the system and associated processes to facilitate nominations, e.g., EPA nominated isocyanates that were recommended for testing in the Committee's 26th Report and aldehydes that were recommended for testing in this Report. Using the computerized system and associated processes to facilitate nominations and transform them into subsequent Committee recommendations allows the nominator to easily access Member Agency information through Committeeactivated interagency networking and provides the nominator with very rapid

access to TSCA section 8 information without notice and comment rulemaking. Member Agency information networking is used to promote cost-effective use of U.S. Government chemical testing resources. The information submitted under TSCA 8(a) may provide access to production, exposure and environmental release confidential business information. Chemical fate, health effects, monitoring, epidemiology and ecological effects studies that could be submitted under TSCA 8(d) are tabulated for the nominator to facilitate identification and review of submissions that appear to be identical to testing recommendations or that appear to indicate a potential concern related to toxicity, exposure or persistence.

The May 17, 1989 ITC meeting during which the Committee discussed the 166 substantially produced chemicals was a planning meeting that was attended by industry and the Chemical Manufactures Association (CMA). After the meeting, CMA requested and received permission to make their members aware of the list of 166 substantially produced chemicals. CMA published the list of 166 substantially produced chemicals in their first issue of CHEMSTAR news with a suggestion that their members submit any unpublished data to the Committee (Ref. 1, CMA, 1989). In response to this suggestion, the Committee received a CBI submission for one chemical. The chemical for which the submission was received was one for which CMA had established a panel of representatives from member companies.

Analysis of the 166 substantially produced chemicals identified by the Committee's computerized system revealed that many chemicals did not have minimum health effects data; 51 chemicals had no subchronic toxicity data. A few of these 51 chemicals had no acute toxicity data; less than onethird of these 51 chemicals had mutagenicity data; most of these 51 chemicals had no reproductive effects, developmental toxicity, chronic toxicity, oncogenicity or neurotoxicity data. At least 22 of these 51 chemicals had NOES information indicating potential exposure to ≥ 1,000 workers; 21 of these 51 chemicals had vapor pressures ≥ 0.1 mmHg at ambient temperature indicating potential for accidental release and 9 of these 51 chemicals had octanol-water partition coefficients ≧ 1,000 indicating bioconcentration/ bioaccumulation potential. At the Committee's request, the EPA's Exposure Assessment Branch estimated the persistence of these 51 chemicals as

well as their potential consumer exposure. Also at the Committee's request, the EPA's Structure Activity Team reviewed available information on these 51 chemicals and expressed at least moderate concerns for the potential of these chemicals to cause adverse effects. Moderate concerns result when there is suggestive evidence in animal studies of mutagenicity, reproductive effects, developmental toxicity, chronic toxicity, oncogenicity or neurotoxicity or there is close homology (structural, functional or mechanistic) to chemicals with known toxicity. At the Committee's request, the EPA's Environmental Effects Branch also reviewed available information on these 51 chemicals and identified a number of testing information deficiencies related to aquatic toxicity. These individual evaluations and more comprehensive analyses of the Toxic **Substances Control Act Test** Submissions database, ITC Member Agency computer files and recently developed OECD SIDS dossiers revealed that subchronic toxicity data were available for 8 chemicals. After the individual evaluations and more comprehensive analyses, subchronic toxicity data could still not be located for 43 chemicals. An additional 8 chemicals for which no subchronic toxicity data were available are not being recommended at this time for subchronic toxicity testing, because these chemicals were recommended for other testing and the Committee wants an opportunity to review the TSCA section 8(d) health and safety study submissions and determine if they include subchronic toxicity studies, before recommending subchronic toxicity testing. The Committee is recommending 35 substantially produced chemicals only for subchronic toxicity testing at this time, because it wants an opportunity to evaluate the production and exposure information and the health and safety studies that will be submitted under TSCA sections 8(a) and 8(d), respectively. The Committee believes that after evaluation of the TSCA 8(a) and 8(d) information, . they will be able to make further recommendations as to which of these 35 chemicals EPA should add to a subchronic toxicity testing listing rule and which of these chemical should be referred to others (e.g., NTP, OECD, etc.) with an option for testing. Information available to the Committee indicates that each of the 35 chemicals is substantially produced in volumes ranging from 1 million to 10 billion pounds per annum, but actual production volumes are CBI.

Summary of recommended studies. The substantially produced chemicals briefly described below and listed in the paragraph following Table 1 are recommended for subchronic toxicity testing.

p.p-Oxybis(benzenesulfonylhydrazide). A search for physical/chemical property data revealed a measured melting (decomposition) point of 160–161 degrees centigrade. It is used as a blowing agent for rubber and expanded plastics. There are considerable potential occupational exposures (NOES = 1494 workers) as well as potential inhalation/dermal consumer exposures. There are moderate concerns for potential adverse effects and it was mutagenic in Salmonella and caused unscheduled DNA synthesis in cultured cells.

Naphthalenedicarboxylic anhydride. A search for physical/chemical property data revealed a measured melting point of 267–269 degrees centigrade and a measured boiling point of 422 degrees centigrade. It is used as an intermediate for dyes, pigments, fluorescent whiteners and pesticides. It was in a class of anhydrides that NCI reviewed.

2-Ethylanthraquinone. A search for physical/chemical property data revealed a measured melting point of 108-111 degrees centigrade. It is used in chemical synthesis. There are potential occupational exposures (NOES = 483 workers) and moderate concerns for adverse effects. The LD₅₀ value in mice was 200 mg/kg.

7-Amino-4-hydroxy-2naphthalenesulfonic acid. A search for physical/chemical property data revealed none. It is used in onecomponent dry diazo copying process. There are potential occupational exposures (NOES = 737 workers) and potential dermal consumer exposures during changing of ink in copying machines. There are moderate concerns for potential adverse effects.

1-Naphthol. A search for physical/ chemical property data revealed a measured melting point of 96 degrees centigrade, a measured boiling point of 288 degrees centigrade, and a measured water solubility of 866 mg/L. It is used as an intermediate for pesticides, drugs and dyes and in synthetic perfumes. There are substantial potential occupational exposures (NOES = 57,116 workers) as well as potential consumer exposures. There are moderate concerns for potential adverse effects; it was mutagenic in Salmonella and bacterial DNA repair assays. The LD50 values in guinea pigs, rabbits, cats, mice and rats

were 2, 9, 134, 275, and 2,400 mg/kg,

respectively.

3-Hydroxy-2-naphthoic acid. A search for physical/chemical property data revealed a measured melting point of 222-223 degrees centigrade. It is used in dyes and pigments. There are considerable potential occupational exposures (NOES = 1641 workers) and potential dermal consumer exposures. There are moderate concerns for potential adverse effects; the LD50 value

in mice was 800 mg/kg.
Triethylene glycol bis(2ethylhexanoate). A search for physical/ chemical property data revealed a measured boiling point of 219 degrees centigrade at 5 torr. It is used as a plasticizer. There are moderate concerns for potential adverse effects; LD50 values in guinea pigs and rats were 21 and 31

mg/kg, respectively.

2-(4-Morpholinyldithio)benzothiazole. A search for physical/ chemical property data revealed none. It is used as an accelerator in rubber processing. There are potential occupational exposures (NOES = 174 workers) and moderate concerns for

adverse effects.

N-butylacrylate. A search for physical/chemical property data revealed a measured melting point of 50 degrees centigrade, a measured boiling point of 160 degrees centigrade, and a measured vapor pressure of 2 mmHg at 20 degrees centigrade. It is used as a monomer for resins, and in solvent coatings, adhesives, oil additives, emulsions for textiles, leathers and paper finishing. There are considerable potential occupational exposures (NOES = 5,136 workers) and potential dermal consumer exposures. There are moderate concerns for potential adverse effects; lowest threshold doses of 2304 and 690 mg/kg were reported for days 5 and 15, respectively, during a rat developmental toxicity study.

m-Benzenedisulfonic acid. A search for physical/chemical property data revealed a measured melting point of 137 degrees centigrade. It is used as an intermediate in resorcinol production and as a nitration catalyst in mononitrotoluene synthesis. There are potential occupational exposures (NOES = 56 workers) and moderate concerns

for adverse effects.

3.4-Dichloronitrobenzene. A search for physical/chemical property data revealed a measured melting point of 40-42 degrees centigrade, a measured boiling point of 257-258 degrees centigrade, and a measured water solubility of 0.63 mg/L. It is used as a pesticide intermediate. There are moderate concerns for potential adverse effects; it was a positive mutagen in

Salmonella and Drosophila. The LD50 value in mice was 1,384 mg/kg.

Isophthaloyl chloride. A search for physical/chemical property data revealed a measured melting point of 43-44 degrees centigrade and a measured boiling point of 276 degrees centigrade. It is used as an intermediate for dyes, synthetic fibers, resins, films, protective coatings and laboratory reagents. There are potential occupational exposures (NOES = 46 workers) and moderate concerns for adverse effects. The LD50 value in mice was 2,200 mg/kg.

Terephthaloyl chloride. A search for physical/chemical property data revealed a measured melting point of 79-81 degrees centigrade and a measured boiling point of 259 degrees centigrade. It is used as an intermediate for plasticizers, resins and polymers. There are potential occupational exposure (NOES = 212 workers) and moderate concerns for adverse effects. The LD50 value in mice was 2,140 mg/kg.

4-Ethoxynitrobenzene. A search for physical/chemical property data revealed a measured melting point of 60 degrees centigrade and a measured boiling point of 283 degrees centigrade. It is used to manufacture dyes and intermediates. There are potential occupational exposures (NOES = 207 workers) and moderate concerns for adverse effects. It produced positive results in a Salmonella assay, a Drosophila dominant lethal assay, a bacterial DNA test and a rat cytogenetic study. The LD₅₀ value in rats was 2,100 mg/kg.

Acetoacetanilide. A search for physical/chemical property data revealed a measured melting point of 85-86 degrees centigrade. It is used as a dyestuff intermediate, in organic synthesis and in rubber compounding. There are considerable potential occupational exposure (NOES = 1108 workers) and moderate concerns for adverse effects. The LD50 value in mice

was 3,400 mg/kg.

Butyric anhydride. A search for physical/chemical property data revealed a measured melting point of -75 degrees centigrade and a measured boiling point of 200 degrees centigrade. It is used to manufacture butyrates, drugs and tanning agents. There are considerable potential occupational exposures (NOES = 4,817 workers) and moderate concerns for adverse effects. The LD₅₀ value in mice was 2,000 mg/kg. It was in a class of anhydrides that NCI reviewed.

Isobutyl acrylate. A search for physical/chemical property data revealed a measured boiling point of 61-63 degrees centigrade, a measured water solubility of 1800 mg/L and a measured vapor pressure of 10.7 mmHg at 20 degrees centigrade. It is used in synthesis of acrylic ester polymers. There are moderate concerns for adverse effects. The LC50 value in rats was 2,000 ppm.

Diethylene glycol dimethylether. A search for physical/chemical property data revealed a measured melting point of -68 degrees centigrade and a measured boiling point of 162 degrees centigrade. It is used as a solvent and in reaction medium for grignard and similar syntheses. There are potential occupational exposures (NOES = 207 workers) and moderate concerns for adverse effects. It was positive in a sperm morphology test and a dominant lethal test and caused adverse reproductive and developmental effects during short-term studies. The LD50 value in mice was 2,978 mg/kg.

Carbinol acetate. A search for physical/chemical property data revealed a measured melting point of -25 degrees centigrade, a measured boiling point of 217 degrees centigrade and a measured vapor pressure of 0.1 mmHg at 20 degrees centigrade. It is used as a solvent for cellulose esters, gums and resins and to manufacture coatings, lacquers and printing inks. There are considerable potential occupational exposures (NOES = 7,649 workers) and moderate concerns for adverse effects and potential consumer exposures.

Bromamine acid. A search for physical/chemical property data revealed none. It is used as a dye intermediate. There are potential occupational exposures (NOES = 737 workers) and moderate concerns for

adverse effects.

4-Methyl-2-nitrophenol. A search for physical/chemical property data revealed a measured melting point of 108 degrees centigrade and a measured boiling point of 234 degrees centigrade. It is used to manufacture dyes. There are moderate concerns for adverse effects. The LD50 value in rats was 3,360

4-(Acetylamino) benzenesulfonyl chloride. A search for physical/chemical property data revealed a measured melting point of 149 degrees centigrade. It is used to manufacture sulfa drugs. There are considerable potential occupational exposures (NOES = 1,481 workers) and moderate concerns for

adverse effects.

2,4-Pentanedione. A search for physical/chemical property data revealed a measured melting point of -23 degrees centigrade, a measured boiling point of 141 degrees centigrade, a measured water solubility of 125,000

mg/L and a measured vapor pressure of 1.3 mmHg at 25 degrees centigrade. It is used as a solvent for cellulose acetate, a chelating agent for metals, as a lubricant additive and in paint dryers. There are considerable potential occupational exposures (NOES = 4,841 workers) and high concerns for adverse effects. It was mutagenic in chinese hamster ovary cells. The LDso value in rats was 1,000 ppm. EPA proposed a Significant New Use Rule based on reported neurotoxicity and production of a nervous system disorder that is characterized by an irreversible cerebellar syndrome in experimental animals, genotoxic effects and reported contact dermatitis and urticaria in humans (Ref. 2, EPA, 1989). In response to this proposal, Union Carbide submitted public comments and publications and reported that 2,4pentanedione produced a "slight dominant lethal effect at the spermatid stage of spermatogenesis" and "no embryotoxicity or teratogenicity" to Fischer 344 rats (Ref. 3, Union Carbide,

Propanoic anhydride. A search for physical/chemical property data revealed a measured melting point of -45 degrees centigrade and a measured boiling point of 167-169 degrees centigrade. It is used as an esterifying agent for fats, oils, cellulose and a dehydrating medium for nitrations and sulfonations, alkyd resins, dyestuffs, and pharmaceuticals. There are potential occupational exposures (NOES = 489 workers) and moderate concerns for adverse effects. The LD50 value in rats was 2,360 mg/kg. It was in a class of anhydrides that NCI reviewed.

Bis(2-ethylhexyl)-2-butenedioate. A search for physical/chemical property data revealed a measured boiling point of 209 degrees centigrade. It is used in emulsions and copolymerized with vinyl acetate. There are considerable potential occupational exposures (NOES = 3,352 workers) and moderate concerns for adverse effects.

Perfluorotributylamine. A search for physical/chemical property data revealed a measured boiling point of 177.

degrees centigrade. It is used in inert fluids and as a solvent. There are slight potential occupational exposures (NOES = 7 workers) and moderate concerns for adverse effects. The LD₅₀ value in mice was 1,200 mg/kg.

Perfluoro-N-hexane. A search for physical/chemical property data revealed a measured melting point of -4 degrees centigrade and a measured boiling point of 57 degrees centigrade. It is used in liquid fluorocarbons.

Trichloromethanesulfenyl chloride. A search for physical/chemical property data revealed a measured boiling point of 148–149 degrees centigrade and a measured vapor pressure of 0.6 mmHg at 20 degrees centigrade. It is used in the synthesis of lubricant additives. There are considerable potential occupational exposures (NOES = 7,790 workers) and moderate concerns for adverse effects. It was a positive mutagen in a bacterial DNA assay. The LD50 value in rats was 8 mg/kg.

1,2-Dichlorobutane. A search for physical/chemical property data revealed a measured boiling point of 124 degrees centigrade and a measured vapor pressure of 2.7 mmHg at 25 degrees centigrade. It is used as a butadiene intermediate. There are moderate concerns for adverse effects.

1,3-Dicyanobenzene. A search for physical/chemical property data revealed a measured melting point of 160-162 degrees centigrade. It is used as an intermediate for amines, synthetic fibers, agricultural chemicals, rust inhibitors and pharmaceuticals. There are potential occupational exposures (NOES = 208 workers) and moderate concerns for adverse effects. The LD₅₀ value in mice was 178 mg/kg.

3,4-Dichlorobutene. A search for physical/chemical property data revealed a measured melting point of -61 degrees centigrade, a measured boiling point of 115-117 degrees centigrade and a measured vapor pressure of 3.5 mmHg at 25 degrees centigrade. It is used as chloroprene and adiponitrile intermediates. There are moderate concerns for adverse effects. The LD₅o value in mice was 724 mg/kg. It was

positive in Salmonella and in vivo cytogenetics assays.

2-(2-Aminoethoxy)-ethanol. A search for physical/chemical property data revealed a measured melting point of -13 degrees centigrade and a measured boiling point of 221 degrees centigrade. It is used to remove acid components from gases. There are considerable potential occupational exposures (NOES = 5,579 workers) and moderate concerns for adverse effects. The LD₅₀ value in rats was 5,660 mg/kg.

Quinacridone. A search for physical/chemical property data revealed none. It is used as a dye and pigment. There are substantial potential occupational exposures (NOES = 23,292 workers) and moderate concerns for adverse

Ammonium carbamate. A search for physical/chemical property data revealed a measured melting point of 133-134 degrees centigrade. It is used in urea manufacture.

Hexa(methoxymethyl) melamine. A search for physical/chemical property data revealed none. It is used during leather manufacturing, rubber bonding and to produce polyester powder coatings. There are substantial potential occupational exposures (NOES = 18,033 workers). The LD50 value in mice was 550 mg/kg.

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