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# Bibliography of Work on the Heterogenous Photocatalytic Removal of Hazardous Compounds from Water and Air Update Number 2 To October 1996

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National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401-3393
A national laboratory of the U.S. Department of Energy
Operated by Midwest Research Institute
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# Summary

The Solar Industrial Program, funded by the United States Department of Energy, has developed processes that destroy hazardous substances in or remove them from water and air. This work was done by the National Renewable Energy Laboratory in Golden, CO, and Sandia National Laboratory in Albuquerque, NM, and by their subcontractors at universities and small or large businesses. The processes of interest in this report are based on the application of heterogeneous photocatalysts, principally titanium dioxide or modifications thereof, but work on other heterogeneous catalysts is included in this compilation.

This report continues bibliographies that were published in May, 1994, and October, 1995. The author compiles published work on the photocatalytic oxidation and reduction of organic or inorganic compounds in air or water. The previous reports included 663 and 574 citations, respectively. This update contains an additional 518 references. These were published during the period from June 1995 to October 1996, or are references from prior years that were not included in the previous reports. The work generally focuses on removing hazardous contaminants from air or water to meet environmental or health regulations. This report also references work on properties of semiconductor photocatalysts and applications of photocatalytic chemistry in organic synthesis. This report follows the same organization as the previous publications. The first part provides citations for work done in a few broad categories that are generic to the process. Three tables provide references to work on specific substances. The first table lists organic compounds that are included in various lists of hazardous substances identified by the United States Environmental Protection Agency (EPA). The second table lists compounds not included in those categories, but which have been treated in a photocatalytic process. The third table covers inorganic compounds that are on EPA lists of hazardous materials or that have been treated by a photocatalytic process. A short update on companies that are active in providing products or services based on photocatalytic processes is provided.

# Table of Contents

# 1.0 Introduction

This update in combination with the previous reports[1],[2] provides a comprehensive bibliography of work available in the open literature for scientists and engineers interested in the use of heterogeneous photocatalytic oxidation or reduction processes in environmental remediation, process emission control, indoor air quality, or other applications. The combined bibliographies include more than 1700 citations to work published between 1970 and the third quarter of 1996. The literature cited includes United States and foreign patents. Information was compiled by manually scanning the literature and searching commercial databases. This update includes about 150 citations to work done prior to 1995 that were not included in the earlier reports. Some citations have doubtless been missed and topics covered in certain papers may not have been identified and covered in every appropriate category. The author is grateful to the many people who have sent references and reprints of their work. Coverage is limited to heterogeneous processes except in a few cases where review material for homogeneous processes is relevant to heterogeneous photocatalytic chemistry. The author invites readers to send references to relevant work that appeared before 1996 that has been missed to the mail or e-mail address included in Section 5.1 of this report.

The photocatalytic oxidation of organic compounds in water has received the most attention but there is a rapidly increasing amount of work on the oxidation of volatile organic or inorganic compounds in the gas phase. Photocatalytic reduction of both organic compounds and metal-containing ions is also receiving increasing attention.

It is widely observed that intermediates and by-products are often formed that persist in the treated stream. These can include acids, oxygenated compounds, and carbon monoxide. The nature of the intermediates is increasingly being used to reveal details of the chemical mechanism of the photocatalytic process. The net process involves oxidizing the organic compound to an intermediate stage of oxygen content or to

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[1]Blake, Daniel M. (1994). *Bibliography of Work on the Photocatalytic Removal of Hazardous Compounds from Water and Air.* NREL/TP-430-6084. Golden, CO: National Renewable Energy Laboratory. 75 pp. [DE94006906] Available from the National Technical Information Service, Springfield, VA 22161.

[2]Blake, Daniel M. (1995). *Bibliography of Work on the Photocatalytic Removal of Hazardous Compounds from Water and Air. Update Number 1, to June, 1995.* NREL/TP-473-20300. Golden, CO: National Renewable Energy Laboratory. 102 pp. [DE95013148] Available from the National Technical Information Service, Springfield, VA 22161.

carbon dioxide, water, and a mineral acid (if a heteroatom such as nitrogen or chlorine is present). Other oxidizing agents may be substituted for oxygen. Certain metal ions can be modified or removed from water when the ions replace oxygen as the electron acceptor in the process and sacrificial electron donor compounds are provided.

Reference to test work on more than 270 compounds is included in the tables in Section 3. The most-studied compounds are phenol derivatives, BTEX (benzene, toluene, ethyl benzene, and xylene) components found in fuel spills, and chlorinated solvents such as trichloroethylene and chloroform. Test work reports that a significant number of pesticides, dye compounds, and surfactants can be completely oxidized (mineralized), and a variety of bacteria and viruses have been killed by irradiation with near-ultraviolet light in the presence of titanium dioxide. The breadth of work attests to the very wide range of applications that are being evaluated for the technology.

The section on companies active in the field notes only additions and changes that have occurred since the last report.[2] The high level of participation of Japanese companies in the Second International Conference on $TiO_2$ Photocatalytic Purification and Treatment of Water and Air[3] and the numerous patents assigned to Japanese companies indicate a high level of activity in that country. However, the author has little information on the individual companies that may be active in this field in Japan.

The following sections discuss reviews written on various aspects of the technology, work in developing and testing photocatalysts and oxidants, engineering issues, other topics, patents, and companies active in bringing photocatalytic processes or services to the marketplace. These sections, which include information that can apply to a range of applications, are followed by tables listing references to work performed on specific substances. References to work on systems in which the compound to be treated is carried in the gas phase are indicated by the suffix "g" in the citation number.

[3]Al-Ekabi, Hussain, *Abstracts of the Second International Conference on $TiO_2$ Photocatalytic Purification and Treatment of Water and Air*, Cincinnati, OH, October 26-29, 1996, Science and Technology Integration, Inc., London, ON.

# 2.0 Generic Information

This section refers to work that pertains to the field of photocatalytic processes.

## 2.1 Reviews and Articles

Reviews describe many aspects of photocatalytic chemistry and technology. This section also includes reviews written in the years prior to 1995 that were not cited in the previous reports. Reviews covering the broad topics given can be found in the following:

Semiconductors and supports - 120, 362, 368, 369, 370, 371, 396, 495, and 506; methodology for comparing reaction systems - 396, 424, and 446; mechanisms/activity - 165, 173, 174, 179, 231, 277, 365, 366, 367, 368, 398, 425, 435, and 439; nanocrystalline semiconductors - 165, 231, and 233; photoelectrochemical systems - 113 and 115; photocatalysis - 46, 47, 104, 105, 106, 107, 113, 114, 115, 119, 121, 127, 132, 146, 157, 173, 231, 365, 366, 367, 368, 372, and 506; solar processes - 112, 355, and 461g; companies active in the field - 16; adsorption - 78; disinfection - 17, 167, 269, 330g, and 489; water treatment - 30, 269, and 297; indoor air quality - 17, 324, 326, 330g, 438g, and 450g; environmental applications - 112, 144, 145, 166, 173, 174, 179, 250, 386, 412, and 461g; energy storage - 193; preparation and applications of semiconductor thin films - 232, 233, and 250; organic synthesis - 372; intercalation compounds - 350; oxidation of phenols - 414 and 435; comparison of advanced oxidation processes - 109, 269, and 406; issues and questions in application of photocatalysis - 355, 412, and 494; reactors - 259; problems of immobilization of catalyst - 45; photocatalytic ammonia synthesis - 52 and 84; activation of oxygen - 103; charge injection into semiconductor particles - 110, 111, 116, 117, and 118; and activating $TiO_2$ with visible light - 217.

## 2.2 Photocatalysts

The nature of the photocatalyst determines the rate and efficiency of the process. The anatase form of titanium dioxide has the desirable properties of being chemically stable, readily available, and active as a catalyst for oxidation processes. The 3.2 eV band gap matches the output of a wide variety of readily available lamps but is not ideal for solar applications. The photoefficiency for reaction of hazardous molecules is generally rather low, particularly for the aqueous-phase processes. Considerable work has been directed toward modifying $TiO_2$ and testing other semiconductors to identify ways to increase process efficiency and to improve the overlap of the absorption spectrum of the photocatalyst with the solar spectrum. This work is broken down into a few broad categories and covered in the references cited.

### 2.2.1 Modified Titanium Dioxide

Titanium dioxide and modified forms, including different commercially available forms, heat treated materials, and materials prepared by a range of techniques:

sol-gel - 2, 3, 13, 14, 21, 91, 164, 212, 239, 241, 253, 254, 311, 316, 336, 343g, 388, 397g, 429, 492, and 508; controlled hydrolysis of $TiCl_4$ - 423; heat treatment - 65, 164, and 252; colloidal or quantized particles - 51, 67, 68, 96, 102, 291, 337, 407, 419, 420, 421, and 453; xerogel/aerogel - 2, 3, 246, 317, and 470; flame synthesis - 77 and 381; or catalysts from different vendors - 35, 51, 285, 334, 389, 413, 424, and 446; spray pyrolysis - 44 and 77; impregnation - 44 and 67; co-precipitation - 44 and 67; microemulsion - 68; reduction - 183; rutile - 432g; potassium pillared layered titanate - 318 and 319; cysteine - 387; and surface modification - 462.

### 2.2.2 Hydrophobic Surface Treatment

No new work was identified in this area.

### 2.2.3 Dye Sensitized Titanium Dioxide

Sensitizers have been used in conjunction with titanium dioxide to improve the response to visible light:

ruthenium complexes - 38, 99, 235, 364, and 476; vanadium(+5) complexes - 41; cobalt(+2) complexes - 31; nickel(+2) complexes - 31; copper(+2) complexes - 31; cobalt(+3) complexes - 40; metal phthalocyanine - 43 and 266; organic dyes - 38, 266, and 278; poly-(10-substituted-2-(9-enthral) ethylmethacrylates) - 122; polypyrrole - 507; or erythrosin B - 234.

### 2.2.4 Metal Ion Doping of Titanium Dioxide or Mixed Oxides

Other metal ions have been introduced into the titanium dioxide lattice to modify the properties. They are covered in the following:

Al - 13; Si - 2, 3, 13, 14, 21, 33, 55, 139, and 329g; V - 39, 190, 407, and 423; Cr - 195, 200, 370, 407, and 423; Fe - 44, 51, 96, 340, 342, 407, and 423; Co - 39; Cu - 69; Ga - 182, 185, 187, and 474g; Zr - 139; Nb - 182, 185, 187, and 474g; Mo - 92; Ce - 55; or W - 92, 299, and 329g.

### 2.2.5 Metallized Titanium Dioxide

Noble metals have been deposited on the titanium dioxide surface to enhance catalytic activity:

Ni - 73, 172, 180, 181, 378, and 380; Rh - 98, 172, 178, 180, and 181; Pd - 146, 156, 218, and 398; Pt - 22, 32, 73g, 74g, 76g, 89, 98, 140g, 172, 175, 176, 178, 180, 181, 191, 192, 194, 197, 201, 278, 287g, 298, 310, 316, 370, 371, 376, 378, 380, 398, 457, 486, 510, and 514; Ag - 198, 199, 226, and 251; Au - 32 and 198; Pt/Rh - 199; Ag/Rh - 199; or Pt/Pd - 199.

### 2.2.6 Other Semiconductors

A wide range of other semiconductors and other materials have been tested for photocatalytic activity. In general they have been found to be less active than titanium dioxide. Relevant work is cited in the following:

$Al_2O_3$ - 60g and 237; $V_2O_5$ - 196g and 375g; $Fe_2O_3$ - 60g, 158, 159, 160, 200, and 402; ZnO - 9, 22, 99, 196g, 200, 202, 237, 375g, 393, 402, and 426; Zn - or CdS - 265, 402, and 486; Pt/CdS - 486; ZnTe - 298; $ZrO_2$ - 133, 196g, 200, 339, and 375g; $ZrTiO_4$ - 75, 339, and 241; $MoS_2$ - 298; $SnO_2$ - 33, 99, 122, 133, 196g, 230, 375g, and 475; $Sb_2O_4$ - 196g, 200, and 375g; $Sn/SbO_2$ - 375g; $CeO_2$ - 196g, 200, and 375g; $WO_3$ - 123, 196g, 200, 202, and 375g; $Nb_2O_5$ - 26; fly ash - 160; furnace slag or core sands - 70; polyaniline - 59; poly(p-phenylene) - 472g; polythiocyanogen - 472g; muscovite - 160; or natural minerals - 134 and 158.

### 2.2.7 Immobilized Photocatalysts

Most experimental work on aqueous systems has used fine particles of photocatalyst suspended in the liquid phase. In a waste treatment application it would be simpler if the catalyst were immobilized in the photoreactor so the material would not have to be separated from the treated fluid in a subsequent process step. Most work on the treatment of gases has used immobilized catalyst. Titanium dioxide has been affixed to a variety of surfaces:

glass (including fibers) - 18, 21, 57, 97, 120, 141, 148g, 239, 252, 254, 255g, 307, 308, 311, 316, 327, 328, 331, 357, 358, 359, 383, 397, 427, 428, 429, 467, 473g, 477, 492, 502, and 514; silica - 49, 67, 326g, 405g, 458g, 463, 471, 498, and 514; metal - 97, 163, 164, 331, 514, and 518; clays - 67 and 120; polymer - 6, 7, 15, 120, 262, 265, 331, 459g, 464, 482, and 483; thin films - 23, 120, 255g, 343g, 397g, 403, 441, 442, 443, and 493; internal light guide - 444; zeolite - 21, 53, 120, 254, 325, 458g, 471, 498, 501, 512, and 515; alumina - 458g and 498; carbon - 215, 216, 220g, 292, 458g, and 471; paper - 305 and 306g; Ambersorb - 514; PHOTOPERM™ - 39, 41, and 42; metal oxides and ceramics - 120, 147, 405g, and 459g; vesicles and micelles - 120; or silica coating on $TiO_2$ films - 441, 442, and 443.

## 2.3 Hydrogen Peroxide and Other Oxidants

Oxygen is the most commonly used oxidant, but other oxidants have been found to improve rates of reaction with a variety of organic substrates under some conditions. This work is covered in the following:

hydrogen peroxide - 9, 29, 35, 48, 206, 364, 373, 511, and 517; superoxide - 373; peroxydisulfate - 35, 303, and 313; chlorite - 303; chlorate - 303; bromate - 303 and 312; periodate - 303; or ozone - 26, 48, 304, 379, and 499.

## 2.4 Engineering Issues

In recent years the success of laboratory work has led to interest in applying the technology to environmental remediation and treatment of process waste streams. Literature now discusses scale-up of the process and resolution of engineering problems. Progress has been significant and many companies are now providing turn-key systems for treating contaminated water and air.

### *2.4.1 Reactor and System Design*

A number of papers address topics relevant to the design of reactors for photocatalytic processes:

photochemical reactors - 251, 252, 300, 301, and 310; non-concentrating reactor - 345 and 460g; parabolic trough - 50, 79, and 313; compound parabolic concentrator - 79; kinetic modeling - 300, 301, 405g, 497, and 513; fixed bed - 91 and 343; filtration - 491 and 508; controlled periodic illumination - 100, 416, 417, and 436; light scattering model - 4, 149; flat plate reactor - 28;

ceramic monolith - 405g; effectiveness factors for reactions in a planar membrane - 94; mass transfer limitations - 95 and 251; photocatalytic membrane reactor - 214; fiber optic cable reactor - 358 and 359; or field tests - 392g.

### *2.4.2 Systems Analysis*

As the technology for the photocatalytic treatment of contaminated air or water has progressed, some work on economic evaluation has appeared in the literature. However, there was limited new information during the last year:

process waste water - 379; or photon costs from lamps and sunlight - 48.

## 2.5 Miscellaneous Topics

This category includes papers of interest that do not fall into the preceding headings:

actinometry - 210; adsorption - 22, 292, 302, 320, 344g, 405g, 426g, and 443g; combined photocatalytic and biological treatment - 48; effect of applied voltage bias on photocatalytic reactions - 477, 478, and 479; non-aqueous solvent systems - 131, 135, 137, 228, 234, 235, 377, 396, 431, 436, and 486; application in chemical analysis - 1, 262, 445, and 457; polymer aging - 6, 7, and 152; photo initiators - 40; "inert" ion effect - 29, 51, 285, and 290; dissolved metal ion effect - 56, 66, 159, 290, 463, 511, and 517; comparison with other advanced oxidation processes - 51, 81, 364, 366, 379, and 418; purification of water for recycle in semiconductor fabs - 63; purification of drinking water - 64; photoelectrode - 71; organic synthesis - 108, 114, 119, 124, 125, 126, 127, 128, 132, 136, 228, 356, 377, 396, 486, and 496; surface science of $TiO_2$ - 150, 286g, and 287g; quantum yield as a function of particle size and light intensity - 151, 420, and 421; photoconductivity/electrical conductivity - 177, 184, 185, 186, 187, 196g, and 201; self cleaning surface - 357, 437, and 459; mixed waste - 418; or treatment of photographic processing effluents - 422.

## 2.6 Patents

The number of patents for aspects of photocatalytic technology has increased rapidly in the last decade. They cover a range of aqueous and gas-phase applications. The general topic of the patents are described in the following:

process for oxidation of hydrocarbons - 229; parts having photocatalytic function - 168, 169, 240, 241, 242, and 258; catalyst formulation - 15, 171, 238, 240, 241, 242, 244g, 258, 263, 268, 308, 327, 331, 336, 353, 360, 381, 399, 447, 449g, 454, 455, 467, 468, 470, 490, and 515; thin silica coating - 441; odor control - 335g; water treatment - 308, 347, 466, 505, and 514; water treatment system - 58, 142, 205, 270, and 447; painted bodies - 204 and 456; photocatalytic tiles - 222; photocatalyst on paper supports - 451 and 452; photocatalyst on flexible supports - 223; membrane for water purification - 279; regeneration of adsorbents - 24g and 449g; metals removal from water - 245; method for activity measurement - 348; removal of chlorinated compounds from air (includes scrubber) - 309g; removal of air pollutants (includes catalysts on exterior walls of buildings) - 24g, 25g, 141g, 143g, 148g, 215g, 238g, 242g, 258g, 308g, 449g, and 467; method for cleaning solid surface - 332; additive to enhance degradation of plastics in the environment - 352; deodorizing agents - 242 and 401; process for killing cells or disinfection - 93, 205, 354, and 448; methanol synthesis - 353; method for preparing hydrocarbons - 390; ethylene oxidation to preserve fruit and vegetables - 400; pigment additive - 55; slurry reactor configuration - 72; catalyst cleaning - 499; or plasma reactor - 500.

### 2.7. Companies Active in the Field

Research and development (R&D) and market assessment activity is underway at many companies in the United States but there is little change in the list of companies that have started business lines that use photocatalytic processes.[2]

The assets, in the field of photocatalytic oxidation, of IT Corporation, NEPCCO, and PHOTOX Corporation have been acquired by a new company, Zentox Corporation:

Zentox Corporation
Mr. J. Sandy Reese, President
2140 N.E. 36th Avenue
Ocala, FL 34470
Telephone: (352) 867-9706 Fax: (352) 867-1320
Products: Advanced oxidation, ozone treatment, electrocoagulation, low temperature distillation, and photocatalytic oxidation systems for groundwater remediation, industrial water treatment, and treatment of contaminated vapor streams for industrial, environmental, consumer, and medical applications.

Universal Air Technology, Inc.

Sanjeev K. Hingorani, Ph.D.

Sid Martin Biotechnology Development Institute

12085 Research Drive

Alachua, FL 32615

Telephone: (904)418-0661 Fax: (904) 462-0875

Products: Stand-alone and HVAC duct integrated products for indoor air disinfection using photocatalytic technology.

# 3.0 Compounds Studied

The tables in this section have the same format as in the first two reports. No compounds have been removed from the tables but new compounds have been added to the second table to incorporate new work. The list of the compounds included in various lists of priority pollutants, air toxics, and the toxic release inventory compiled by the EPA[4] provided the starting point for these tables. Table 1 lists compounds in the EPA categories; Table 2 lists organic compounds that are not in EPA lists; and Table 3 covers inorganic compounds in EPA lists or that have been treated by a photocatalytic process. The inorganic compounds are arranged by element unless a significant number of citations referred to work on a specific ion or compound. Formulas of compounds, when given, are not in the standard format because the software used to prepare the tables does not support subscripts. A few broad categories are included in Table 2 that reflect new applications: bacteria, algae, and virus; coal or carbon; adsorbable organic halides (AOX); color or chemical oxygen demand (COD); and oil or petroleum, for example. In these tables the citation suffix "g" indicates a gas-phase study. The treatability of compounds that have not been tested can usually be inferred from results for related compounds in the tables.

[4]"Notice of the Second Priority List of Hazardous Substances Commonly Found at Superfund Sites," *Environmental Reporter*, October 28, 1988, 1255-1260.

Table 1. Organic Compounds in EPA Lists of Priority Pollutants, Air Toxics, or Toxic Release Inventory

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| 1,1,1-Trichloroethane | CHCl2CH2Cl | Cl | | 206,392g |
| 1,1,2,2-Tetrachloroethane | CHCl2CHCl2 | Cl | | 206 |
| 1,1,2-Trichloroethane | CHCl2CH2Cl | Cl | | 206 |
| 1,1,2-Trichloro-1,2,2-trifluoroethane | CCl2FCClF2 | Cl,F | | |
| 1,1-Dichloroethane | CH3CHCl2 | Cl | | 206 |
| 1,1-Dimethyl hydrazine | (CH3)2NNH2 | | N | |
| 1,2,3-Trichloropropane | CH2ClCHClCH2Cl | Cl | | |
| 1,2,4-Trichlorobenzene | C6H3Cl3 | Cl | | |
| 1,2,4-Trimethylbenzene | C6H3(CH3)3 | | | |
| 1,2-Butylene oxide | H2COCHCH2CH3 | | | |
| 1,2-Dibromoethane | BrCH2CH2Br | Br | | |
| 1,2-Dibromo-3-chloropropane (DBCP) | CH2BrCHBrCH2Cl | Br,Cl | | |
| 1,2-Dichlorobenzene | C6H4Cl2 | Cl | | |
| 1,2-Dichloroethane | ClCH2CH2Cl | Cl | | 206,257g |
| 1,2-Dichloroethylene | ClHC:CHCl | Cl | | 206,392g |
| 1,2-Dichloropropane | CH3CHClCH2Cl | Cl | | |
| 1,2-Dinitrotoluene | C6H3CH3(NO2)2 | | N | |
| 1,2-Diphenylhydrazine | C12H12N2 | | N | |
| 1,2-Trans-dichloroethene | C2H2Cl2 | Cl | | |
| 1,3,5-Trinitrobenzene | C6H3(NO2)3 | | N | 87,408 |
| 1,3-Butadiene | H2C:CHHC:CH2 | | | |
| 1,3-Dichlorobenzene | C6H4Cl | Cl | | |
| 1,3-Dichloropropene | CHCl:CHCH2Cl | Cl | | |
| 1,4-Dichlorobenzene | C6H4Cl2 | Cl | | 292 |
| 1,4-Dioxane | OCH2CH2OCH2CH2 | | | |
| 1-Amino-2-methylanthraquinone | C6H4[C(O)]2C6H2NH2CH3 | | | |
| 1-Bromo-4-phenyoxybenzene | p-BrC6H4OC6H5 | Br | | |
| 2,2,4-Trimethylpentane | (CH3)3C5H9 | | | |
| 2,3,7,8-Tetrachlorodibenzo-p-dioxin | C12H4Cl4O2 | Cl | | |
| 2,4,5-Trichlorophenoxyacetic acid | C6H2Cl3OCH2CO2H | Cl | | 333 |
| 2,4,5-TP acid (silvex) | Cl3C6H2OCH(CH3)COOH | Cl | | |
| 2,4,5-Trichlorophenol | C6H2Cl3OH | Cl | | 26,82,208 |
| 2,4,6-Trichlorophenol | C6H2Cl3OH | Cl | | 82,208 |
| 2,4,6-Trinitrotoluene | CH3C6H2(NO2)3 | | | 48,87,408,408,409,410,411 |
| 2,4 Diaminoanisole | (NH2)2C6H3OCH3 | | N | |
| 2,4-Dichlorophenoxyacetic acid (2,4-D) | Cl2C6H3OCH2COOH | Cl | | 81,294,333,364,389,440 |
| 2,4-Diaminoanisole sulfate | (NH2)2C6H3OCH3.H2SO4 | | N | |
| 2,4-Dichlorophenol | Cl2C6H3OH | Cl | | 82,247,511 |
| 2,4-Dimethylphenol | (CH3)2C6H3OH | | | 465 |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| 2,4-Dinitrophenol | C6H3OH(NO2)2 | | N | |
| 2,4-Dinitrotoluene | C6H3CH3(NO2)2 | | | 87 |
| 2,4-Toluene diamine | CH3(NH2)2C6H3 | | N | |
| 2,6-Dinitrotoluene | C6H3CH3(NO2)2 | | N | 87 |
| 2,6-Xylidine | (CH3)2C6H3NH2 | | N | |
| 2-Acetylaminofluorene | CH3C(O)NHC6H3CH2C6H4 | F | N | |
| 2-Aminoanthraquinone | C6H4(CO)2C6H3NH2 | | N | |
| 2-Butanone | CH3COCH2CH3 | | | |
| 2-Chloroacetophenone | C6H5COCH2Cl | Cl | | |
| 2-Chloroethyl vinyl ether | CH2ClCH2OCHCH2 | Cl | | |
| 2-Chlorophenol | C6H4OHCl | Cl | | 59,82,267 |
| 2-Ethoxyethanol | H3CCH2OCH2CH2CH2OH | | | |
| 2-Methoxyethanol | MeOCH2CH2OH | | | |
| 2-Methylnaphthalene | C10H7CH3 | | | |
| 2-Nitrophenol | NO2C6H4OH | | N | 413,414 |
| 2-Nitropropane | CH3CHNO2CH3 | | N | |
| 2-Pentanone, 4-Methyl | CH3(CH2)2COCH3 | | | |
| 2-Phenylphenol | C6H5C6H4OH | | | |
| 3,3'-Dichlorobenzidine | C6H3ClNH2C6H3ClNH2 | Cl | N | |
| 3,3'-Dimethoxybenzidine | [C6H3(OCH3)NH2]2 | | N | |
| 3,3'-Dimethylbenzidine (o-Tolidine) | [C6H3(CH3)NH2]2 | | N | |
| 4,4'-Dichlorodiphenyldichloroethylene | (ClC6H4)2CCCl2 | Cl | | |
| 4,4'-Diaminodiphenyl ether | NH2(C6H4)2NH2 | | N | |
| 4,4'-Isopropylidenediphenol | (CH3)2C(C6H4OH)2 | | | |
| 4,4'-Methylenebis(N,N-dimethyl) benzenamine | C17H22N2 | | N | |
| 4,4'-Methylenedianiline | H2NC6H4CH2C6H4NH2 | | N | |
| 4,4'-Methylene-bis-(2-chloroaniline) | CH2(C6H4ClNH2)2 | Cl | N | |
| 4,4'-Thiodianiline | C12H12N2S | | S,N | |
| 4,6-Dinitro-o-cresol | CH3C6H2(NO2)2OH | | N | |
| 4,6-Dinitro-2-methylphenol | C7H6N2O5 | | N | |
| 4-Aminoazobenzene | C6H5NNC6H4NH2 | | N | |
| 4-Aminobiphenyl | C6H5C6H4NH2 | | N | |
| 4-Chloroaniline | ClC6H4NH2 | Cl | | |
| 4-Chlorophenyl phenyl ether | p-ClC6H4OC6H5 | Cl | | |
| 4-Dimethylaminoazobenzene | (CH3)2C6H3NH2 | | N | |
| 4-Methylphenol | p-CH3C6H4OH | | | |
| 4-Nitrobiphenyl | C6H5C6H4NO2 | | N | |
| 4-Nitrophenol | NO2C6H4OH | | N | 85,86,299,413,414 |
| 5-Nitro-o-anisidine | NO2C6H3(NH2)(OCH3) | | N | |
| Acenaphthene | C10H6(CH2)2 | | | |
| Acenaphthylene | C12H8 | | | |
| Acetaldehyde | CH3CHO | | | 158,305g,306g,343g,344g, |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| | | | | 397g,405g,432g,450g |
| Acetamide | CH3CNOH2 | | N | 293 |
| Acetone | CH3COCH3 | | | 282g,329g |
| Acetonitrile | CH3CN | | N | 282g,283,283g,284g |
| Acetophenone | CH3C(O)C6H5 | | | |
| Acrolein | CH2CHCHO | | | |
| Acrylamide | CH2CHCONH2 | | N | |
| Acrylic acid | H2C:CHCOOH | | | |
| Acrylonitrile | H2C:CHCN | | N | |
| Aldrin | C12H8Cl6 | Cl | | |
| Allyl chloride | H2C=CHCH2Cl | Cl | | |
| Aniline | C6H5NH2 | | N | |
| Anthracene | C6H4(CH)2C6H4 | | | 134 |
| Aramite | (CH3)3CC6H4OCH2CH(CH3)-SO3C2H4Cl | Cl | S | |
| Atrazine | C18H14ClN5 | Cl | N | 41,42,313,383 |
| Benzal chloride | C6H5CHCl2 | Cl | | |
| Benzamide | C6H5CONH2 | | N | 81 |
| Benzene | C6H6 | | | 140g,224g,282g,429 |
| Benzidine | NH2(C6H4)2NH2 | | N | |
| Benzoic acid | C6H5COOH | | | 160 |
| Benzoic trichloride | C6H5CCl3 | Cl | | |
| Benzoyl chloride | C6H5COCl | Cl | | |
| Benzoyl peroxide | (C6H5CO)2O2 | | | |
| Benzo(a)anthracene | C22H14 | | | |
| Benzo(a)pyrene | C20H12 | | | |
| Benzo(b)fluoranthene | C20H12 | | | |
| Benzo(g,h,i) perylene | C22H12 | | | |
| Benzyl alcohol | C6H5CH2OH | | | |
| Benzyl chloride | C6H5CH2Cl | Cl | | |
| BHC (Benzenehexachloride) | C6H6Cl6 | Cl | | |
| Biphenyl | C6H5C6H5 | | | |
| Bis(2-Chloroethoxy)methane | CH2(2-ClC2H5O)2 | Cl | | |
| Bis(2-chloroethyl) ether | ClCH2CH2OCH2CH2Cl | Cl | | |
| Bis(2-chloro-1-methylethyl) ether | [ClCH2(CH3)CH]2O | Cl | | |
| Bis(2-ethylhexyl) adipate | (C7H13)2C4H8(CO2)2 | | | |
| Bis(2-ethylhexyl)phthalate | (C4H9CH(CH2))2OOC | | | |
| Bis(chloromethyl)ether | (CH2Cl)O(CH2Cl) | Cl | | |
| Bromochloromethane | BrCH2Cl | Br,Cl | | |
| Bromodichloromethane | CHCl2Br | Cl,Br | | |
| Bromoethane | C2H5Br | Br | | |
| Bromoform (Tribromomethane) | CHBr3 | Br | | 43 |
| Bromomethane (Methyl bromide) | CH3Br | Br | | |

| Substance | Formula | Halogen | Het. Atom | Reference |
|---|---|---|---|---|
| Butyl acrylate | CH2:CHCOOC4H9 | | | |
| Butylbenzyl phthalate | C4H9OOCC6H4COOC7H7 | | | |
| Butyraldehyde | CH3(CH2)2CHO | | | |
| Calcium cyanamide | NCNCa | | N | |
| Caprolactam | CH2(CH2)4NHCO | | N | |
| Captan (N-Trichloromethylmercapto-tetrahydrophthalimide) | C9H8Cl3NO2S | Cl | N,S | |
| Carbaryl [1-Naphthalenol, methylcarbamate] | C10H7OOCNHCH3 | | N | |
| Carbon disulfide | CS2 | | S | |
| Carbon tetrachloride | CCl4 | Cl | | 206,282g,404g,513 |
| Carbonyl sulfide | COS | | | |
| Catechol | C6H4(OH)2 | | | 302 |
| Chloramben (Benzoic acid, 3-amino-2, 5-dichloro-) | C6H(CO2H)(NH2)Cl2 | Cl | N | |
| Chlordane | C10H6Cl8 | Cl | | |
| Chloroacetic acid | CH2ClCOOH | Cl | | 101 |
| Chlorobenzene | C6H5Cl | Cl | | |
| Chlorobenzilate (Benzeneacetic acid, 4-chloro-alpha-(4-chlorophenyl)-) | (C6H4Cl)2C(OH)COOC2H5 | Cl | | |
| Chlorodibenzodioxins, various | C12O2H8-xClx | Cl | | |
| Chlorodibenzofurans | C12OH8-xClx | Cl | | |
| Chlorodibromomethane | ClBr2CH | Br,Cl | | |
| Chlorodifluoromethane | CHClF2 | Cl,F | | |
| Chloroethane | C2H5Cl | Cl | | |
| Chloroform | CHCl3 | Cl | | 206,276,282g,300,301,404g |
| Chloromethane | CH3Cl | Cl | | |
| Chloromethyl methyl ether | C2H5ClO | Cl | | |
| Chloroprene | H2C:CHCCl:CH2 | Cl | | |
| Chlorothalonil (1,3-Benzendedicarbonitrile, 2,4,5,6-tetrachloro-) | C6Cl4(CN)2 | | N | 254 |
| Chrysene | C18H12 | | | |
| cis-1,2-Dichloroethylene | ClHC:CHCl | Cl | | |
| cis-1,3-Dichloropropene | CHCl:CHCH2Cl | Cl | | |
| o-,m-,p-Cresols | CH3C6H4OH | | | |
| Cumene | C6H5CH(CH3)2 | | | |
| Cumene hydroperoxide | C6H5C(CH3)2OOH | | | |
| Cupferron (Benzeneamine, N-hydroxy-N-nitrose, ammonium salt) | C6H5N(NO)ONH4 | | N | |
| Cyclohexane | C6H12 | | | 323,413 |
| Cyclohexanone | C6H10O | | | |
| Cyclonite (RDX) | (CH2)4(NNO2)4 | | N | 48 |
| Decabromodiphenyl oxide | (C6Br5)2O | Br | | |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Dialate [Carbamothioic acid, bis (1-methylethyl)-, S-(2,3-dichloro-2-propenyl) ester] | [(CH3)2CH]2NCOSCH2CClCHCl | Cl | N,S | |
| Diaminotoluene (mixed isomers) | CH3C6H3(NH2)2 | | N | |
| Diazomethane | CH2N2 | | N | |
| Dibenzofuran | C12H8O | | | |
| Dibenzo(a,h)anthracene | C22H14 | | | |
| Dibromochloropropane | CH2BrCHBrCH2Cl | Br,Cl | | |
| Dibutyl phthalate | C6H4(COOC4H9)2 | | | |
| Dichlorobenzene (mixed isomers) | C6H4Cl2 | Cl | | |
| Dichlorobromomethane | CHBrCl2 | Cl,Br | | |
| Dichlorodifluoromethane | CCl2F2 | Cl,F | | |
| Dichlorvos (Phosphoric acid, 2 dichloroethenyl dimethyl ester) | (CH3O)2P(O)OCH:CCl2 | Cl | P | 427,428,517 |
| Dicofol ,4,4'-Dichloro-alpha-trichloro-methylbenzhydrol | C14H9Cl5O | Cl | | |
| Dieldrin/aldrin | C12H10OPCl6 | Cl | P | |
| Diepoxybutane | C4H6O2 | | | |
| Diethanolamine | (HOCH2CH2)2NH | | N | |
| Diethyl phthalate | C6H4(CO2C2H5)2 | | | |
| Diethyl sulfate | (C2H5)2SO4 | | S | |
| Dimethyl aminoazobenzene | C6H5NNC6H4N(CH3)2 | | N | |
| Dimethyl formamide (DMF) | HCON(CH3)2 | | N | 293 |
| Dimethyl phthalate | C6H4(COOCH3)2 | | | |
| Dimethyl sulfate | (CH3)2SO4 | | S | |
| Dimethylcarbamyl chloride | (CH3)2NCOCl | Cl | N | |
| Disulfoton | (C2H5O)2P(S)SCH2CH2SCH2CH3 | | P,S | |
| Di-n-butyl phthalate | C6H4(COOC4H9)2 | | | |
| Di-n-octyl phthalate | C6H4(CO2)(n-C8H17)2 | | | |
| Di-(2-ethylhexy) phthalate (DEHP) | C6H4[COOCH2CH(C2H5)C4H9]2 | | | |
| Endosulfan | C9H6Cl6O3S | Cl | | |
| Endrin aldehyde/ endrin | (C12H8OCl6) | Cl | | |
| Epichlorohydrin | CH2OCHCH2Cl | Cl | | |
| Ethyl acrylate | CH2:CHCOOC2H5 | | | |
| Ethyl chloroformate | ClCOOC2H5 | Cl | | |
| Ethylbenzene | C6H5C2H5 | | | |
| Ethylene | H2C:CH2 | | | 493g |
| Ethylene glycol | CH2OHCH2OH | | | |
| Ethylene oxide | CH2CH2O | | | |
| Ethylene thiourea | NHCH2CH2NHCS | | N,S | |
| Ethyleneimine (Aziridine) | CH2NHCH2 | | N | |
| Fluometuron [Urea, N,N-dimethyl-N'-[3-(trifluoromethyl)phenyl]-] | C10H11F3N2O | F | N | |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Fluoranthene | C16H10 | | | |
| Fluorene | C6H4CH2C6H4 | | | |
| Fluorotrichloromethane | CCl3F | Cl,F | | |
| Formaldehyde | HCHO | | | 344g,405g |
| Heptachlor/heptachlor epoxide | C10H7Cl7 | Cl | | |
| Heptane | CH3(CH2)5CH3 | | | |
| Hexachlorobenzene | C6Cl6 | Cl | | |
| Hexachlorobutadiene | Cl2C:CClCCl:CCl2 | Cl | | |
| Hexachlorocyclopentadiene | C5Cl6 | Cl | | |
| Hexachloroethane | Cl3CCCl3 | Cl | | |
| Hexachloronaphthalene | C10H2Cl6 | Cl | | |
| Hexamethylphosphoramide | [(N(CH3)2]3PO | | P,N | |
| Hexamethylene-1,6-diisocyanate | OCN(CH2)6NCO | | N | |
| Hexane | CH3(CH2)4CH3 | | | |
| Hydroquinone | C6H4(OH)2 | | | 57 |
| Indeno(1,2,3-cd)pyrene | C22H12 | | | |
| Isophorone | C(O)CHC(CH3)CH2C(CH3)2CH2 | | | |
| Isopropyl alcohol | (CH3)2CHOH | | | 55,101,207,228,271,274g,282g 339,374,413 |
| Lindane (gamma-Benzenehexachloride) | C6H6Cl6 | Cl | | 161,280 |
| Malachite Green | C23H25ClN2 | Cl | N | |
| Malathion | (CH3O)2P(S)SCH(CO2C2H5)-CH2CO2C2H5 | | P,S | |
| Maleic anhydride | HC:CHC(O)OC(O) | | | |
| Maneb (Carbamodithioic acid, 1,2-ethanediylbis-,manganese complex) | (SSCNCH2CH2NHCSS)Mn | | N,S | |
| Mechlorethamine | CH3N(CH2CH2Cl)2 | Cl | N | |
| Melamine | H2NCNC(NH2)NC(NH2)N | | N | |
| Methanol | CH3OH | | | 207,228,274g,282g,283,283g, 344g,374,376,378,380,482, 483,510 |
| Methoxychlor | Cl3CCH(C6H4OCH3)2 | Cl | | |
| Methyl acrylate | CH2:CHCOOCH3 | | | |
| Methyl butyl ketone | CH3COC4H9 | | | |
| Methyl ethyl ketone | CH3COCH2CH3 | | | 513 |
| Methyl iodide | CH3I | I | | |
| Methyl isobutyl ketone | (CH3)2CHCOCH3 | | | |
| Methyl isocyanate | CH3NCO | | N | |
| Methyl methacrylate | CH2:C(CH3)COOCH3 | | | |
| Methyl tert-butyl ether | (CH3)3COCH | | | |
| Methylene bromide | CH2Br2 | Br | | |
| Methylene chloride | CH2Cl2 | Cl | | 206,282g,283,283g,404g |
| Methylenebis(phenylisocyanate) (MBI) | CH2(C6H4NCO)2 | | N | |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Methylhydrazine | CH3NHNH2 | | N | |
| Michler's ketone | CO[C6H4N(CH3)2]2 | | N | |
| Mirex | C10Cl12 | Cl | | |
| Mustard gas | S(CH3CH2Cl)2 | Cl | S | |
| m-Nitroaniline | NO2C6H4NH2 | | N | |
| N,N-Dimethylaniline | C6H5N(CH3)2 | | N | |
| Naphthalene | C10H8 | | | 158,160 |
| Naphthylamine (alpha-, beta-) | C10H7NH2 | | N | |
| Nitrilotriacetic acid | N(CH2COOH)3 | | N | |
| Nitrobenzene | C6H5NO2 | | N | 81,87,356 |
| Nitrofen [Benzene, 2,4-dichloro-1-(4-nitrophenoxy)-] | C12H7Cl2NO3 | Cl | N | |
| Nitrogen mustard (2-Chloro-N-(2-chloroethyl)-N-methylethanamine) | (ClCH2CH2)2NCH3 | Cl | N | |
| Nitroglycerin | CH2NO3CHNO3CH2NO3 | | N | 329g |
| Nitrophenol | NO2C6H4OH | | N | |
| n-Butyl alcohol | CH3(CH2)2CH2OH | | | |
| n-Dioctyl phthalate | (C8H17OOC)2C6H4 | | | |
| N-Nitrosodiethylamine | C4H10N2O | | N | |
| N-Nitrosodimethylamine | (CH3)2N2O | | N | |
| N-Nitrosodiphenylamine | (C6H5)2NNO | | N | |
| N-Nitrosodi-n-butylamine | ONN(n-C4H9)2 | | N | |
| N-Nitrosodi-n-propylamine | ONN(n-C3H7)2 | | N | |
| N-Nitrosomethylvinylamine | ONN(CH3)(C2H3) | | N | |
| N-Nitrosomorpholine | ONNC4H8O | | N | |
| N-Nitrosonornicotine | | | N | |
| N-Nitrosopiperidine | C5H10NHNO | | N | |
| N-Nitroso-N-ethylurea | C(O)(NH2)N(NO)C2H5 | | N | |
| N-Nitroso-N-methylurea | C(O)(NH2)N(NO)(CH3) | | N | |
| n-Pentane | CH3(CH2)3CH3 | | | |
| Octachloronaphthalene | C10Cl8 | Cl | | |
| Octane | CH3(CH2)6CH3 | | | |
| Oxirane | H2COCH2 | | | |
| o-Anisidine | CH3OC6H4NH2 | | N | |
| o-Anisidine hydrochloride | CH3OC6H4NH2.HCl | Cl | N | |
| o-Nitroaniline | NO2C6H4NH2 | | N | |
| o-Toluidine | CH3C6H4NH2 | | N | |
| o-Toluidine hydrochloride | CH3C6H4NH2.HCl | Cl | | |
| Parathion (DNTP) | (C2H5O)2P(S)OC6H4NO2 | | P,S | 427,428,517 |
| PCBs (Aroclor 1260,1254,1248, and1242) | C12ClxH10-x | Cl | | 70,209,351 |
| Pentachlorobenzene | C6Cl5H | Cl | | |
| Pentachlorophenol | C6Cl5OH | Cl | | 208,280,359 |
| Peracetic acid | CH3COOOH | | | |

| Substance | Formula | Halogen | Het. Atom | Reference |
|---|---|---|---|---|
| Phenanthrene | C4H10 | | | |
| Phenol | C6H5OH | | | 28,29,56,57,67,68,79,91,102, 276,311,318,319,349,382,413, 414,424,446,464,488,492 |
| Phenol,2-methyl | CH3C6H4OH | | | |
| Phosgene | COCl2 | Cl | | 225g,328g |
| Phthalic anhydride | C6H4(CO)2O | | | |
| Picric acid | C6H2(NO2)3OH | | N | |
| Polybrominatedbiphenyls | C12BrxH10-x | Br,Cl | | |
| Propane sultone | C3H6SO2 | | S | |
| Propionaldehyde | C2H5CHO | | | 458g |
| Propiolactone, beta- | OCH2CH2CO | | | |
| Propoxur [Phenol, 2-(1-methylethoxy)-methylcarbamate] | C11H15NO3 | | N | 294 |
| Propylene oxide | CH2OCHCH3 | | | |
| Propylene (Propene) | CH3CH:CH2 | | | |
| Propyleneimine | CH3HCNHCH2 | | N | |
| Pyrene | C16H10 | | | |
| p-Anisidine | CH3OC6H4NH2 | | N | 10 |
| p-Chloro-m-cresol | C6H3CH3OHCl | Cl | | |
| p-Cresidine | CH3C6H3(NH2)OCH3 | | N | |
| p-Nitrosodiphenylamine | (C6H5)2NNO | | N | |
| p-Phenylenediamine | C6H4(NH2)2 | | N | |
| Quinoline | C9H7N | | N | 61 |
| Quinone | C6H4O2 | | | |
| Quintozene (Pentachloronitrobenzene) | C6Cl5NO2 | Cl | N | |
| Safrole | C3H5C6H3O2CH2 | | | |
| sec-Butyl alcohol | CH3CH2CHOHCH3 | | | |
| Sevin (carbaryl) | C10H7OOCNHCH3 | | | |
| Sodium Alizarinsulfonate | SO3C6H3(CO)2C6H2(OH)2Na | | N,S | |
| Styrene | C6H5CH:CH2 | | | |
| Styrene oxide | C6H5CHOCH2 | | | |
| Terephthalic acid | C6H4(COOH)2 | | | |
| tert-Butyl alcohol | (CH3)3COH | | | 282g |
| tert-Butylformate | (CH3)3COC(O)H | | | |
| Tetrachloroethylene | Cl2C:CCl2 | Cl | | 162,206,282g,392g,463,504g, |
| Tetrachlorvinphos | C10H0Cl4O4P | Cl | P | 248 |
| Tetrahydrofuran | CH2CH2CH2CH2O | | | |
| Thioacetamide | CH3CSNH2 | | S,N | |
| Thiourea | (NH2)2CS | | S,N | |

| Substance | Formula | Halogen | Het. Atom | Reference |
|---|---|---|---|---|
| Toluene | C6H5CH3 | | | 49g,53g,60g,224g,340,404g, |
| Toluene diisocyanate | CH3C6H3(NCO)2 | | N | |
| Total xylenes | C6H4(CH3)2 | | | |
| Toxaphene | C10H10Cl8 | Cl | | |
| Triaziquone | C12H13N3O2 | | N | |
| Trichlorfon | (CH3O)2P(O)CH(OH)CCl3 | Cl | P | |
| Trichloroethylene | CHCl:CCl2 | Cl | | 39g,41,42,206,213g,225g,255g 257g,275,276,282g,283,283g, 292,328g,392g,404g,463, 493g,504g,505,513 |
| Triethylamine | N(C2H5)3 | | N | |
| Trifluralin | F3C(NO2)2C6H2N(C3H7)2 | F | N | |
| Trinitrophenylmethylnitramine | (NO2)3C6H2N(NO2)CH3 | | N | |
| Tris(2,3-dibromopropyl) phosphate | (CH2BrCHBrCH2O)3PO | Br | P | |
| Urethane (ethyl carbamate) | CO(NH2)OC2H5 | | N | |
| Vinyl acetate | CH3COOCH:CH2 | | | |
| Vinyl bromide | CH2CHBr | Br | | |
| Vinyl chloride | CH2:CHCl | Cl | | |
| Vinylidene chloride | CH2:CCl2 | Cl | | |
| Xylene (mixed isomers) | C6H4(CH3)2 | | | 49g,322g,496 |
| Zineb | Zn(CS2NHCH2)2 | | S,N | |

Table 2. Other Organic Compounds Treated by a Photocatalytic Process

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| 1,1,1,2-Tetrachloroethane | Cl3CCH2Cl | Cl | | |
| 1,3,5,7-Tetramethylcyclotertrasiloxane | | | Si | 441,442,443 |
| 1,1,1-Trifluoro-2,2,2-trichloroethane | F3CCCL3 | F,Cl | | 282g |
| 1,1,1-Trifluorobromochloroethane | C2HF3ClBr | F | | |
| 1,1,3-Trichloropropene | Cl2CCHCH2Cl | Cl | | 404g |
| 1,1-Difluoro-1,2,2-trichloroethane | ClF2CCHCl2 | F,Cl | | |
| 1,1-Difluoro-1,2-dichloroethane | FClCCClH2 | F,Cl | | |
| 1,1-Difluoroethylene | CH2CF2 | F | | |
| 1,1-Dimethyl-3-phenylurea | C6H5NHC(O)N(CH3)2 | | N | 393 |
| 1,1-Diphenylethylene | (C6H5)CCH2 | | | 125 |
| 1,2-Dimethoxybenzene | (CH3O)2C6H4 | | | 8,9,12,373 |
| 1,2-Bis(2-chloroethoxy)ethane | (ClC2H4)2C2H4 | Cl | | |
| 1,2-, 1,3-, or 1,4-Dinitrobenzene | (NO2)2C6H4 | | N | 87 |
| 1,2,4,5-Tetramethylbenzene | (CH3)4C6H2 | | | |
| 1,3-Dimethoxybenzene | (CH3O)2C6H4 | | | 12 |
| 1,3-Diphenylisobenzofuran | (C6H5)2C6H2OC6H4 | | | 237 |
| 1,4-Dinitrobenzene | (NO2)C6H4 | | N | 296 |
| 1,4-Napthoquinone | C10H6O2 | | | 160 |
| 1,4-Pentanediole | CH3CH(OH)(CH2)3OH. | | | 133 |
| 1-Benzylnicotinamide | (C6H5)CH2(C5H3N)C(O)NH2 | | N | |
| 1-Bromodecane | BrC10H21 | Br | | |
| 1-Bromododecane | BrC12H25 | Br | | |
| 1-Butanol | CH3(CH2)3OH | | | 101,374 |
| 1-Dodecanol | CH3(CH2)11OH | | | |
| 1-Hexene | C6H12 | | | |
| 1-(Methoxyphenyl)-2-propanol | (CH3OC6H4)(CH3)CHOH | | | |
| 1-Phenylethanol | CH3CH(C6H5)OH | | | 485 |
| 1-Propanol | n-C3H7OH | | | 101,374,376,378,380 |
| 1-Nitronaphthalene | C10H7NO2 | | N | 296 |
| 2,2-Dichloropropionic acid | CH3CCl2CO2H | Cl | | 69 |
| 2,3- , 2,4- or 3,4-Difluorophenol | F2C6H3OH | F | | |
| Tris-(2,4-dichlorophenoxy)ethyl-phosphite | C2H5P[OC6H3Cl2]3 | Cl | P | |
| 2,6-Dichlorophenol | C6H3Cl2OH | Cl | | 82,315 |
| 2,7-Dichlorodibenzo-p-dioxin | Cl2C12H6O2 | Cl | | |
| 2-, 3-, or 4-Chlorobenzoic acid | | | | 80 |
| 2-, 3-, or 4-Fluorophenol | FC6H4OH | F | | |
| 2-,3-, or 4-Nitrotoluene | N02C6H4CH3 | | N | 87 |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| 2,3-Benzofuran | C8H6O | | | 11 |
| 2,3- and 2,5-Dichlorophenol | Cl2C6H3OH | Cl | | 82,208,291,315 |
| 2,3-Dihydrobenzofuran | C8H8O | | | 377 |
| 2,4-Dimethoxybenzene | (CH3O)2C6H4 | | | 8,12 |
| 2,5-Dinitrophenol | (NO2)2C6H3OH | Cl | N | |
| 2,6-Dichloroindophenol | C8H2N(OH)Cl2 | | | |
| 2,5-Furandimethanol | C4H2O(CH2OH)2 | | | |
| 2,4,6-Trinitrobenzoic acid | (NO2)3C6H2CO2H | | N | 408 |
| 2-Chloroaniline | ClC6H4NH2 | Cl | N | |
| 2-Chlorobiphenyl | ClC6H4C6H5 | Cl | | 513 |
| 2-Chlorodibenzo-p-dioxin | ClC12H7O2 | Cl | | |
| 2-Chloroethylethylsulfide | (ClC2H4)C2H5S | Cl | S | 130 |
| 2-Chloroethylmethylsulfide | (ClC2H4)CH3S | Cl | S | 130 |
| 2-Coumaranone | C8H6O2 | | | 11 |
| 2-Furoic Acid | (CH2)3CHOCO2H | | | |
| 2-Hydroxypyridine | HOC5H4N | | N | |
| 2-Hydroxytetrahydropyran | HOC5H9O | | | |
| 2-Methyl-1,4-hydroquinone | CH3C6H3(OH)2 | | | 100 |
| 2-Naphthol | C10H7OH | | | 160 |
| 2-Tolualdehyde | CH3C6H4CHO | | | 60g |
| 2,2'-Dihydroxybiphenyl | C12H8(OH)2 | | | 54 |
| 3,3,3-Trifluoropropene | CH2CHCF3 | | | |
| 3,3'-Dichlorobiphenyl | (ClC6H4)2 | Cl | | |
| 3,4,5-Trichlorophenol | Cl3C6H2OH | Cl | | 82 |
| 3,4-Dichlorophenol | 3,4-Cl2C6H3OH | Cl | | 82 |
| 3-Aminoanisole | CH3OC6H4NH3 | | N | 10 |
| 3-Chloroanisole | CH3OC6H4Cl | Cl | | 10 |
| 3-Chlorophenol | m-ClC6H4OH | Cl | | 59,81,82 |
| 3-Chlorosalicylic acid | C7H5ClO3 | Cl | | |
| 3-Chlorotoluene | CH3C6H4Cl | Cl | | 496 |
| 3-Fluoroanisole | CH3OC6H4F | F | | 10 |
| 3-Fluorotoluene | CH3C6H4F | F | | 496 |
| 3-hydroxyanisole | CH3OC6H4OH | | | 10 |
| 3-Methyl-2-oxobutanoic acid | (CH3)CHC(O)CO2H | | | 486 |
| 3-Nitroanisole | CH3OC6H4NO2 | | | 10 |
| 3-Nitrotoluene | CH3C6H4NO2 | N | | 496 |
| 4-Acetobenzaldehyde | CH3C(O)C6H4CHO | | | 228 |
| 4-Aminoanisole | CH3OC6H4NH2 | | N | 10 |
| 4-Chloroanisole | CH3OC6H4Cl | Cl | | 10 |
| 4-Chlorotoluene | CH3C6H4Cl | Cl | | 496 |
| 4-Fluoroanisole | CH3OC6H4F | F | | 10 |
| 4-Fluorotoluene | CH3C6H4F | F | | 496 |
| 4-Hydroxyanisole | CH3OC6H4OH | | | 10 |

| Substance | Formula | Halogen | Het. Atom | Reference |
|---|---|---|---|---|
| 4-Nitroanisole | CH3OC6H4NO2 | | N | 10 |
| 4-Bromophenol | BrC6H4OH | Br | | |
| 4-t-Butyltoluene | p-(t-C4H9)C6H4CH3 | | | 496 |
| 4-Chloro-3-nitro-benzotrifluoride | C6HCl(NO2)F3 | F,Cl | N | |
| 4-Chlorophenol | ClC6H4OH | Cl | | 59,81,82,85,157g,303,358,359, 434,435,478,485,487,498 |
| 4-Chlorophenylisocyanate | ClC6H4NCO | Cl | N | |
| 4-Fluorophenol | FC6H4OH | F | | |
| 4-Hydroxyacetophenone | HOC6H4C(O)CH3 | | | |
| 4-Hydroxybenzyl Alcohol | p-HO(C6H4)CH2OH | | | |
| 4-Hydroxybiphenyl | C12H9OH | | | 54 |
| 4-Iodophenol | IC6H4OH | I | | |
| 4-Methoxybenzyl(3-phenylpropyl)-ether | CH3OC6H4CH2O(CH2)3C6H5 | | | 377 |
| 4-Methoxyphenol | CH3C6H4OH | | | |
| 4-Nitroaniline | NO2C6H4NH2 | | N | |
| 4-Nitrobenzaldehyde | NO2C6H4CHO | | N | 228 |
| 4-Nitrocatechol | (NO2)C6H3(OH)2 | | N | |
| 4-Nitrophenylethylphosphinate | (NO2)C6H4(C2H5)PO2 | | N,P | |
| 4-Nitrophenylisopropylphosphinate | (NO2C6H5)(C3H7)HPO3 | | N,P | |
| 4-Nitrophenyldiethylphosphate | (NO2C6H5)(C2H5)2PO4 | | N,P | |
| 4-Nitrotoluene | CH3C6H4NO2 | | N | 296,496 |
| 4-Phenylbutylamine | C6H5(CH2)4NH2 | | N | 128 |
| 4-Picoline | CH3C5H4N | | N | 340 |
| 4-Thiophenyl-1-butanol | C6H5S(CH2)4OH | | S | |
| 4-Trifluoromethylphenol | CF3C6H4OH | F | | |
| 4,4'-Dihydroxybiphenyl | C12H8(OH)2 | | | 54 |
| 5-Bromouracil | BrC4H(NH)2(O)2 | Br | N | 5 |
| 5-Chlorouracil | ClC4H(NH)2(O)2 | Cl | N | 5 |
| 5-Fluorouracil | FC4H(NH)2(O)2 | F | | 5 |
| 5-Hydroxypentanoic acid | HO(CH2)4CO2H | | | |
| 6-Methoxytetralin | CH3OC8H5O | | | 377 |
| 5-Methylresorcinol | CH3C6H5O2 | | | 382 |
| 12-Nitrododecanoic acid | NO2C11H22CO2H | | N | 296 |
| 12-phenyldodecanesulfonate, sodium salt | C6H5(CH2)12SO3H | | | |
| Acenapthane | C10H16(CH2)2 | | | |
| Acetic Acid | CH3CO2H | | | 90,239,344g,405g |
| Acetophenone | CH3COC6H5 | | | 160,485,498 |
| Acetylene | C2H2 | | | |
| Acid orange 7 | Na,O3SC6H4N2C10H6OH | | N,S | 477,478,479,481 |
| Adipic acid | C5H11CO2H | | | |
| Aldicarb | CH3SC(CH3)2CHN(O)C(O) NHCH3 | | N,S | |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| p-Alkylphenol (various) | R(C6H4)OH | | | |
| Allyl alcohol | C3H5OH | | | |
| Alochlor | | | | |
| p-Aminophenol | NH2(C6H4)OH | | N | |
| Anthraquinone-2-sulfonic acid | HO3SC14H7O2 | | S | |
| AOX or Haloform Precursors | | | | |
| Asulam | | | | 304 |
| Azobenzenes (various) | XC6H4NNC6H4X | | N | |
| Azobisformamidoacetic acid | | | N | |
| Bacteria/Algae/Virus | | | | 36,147,167,273,281,305,307, 330g,347,430,473,489 |
| Basagran | | | | 256 |
| Benzaldehyde | C6H5C(O)H | | | 160,228 |
| Benzophenone | (C6H5)2CO | | | |
| Benzoquinone | C6H4O2 | | | |
| Benzyldodecyldimethylamonium chloride | (C6H5CH2)(C12H25)(CH3)2N,Cl | Cl | N | |
| Benzyl ethers | C6H5CH2O-R R=CH3, n-C6H13, t-C4H9, (CH2)3C6H5, CH2C6H5 | | | 377 |
| Benzyltetradecyldimethylamonium chloride | (C6H5CH2)(C14H27)(CH3)2N,Cl | Cl | N | |
| Biomass | | | | |
| Biphthalate | (C6H4)(CO2H)CO2)(-1) | | | |
| Bromobenzene | BrC6H5 | Br | | 485 |
| Butane | C4H10 | | | |
| But-1-ene | CH2CHCH2CH3 | | | 19 |
| But-2-ene, trans | CH3CHCHCH3 | | | |
| Butylamine | n-C4H7NH2 | | N | 62 |
| t-Butylazine | | | N | 415 |
| n-Butyltin chloride | C4H9SnCl3 | | Sn | 338 |
| But-1-yne | CHCCH2CH3 | | | 19 |
| Butyric acid | C3H7CO2H | | | |
| Carbetamide | | | N | 361 |
| Carbon dioxide (reduction) | CO2 | | | 18,20,31,156,271,298,320g, 466,503 |
| Carbon monoxide | CO | | | 175g, 182g, 186g,188g, 189g, 474 |
| Carbon tetrabromide | CBr4 | Br | | 243g,286g,287g |
| Catechol | C6H4(OH)2 | | | 57 |
| C12-Betaine | (C12H25)(CH3)2NCO2 | | N | 202,203 |
| C12-Amidobetaine | | | | 202 |

| Substance | Formula | Halogen | Het. Atom | Reference |
|---|---|---|---|---|
| Cetyldimethylbenzylamonium chloride | CH3(CH2)15(CH3)2-(C6H5CH2)N,Cl | | N | |
| Cetylpyridinium chloride | N-[CH3(CH2)15](C5H5N),Cl | | N | 92,334 |
| Cetyltrimethylammonium bromide | CH3(CH2)15(CH3)3N,Cl | | N | 202 |
| Chloroacetaldehyde | CH2ClC(O)H | Cl | | |
| Chlorobenzoic acids, o-, m-, or p- | Cl(C6H4)CO2H | Cl | | |
| Chlorofluorocarbons, various | | F,C | | |
| Chloral hydrate | Cl3CO(OH)2 | Cl | | |
| Chloranil, o- and p- | C6Cl4O2 | Cl | | |
| Chloroethylammonium chloride | ClH3N,Cl | Cl | N | |
| Chlorpyrifos | | Cl | S,N | |
| Ciba Orange RI | | | | |
| Citric acid | HO2CCH2C(OH)(CO2H)CH2CO2H | | | 48,101 |
| Coal or Carbon | | | | |
| Color and/or COD (in wastewater) | | | | 34 |
| Congo Red | C32H22O6N6S2Na2 | | | |
| Cresol violet | C16H8NO(NH2),Cl | | N | |
| Creosote phenolics | | | | |
| Cyanuric acid | C3N3(OH)3 | | N | |
| Cyclododecanol | C12H23OH | | | |
| Cyclohexanedicarboxylic acids | C6H10(CO2H)2 | | | |
| Cyclohexanol | C6H11OH | | | 323 |
| Cyclohexene | C6H10 | | | |
| Cyclohexene oxide | C6H10O | | | |
| Cyclooctatetraene | C8H8 | | | 135 |
| Cyclopentane | C5H10 | | | 73g,74g,370g |
| Cyclophosphamide | OPONHC3H6[N(C2H4Cl)2] | | P,N | |
| Cynnamyl alcohol | C6H4C2H2OH | | | |
| DDT | (ClC6H4)2CHCCl3 | Cl | | 333 |
| Decalin | C10H18 | | | |
| Decamethyltetrasiloxane | (CH3)10Si4O3 | | Si | |
| Decanoic acid | C9H19CO2H | | | |
| Decanol | HOC10H21 | | | |
| Desipramine | (C6H4)2(CH2)2N(CH2)3NHCH3 | | | |
| Diazinon | [(CH3)2CHC4N2H(CH3)O]-PS(OC2H5)2 | | N,P,S | 304 |
| Dibenzo-p-dioxines, various | XnC12H(8-n)O2 | Cl | | 516 |
| Dibromomethane | CH2Br2 | Br | | |
| Dimethylacetamide | CH3C(O)N(CH3)2 | | N | 293 |
| Dichloroacetic acid | Cl2CHCO2H | Cl | | 51,253,285,345,358 |
| Dichloroacetyl Chloride | Cl2CHCOCl | Cl | | 225g,328g |
| Dimethylamine | (CH3)2NH | | N | |
| Dimethylphenols (Xylenols) | (CH3)2C6H3OH | | | 465 |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Dimethylsulfide | (CH3)2S | | S | |
| Dimethyl-2,2-dichlorovinyl phosphate | (CH3)2(Cl2CCH)PO4 | Cl | P | |
| Diphenylacetylene | (C6H5)2C2 | | | 207 |
| Diphenylmethane | (C6H5)2CH2 | | | |
| Diphenylsulfide | (C6H5)2S | | S | |
| Direct blue 1 | [(Na,O3S)C16H6(NH2)(OH)-(OCH3)N2]2 | | N,S | |
| Diquat | | | | 256 |
| Disinfection by-products | | | | 394,514 |
| Disperse red 74 | | | | 509 |
| Diuron | C6H3Cl2NHC(O)N(CH3)2 | | N | 256 |
| Dodecane | C12H26 | | | |
| Dodecyl sulfate | (C12H25)2SO4 | | | |
| Dodecylbenzenesulfonate | (C12H25)C6H4SO3(-1) | | S | 92,202,334 |
| Dodecyldecaoxyethylenephosphates | | | P | |
| Dodecylpyridinium chloride | (C12H25)C5H5NH,Cl | Cl | N | 202,203 |
| Doxycycline | | | | |
| Dyes, unidentified | | | | 96,226,227 |
| Eosin | | | | |
| Ethambutol | | | N | |
| Ethane | C2H6 | | | |
| Ethanol | C2H5OH | | | 32,101,228,264,274g,329g, 374,405g |
| Ethylacetate | CH3CO2C2H5 | | | |
| Ethylenediaminetetraacetic acid | (O2CCH2)4N2C2H4 | | N | 48,101,342,484 |
| 2-, 3-, or 4-Ethylphenol | (C2H5)C6H4OH | | | |
| Fenitrothion | C9H12NO5PS | | NSP | 249 |
| Fluorescein | C20H12O5 | | | |
| Folicur | | | N | |
| Formamide | HC(O)NH2 | | N | 293 |
| Formic Acid | HCO2H | | | 48,90,101,163,214,251,252, 344g,416,444 |
| Fullerenes | C60, C70, and C84 | | | 236 |
| Fulvic acid | | | | 1 |
| Glucose | C6H11O6 | | | 48 |
| Glycerol | C3H5(OH)3 | | | |
| HCFC or HFC | | Cl,F | | |
| Heparin | | | | |
| Heptanal | C6H13CHO | | | 228 |
| Hexafluorobenzene | C6F6 | F | | |
| Hexafluoropropene | CF2CFCF3 | F | | |
| HMX | (CH2)4(NNO2)4 | | N | 48 |
| Hexanol | C6H13OH | | | |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Humic Acids | | | | 34,37,480 |
| Hydroxybenzoic acid (various) | HOC6H4(OH)CO2H | | | |
| Hydroxycarboxylic acids, alpha | RCH(OH)CO2H | | | |
| Hydroxyethylcellulose | | | | |
| Imidazole | C3H4N2 | | N | 346 |
| Indole | C8H6NH | | N | |
| Isobutane | C4H10 | | | 88g |
| Isobutanol | CH3CH(CH3)CH2OH | | | |
| Isobutene | C4H8 | | | |
| Isobutyric Acid | CH3CH(CH3)CO2H | | | 101 |
| Isonicotinaldehyde | C5H4NCHO | | N | 228 |
| Isoprene | CH2C(CH3)CHCH2 | | | |
| Isosorbide dinitrate | C6O2H8(ONO2)2 | | N | |
| Iso-octane | (CH3)2CH(CH2)4CH3 | | | 282g |
| L-Lysine | NH2(CH2)4CH(NH2)CO2H | | | 101 |
| Lactic acid | C3H6O3 | | | |
| Landfill leachate | | | | 35 |
| Kraft lignin | | | | |
| Malachite green oxalate | (C6H5)[C6H4N(CH3)2][C6H4N-(CH3)2]C,(C2O4H)2.H2C2O4 | | N | 153,154 |
| Maleic acid | HO2CCHCHCO2H | | | |
| Malic acid | HO2CCH2CH(OH)CO2H | | | 97 |
| Malonic acid | CH2(CO2H)2 | | | 219 |
| Methane | CH4 | | | |
| Methanethiol | CH3SH | | S | 450g |
| Methylcyclohexane | CH3C6H11 | | | |
| Methyl orange | Na,O3SC6H4N2C6H4N(CH3)2 | | N,S | |
| alpha-Methylstyrene | C6H5(CH3)CCH2 | | | 396 |
| Methyl viologen | (CH3C5H4N)2,Cl2 | Cl | N | |
| Methylene blue | (CH3)2NC6H3NSC6H3N(CH3)2,Cl | Cl | N,S | 26,272 |
| Methylvinylketone | CH3COC2H3 | | | |
| Mixed waste | | | | 418 |
| Molasses | | | | 402 |
| Monocrotophos | | | P | 428,428,517 |
| Monuron | ClC6H4NHCON(CH3)2 | Cl | N | 27 |
| Morpholine | C4H8ONH | | N | 90 |
| m-Phenoxytoluene | m-C6H5O-C6H4CH3 | | | |
| N-Benzyldiphenylamine | (C6H5CH2)(C6H5)2N | | N | 108,129 |
| N-Dodecanoyl-N-(2-hydroxyethyl)amide | CH3(CH2)10C(O)NH(CH2)2OH | | N | 202,203 |
| N-Dodecanoyl-N,N-bis(2-hydroxyethyl)-amide | CH3(CH2)10C(O)N[(CH2)2OH]2 | | N | 203 |
| N-Hydroxysuccinimide | C2H4(C(O))2NOH | | N | 346 |
| N,N,N',N'-Tetraethyloxonine | | | N | |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Naphthol | C10H7OH | | | |
| Naphthol blue black | (C6H5N2)C12H2(OH)(NH2)-(SO3Na)2 | | N,S | 337,475,477 |
| Nicotine | C5H4NC4H7NCH3 | | N | 305 |
| Nile Blue A | C16NO(NH2)N(C2H5)2,SO4 | | N,S | |
| Nitrocellulose | | | N | |
| p-Nitrotoluenesulfonic acid | (CH3)(NO2)C6H3SO3H | | N,S | |
| Nitrotoluene, various | NO2C6H4CH3 | | N | |
| Nonylphenolethoxylate | C9H17C6H4OC2H5 | | | |
| n-Octanol | C8H17OH | | | 436,502 |
| Octanal | C7H15CHO | | | 228 |
| Octaphenylcyclotetrasiloxane | (C6H5)8(SiO2)4 | | Si | 314 |
| Oil/Petroleum | | | | 170 |
| Oxalic acid | C2O4H2 | | | 101,159,200,342,358,423 |
| PCB - polyhydroxy | | Cl | | 315 |
| Pendimethalin | | | | 195 |
| Pentaethyleneglycol n-dodecyl ether | (HO)(CH2CH2O)5(C12H23) | | | 202 |
| Pentafluorophenol | C6F5OH | F | | |
| n-Pentyl amine | n-C5H11NH2 | | N | |
| Permethrin | | | | |
| Pesticides - unspecified | | | | 221 |
| Phenacylstyrylthioether | PhCH2SCH2C(C6H5)CH2 | | S | 138 |
| Phenosafranin | C6H5N2C12H4(NH2(CH3)2 | | N | |
| p-Phenylenediamine | H2NC6H4NH2 | | N | 288,289,291 |
| Phenylmercaptotetrazole | | | | 484 |
| Phorate | (C2H5O)P(S)SCH2SC2H5 | | P,S | 427,428,517 |
| Phthaldialdehyde | C6H4(CHO)2 | | | 160 |
| Phthalan | | | | 377 |
| Phthalic acid | C6H4(CO2H)2 | | | 160 |
| Picoline | CH3C5H4N | | N | |
| Piperidene | C5H10NH | | N | 62 |
| Polyethoxylene alkyl ethers | R2(OC2H4)n | | | |
| Polyethylene | (CH2CH2)n | | | |
| Poly(methylphenylsiloxane) | [(C6H5)(CH3)SiO]n | | Si | 314 |
| Polypropylene | [(CH3)CHCH2]n | | | |
| Polyvinylalcohol | (C2H3OH)n | | | |
| Polyvinylchloride | (CH2CHCl)n | Cl | | 152 |
| Proline | C4H8NCO2H | | N | |
| Prometon | | | | |
| Prometryn | | | | |
| Propane | C3H8 | | | 194 |
| Propionamide | CH3CH2C(O)NH2 | | N | 293 |
| Propionic acid | C2H5CO2H | | | 101 |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Propylene | C3H6 | | | 375g |
| Propylene glycol dinitrate | CH3CH(NO3)CH2(NO3) | | N | |
| Propyne | CH3CCH | | | |
| Propyzamide | | | N | 471 |
| Pyridine | C5H5N | | N | 62,224g |
| Pyrocatechol | o-C6H4(OH)2 | | | |
| Pyrrole | C4H5N | | N | |
| Quinoline acid yellow | | | | 260 |
| Reactive Dyes | | | | |
| Red Dye 79 | | | N,S | |
| Resorcinol | C6H6O2 | | | 382 |
| Rhodamine B | CH3OC(O)(C6H4)C13H6O(NH2)2 | | N | |
| Rhodamine 6G | C2H5OC(O)C6H4C13H4(CH3)2-[N(C2H5)]2,Cl | Cl | N | 14 |
| Rhodamine 6ZH | | | | |
| Rose Bengal | Na2,O2CC6Cl4C13H2OI4O2 | Cl,I | | |
| S-Dodecyl thioether carboxylates | | | S | |
| S-Ethyl-N,N-dipropyl thiocarbamate (EPTC) | (C2H5)SC(O)N(C3H7)2 | | N,S | |
| S-Ethyl-N,N-diisopropylthiocarbamate (Butylate) | (C2H5)SC(O)N(i-C3H7)2 | | N,S | |
| S-Ethyl-4-hexahydro-1-H-azepine-1-carbothionate (molinate) | | | N,S | |
| S-Propyl-N-cyclohexyl thiocarbamate (cycloate) | (C3H7)SC(O)NH(C6H11) | | N,S | |
| S-Propyl-N,N-dipropyl thiocarbamate (vernolate) | (C3H7)SC(O)(NC3H7)2 | | N,S | |
| Salicylaldehyde | C7H6O2 | | | 11 |
| Salicylic acid | C7H6O3 | | | 48,91,102,246,469 |
| Simazine | (C2H5)Cl(NHC2H5)C3N3 | | N | |
| Sodium chloroacetate | CH3CO2Na | Cl | | |
| Sodium dodecylbenzene sulfonate | C12H25C6H4SO3Na | | S | |
| Stearic acid | CH3(CH2)16CO2H | | | 429 |
| Stilbene | C6H5CHCHC6H5 | | | 131 |
| Succinic acid | HO2CCH2CH2CO2H | | | |
| Sucrose | C12H22O11 | | | |
| Sulfones | RS(O)2R' | | S | |
| Surfactants - unspecified | | | | 295 |
| Tetrachlorvinphos | CHClCH(2,4,5-Cl3C6H2)(CH3)PO4 | Cl | P | |
| Tetrafluoroethylene | C2F4 | F | | |
| Tetralin | C10H12 | | | 377 |
| Tetramethylenediamine | NH2(CH2)4NH2 | | N | |
| Tetrabutylammonium phosphate | [(n-C4H9)4N]4,PO4 | | P | |

| Substance | Formula | Halo-gen | Het. Atom | Reference |
|---|---|---|---|---|
| Tetradecyldimethylbenzylammonium-chloride | CH3(CH2)13(CH3)2(C6H5CH2)-NCl | | N | 202,203 |
| Theophylline | C7H8N4O2.H2O | | N | |
| Thioethers | RSR' | | S | |
| Thiobencarb | | | | |
| Thymine | C5H6N2O2 | | N | |
| Thionine | C12NS(NH2),O2CCH3 | | S,N | |
| p-Toluenesulfonic acid | CH3(C6H4)SO3H | | S | |
| s-Triazines | | | N | 38 |
| Trichloroacetic acid | Cl3CCO2H | Cl | | 433 |
| Trietazine | | | N | |
| Triethanolamine | N(CH2CH2OH)3 | | N | |
| Trifluoroacetic acid | CF3CO2H | F | | |
| Trihydrazinotriazine | | | N | |
| Trihydroxybenzene | (HO)3C6H3 | | | |
| Trimethylamine | (CH3)3N | | N | |
| Trinitrophenol | (NO2)3C6H2OH | | | |
| Triphenylacetic acid | (C6H5)3CCO2H | | | |
| Triphenylbismuthine | (C6H5)3Bi | | Bi | 431 |
| Triphenylphosphine | (C6H5)3P | | P | 431 |
| Triphenylstibine | (C6H5)3Sb | | Sb | 431 |
| Tri-(p-Tolyl)arsine | (CH3C6H4)3As | | As | 431 |
| Triton X-100 | C8H17C6H4(OCH2CH2)xOH | | | 92,334 |
| Umbelliferone | C9H6O3 | | | |
| Uracil | HNC(O)NHC(O)CHCH | | N | 5 |
| Urea | C(O)(NH2)2 | | N | 1 |

Table 3. Inorganic Substances Included in EPA Lists of Hazardous Substances and/or Treated by a Photocatalytic Process

| Substance/Element | Formula/Symbol | Reference |
|---|---|---|
| Actinides | Th,Pa,U,Np,Pu | 418 |
| Aluminum (fume or dust) | Al | |
| Aluminum oxide | Al2O3 | |
| Ammonia | NH3 | 261g,321g,472g |
| Ammonium nitrate (soln) | NH4NO3 | |
| Ammonium sulfate (soln) | (NH4)2SO4 | |
| Antimony | Sb | |
| Arsenic | As | |
| Asbestos | Mg,Si | |
| Azide ion | N3(-) | |
| Barium | Ba | |
| Beryllium | Be | |
| Bismuth | Bi | |
| Boron | B | |
| Cadmium | Cd | |
| Chlorine | Cl | |
| Chlorine dioxide | ClO2 | |
| Chromium | Cr | 154 |
| Cobalt | Co | |
| Copper | Cu | 101,197,198 |
| Cyanide and Complexes | CN(-1) and M(CN)x | 2,3,218,384,385 |
| Cyanate ion | CNO(-1) | |
| Gold | Au | 197 |
| Halide ion | X(1-), X = F, Cl, Br, or I | 33,137,484 |
| Hydrazine | H2NNH2 | |
| Hydrogen sulfide | H2S | |
| Hypophosphorus acid | H2PO2 | 48 |
| Iridium | Ir | 197 |
| Iron | Fe | |
| Lead | Pb | 387 |
| Manganese | Mn | |
| Mercury | Hg | |
| Molybdenum | Mo | |
| Nickel | Ni | 197 |
| Nitrates/nitrites | NO3(-1),NO2(-1) | 388 |

| Substance | Formula | Reference |
|---|---|---|
| Nitrogen oxides | NOX | 18.25g.143g.216g.220g.<br>243g.244g.261g.262g.<br>449g.459g.460g.461g.<br>472.501.512 |
| Nitrogen | $N_2$ | |
| Oxalate ion | $C_2O_4^{(2-)}$ | |
| Oxygen | $O_2$ | |
| Ozone | $O_3$ | |
| Palladium | Pd | 197.199.264 |
| Phosphorus | P | |
| Platinum | Pt | 98.197.199.264.444 |
| Radium | Ra | |
| Radon | Rn | |
| Rhodium | Rh | 98.197.199.264 |
| Selenium | Se | |
| Silicon | Si | |
| Silver | Ag | 197.198.199.211.290 |
| Strontium | Sr | |
| Sulfate radical | $SO_4^{(2-)}$ | |
| Sulfite | $SO_3^{(1-)}$ | |
| Sulfur | S | |
| Sulfur oxides | SOx | 449g |
| Sulfuric acid | $H_2SO_4$ | |
| Thallium | Tl | |
| Thiocyanate | $SCN^{(1-)}$ | 33 |
| Thiosulfate | $S_2O_3^{(2-)}$ | 48.198.484 |
| Thorium | Th | |
| Tin | Sn | |
| Tritium | H.(T) | |
| Tungsten | W | |
| Vanadium | V | |
| Zinc | Zn | |

# 4.0 Conclusions

The level of activity in this field remains high. The potential to develop new technology for environmental remediation is still a major driving force for R&D activity. However, it is clear that many companies see potential markets for VOC removal in indoor air quality applications. The application of photocatalytic chemistry for the disinfection of water and air has been the subject of sporadic reports over the last 9 years. The potential impact of this application is very large and it is drawing increased attention. In the work to date no clear mechanism for the killing of micro-organisms has been established. The magnitude of the contribution of a photocatalytic effect versus the effect of heat, light, or extraneous agents such as hydrogen peroxide or transition metal ions is often difficult to determine.

In research, more attention is being paid to the detection and identification of intermediates and by-products that can be formed during the photocatalytic process, both in aqueous and gas phase systems. Defining intermediates helps researchers understand the chemical mechanisms of the processes and is necessary to insure that potentially harmful substances are not left in the processed stream. Key areas of work identified in the last report continue to be important. Few studies include mass balances for the reactions and kinetic models that can be used to size treatment systems are still rare. As systems are deployed in the field, it is increasingly important that the issues of catalyst lifetime and regeneration be addressed. Related to this is the need to identify those components of an air or water stream that can inhibit or kill activity. All of these are important to the design of efficient and economical treatment systems. Questions concerning the economic viability of photocatalytic processes are being raised more often. The significance of simple mineralization of one more organic compound without regard to the amount of energy or time that it took is questioned by those who want to see the process efficiency improved. This may be taken as a sign that the field is maturing. There are entrepreneurs and companies that would like to capitalize on the scientific foundation that has been developed for photocatalytic chemistry.

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## 5.1. Address to Send Corrections or References to Work Appearing Prior to 1996 that May Have Been Left out of the List of References in this and the Previous Report.

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