

Bibliography of Work on the Heterogeneous Photocatalytic Removal of Hazardous Compounds from Water and Air Update Number 1 To June, 1995

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Summary

The Solar Industrial Program, funded by the United States Department of Energy, is carrying out research and development on processes for the destruction or removal of hazardous substances from water and air. The work is being done at the National Renewable Energy Laboratory in Golden, CO, and Sandia National Laboratory in Albuquerque, NM, and by their subcontractors. The processes of interest in this report are based on the application of heterogeneous photocatalysts. The current state of the art in catalysts are forms of titanium dioxide or modifications thereof but work on other heterogeneous catalysts is included in this compilation.

This report is an update of a bibliography of work done on the photocatalytic oxidation of organic or inorganic compounds in air or water and on the photocatalytic reduction of metal containing ions in water that was published in May, 1994. The previous report included 663 citations obtained through the middle of 1993 and some selected references from the balance of that year. This update contains an additional 574 references. These were published during the period from January 1993 to June 1995, or are references from prior years that were not included in the initial report. The general focus of the work is removing hazardous contaminants from air or water to meet environmental or health regulations. This report follows the same organization as the previous publication. 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 covers 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 new section has been added which gives information about companies that are active in providing products based on photocatalytic processes or that can provide pilot, demonstration, or commercial-scale water- or air-treatment systems. Key words, assigned by the author of this report, have been included with the citations in the listing of the bibliography.

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1.0 Introduction

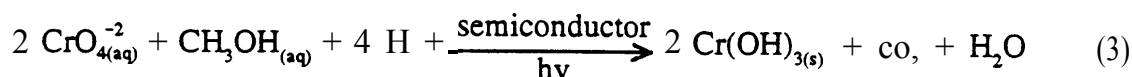
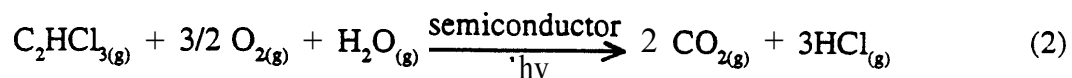
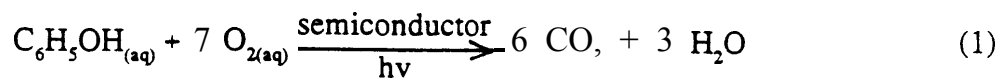
This update in combination with the previous report¹ provides a comprehensive bibliography of work available in the open literature for scientists and engineers interested in the use of heterogeneous photocatalytic oxidation or reduction processes in environmental remediation, process emission control, indoor air quality, or other applications. The combined bibliographies include more than 1200 citations to work published between 1970 and the middle of 1995. 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 100 citations to work done prior to 1993 that were not included in the initial report. Some citations have doubtless been missed and topics covered in certain papers may not have been identified and covered in every appropriate category. The limitation to heterogeneous processes means that work on homogeneous photocatalytic processes is not included. Examples of these are the recently patented process based on the **iron(III)-oxalate-hydrogen** peroxide system² and the systems based on soluble **polyoxometalates**.³ The author invites readers to send **references** to relevant work that appeared before 1995 that has been missed to the mail **or e:mail** address included in Section 5.3 of this report.

The photocatalytic oxidation of organic compounds in water is the subject of a large body of research that has been performed in laboratories all over the world. A lesser but rapidly increasing amount of work has been devoted to 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. Representative reactions are shown below:

¹Blake, 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**Safarzedeh-Amiri, Ali**, inventor. "Photocatalytic Method for Treatment of Contaminated Water." Cryptonics Corporation, assignee. United States Patent, **5,266,214**. November 30, 1993.

³Hill, C. L. and C. M. **Prosser-McCartha**. "Photocatalytic and Photoredox Properties of Polyoxometalate Systems." *Photosensitization and Photocatalysis Using Inorganic and Organometallic Compounds*, eds. K. Kalyanasunderam and M. Gratzel, 307-30, Dordrecht: Kluwer Academic Publishers, 1993.



Reactions are shown in the idealized case of complete oxidation or reduction. It is widely observed that intermediates and by-products are often formed that persist in the treated stream. These can include a variety of acids, oxygenated compounds, and carbon monoxide.

The net process involves oxidizing the organic compound to an intermediate stage of oxygen content or to 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. Modifying or removing certain metal ions from water can be accomplished when the ions replace oxygen as the electron acceptor in the process and sacrificial electron donor compounds are provided.

A survey of the literature collected reveals that about 20% of the new citations are for work in which the target compound is carried in the gas phase rather than in water. Twenty-four citations cover work on disinfection of water or air or to potential medical applications. Control of odor compounds or application to removal of volatile organic compounds specifically for indoor air purification was the subject of nine papers. Use of the sun as the light source was identifiable in more than 80 papers. Engineering issues were addressed in more than 70 papers. Of the 46 patents that are included in the new list, 35 have assignees in Japan.

Reference to test work on more than 150 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. A significant number of pesticides, dye compounds, and surfactants have been shown to be mineralized and a variety of bacteria and virus have been found to be 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.

A new section has been added which lists the names and addresses of companies that offer products or services based on a heterogeneous photocatalytic process. These are mainly in the United States and Canada but a few are from Europe and Japan. The author has attempted to obtain information directly from the company or used information from the open literature in **the** preparation of the entries which identify the product or service. Companies not listed are invited to send information, to the address in Section 5.3, that can be included in the next update of the bibliography.

The following sections cover 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 devices 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. Documents referring to work on systems in which **the** compound to be treated is carried in the gas phase are indicated by the prefix "**g**" in **the** citation number.

2.0 Generic Information

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

2.1 Review Articles

Many new reviews have been written that cover various aspects of photocatalytic chemistry and technology. This section also includes reviews written in the years prior to 1993 that were not cited in the first report. Reviews covering the broad topics given can be found in the following references:

methodology for comparing reaction systems - 21,350, and 428; mechanisms/activity - 27, 50, 63, 133, 205, 258, 290, 325, 338, 425, 426, 427, 429, 535, 537, 546, 549, 550, 561, and 569; ultra small particles - 28,206, 326, and 547; photoelectrochemical systems - 32 and 33; solar facilities - 36; photocatalysis - 45, 116, 124, 309, 366, 543, 549, 564, 568, and 570; solar processes - 51, 509, 531, and 574; companies active in the field - 69; adsorption - 90, 91, and 537; metallized photocatalysts - 145; disinfection - 150 and 319; indoor air quality - 150,319, and 565; oil spills - 150; surfactant degradation - 159 and 360; environmental applications - 171, 266, 286, 300, 316, 342, 343, 358, 381, 421, 422, 424, 425, 429, 517, 556, 558, 559, 560, 562, 565, and 571; production and applications of ultra-fine TiO_2 - 201; preparation and applications of semiconductor thin films - 204; microfabrication and integrated chemical systems - 226; overview of Department of Energy R&D in photocatalysis - 289; Degussa P25 properties - 321; new photocatalytic processes - 338; titanium dioxide pigments and the control of photodegradation of polymers - 339; comparison of advanced oxidation processes - 340 and 557; issues and questions in application of photocatalysis - 341; solar production of fuels and chemicals - 381; and photochemical reactors - 390.

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. On the negative side, its 3.2 eV band gap results in only a small overlap of its action spectrum with the solar spectrum. Also, the efficiency for converting photons absorbed to hazardous molecules destroyed is generally low, particularly for the aqueous phase processes. In order to identify ways to increase process **efficiency** and to improve the overlap of the absorption spectrum of the photocatalyst with

the solar spectrum, a great deal of work has been done on modifying TiO_2 and testing other semiconductors. 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 -11, 167, 211, 212, 355, 376, 520, and 523; rutile -12, 46, 48, 160, 167, 219, 220, 292, and 389; heat treatment -22, 49, 78, 167, 303, 337, 352, 353, 406, 520, and 526; colloidal or quantized particles -28, 67, 81, 114, 115, 136, 170, 200, 241, 254, 277, 278, 279, 389, 510, 511, 519, and 548; modified -29; xerogel/aerogel -94, 95, 96, 97, 230, 413, and 466; flame synthesis - 119 and 376; or catalysts from different vendors - 405.

2.2.2 Hydrophobic Surface Treatment

Titanium dioxide has been modified to make the surface hydrophobic to alter the interaction with organic compounds in water. This work is covered in the following: silica - 94.

2.2.3 Dye Sensitized Titanium Dioxide

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

ruthenium complex - 38, 200, and 460; eosin - 151; cobalt tetraphenylporphine - 187; cobalt tetrasulfophthalocyanine - 235; organic dyes - 209 and 393; polyviologen - 397; $[\text{Mo}_2\text{S}_4(\text{S}_2\text{C}_2\text{H}_4)](-2)$ - 254; iron-porphyrin - g368; coupled semiconductors - 423; or Ni-phthalocyanines - 499.

2.2.4 Metal Ion Doping of Titanium Dioxide

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

Si - 323; Al - 82 and 323; V - 40, 81, 82, and 279; Fe - 28, 40, 47, 49, 81, 82, 259, 278, 311, and 348; Co - 40 and 82; Zr - 230; Ni - 474; Nb - 89, 223, and 230; Mo - 81, 82, 242, 352, 353, and 380; W - 104, 105, 269, 270, 352, 353, and 380; Re - 81 and 82; Ru - 81 and 82; Rh - 81 and 82; or Os - 81.

2.2.5 Metallized Titanium Dioxide

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

Cu - 311,504, and 515; Ru - 203; Os - 203; Rh - 203; Ir - 203; Pd - 151, 203, 269, 270, 333, and 335; Ag - 243, 269, 270, 311, 337, and 459; Au - 31, 244, 269, 270, and 337; or Pt - 23, 24, 87, 88, 146, 147, 160, 164, 191, 203, 269, 270, 273, 317, 327, 337, 370, 401, 413, 467, and 486.

2.2.6 Other Semiconductors

A wide range of other semiconductors 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:

Al₂O₃ - 148 and g436; Sr - or BaTiO₃ - 219 and 220; V₂O₅ - g14 and g367; Fe₂O₃ - 28, 87, 106, 114, 148, 184, 259, 356, 364, 423, 461, 541, and 542; FeO(OH) - 135,354, and 524; CaFe₂O₄ - 282; ZnO - 9, 23, 28, 30, 106, 157, 160, 204, 217, 261, 278, 292, 337, 356, 357, 364, g367, 385, 386, 388, 423, g436, 461, g487, 499, 545, 566, and 573; Zn- or CdS - 106, 112, 143, 301, 337, 423, 433, 519,539, and 540; ZrO₂ - 87 and g367; ZrPO₄ - 313; MoO₃ - g14; MoS₂ - 160; SnO₂ - 9, 38, 87, 204, 356, g367, 482, and 484; Sb₂O₄ - g367; CeO₂ - g367; WO₃ - 9, 39, 106, 160, 204, 337, 356, g367, 499,541, and 542; SiO₂ - 148, ; SiC - 221; Nb₂O₅ - 17; RuS₂ - 18; fly ash - 148 and 555; polyaniline - 296; or natural minerals - g192 and 354.

2.2.7 Immobilized Photocatalysts

Most experimental work on aqueous systems has been performed using the photocatalyst in the form of **fine** particles 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. For the treatment of gases most work has involved immobilized catalyst. Titanium dioxide has been affixed to a variety of surfaces:

glass (including fibers) - g14, 42, 152, 153, 172, 173, 174, 194, 212, 265, 280, 281, 304, 314, 315, 320,345, g440, 481, 484, 485, 552, 553, 554, and 572; silica - 186 and 532; metal - 178 and 446; ceramic-2, 10, g16, 168, 403, g407; clays - 260,449, and g452; polymer -1, 12, 40, 41, 60, 70, 145, 149, 296, 345, 401, and 474; thin films - 26, 38, 83, 84, 144, 210, 223, 334, 398, 406, and 523; zeolite - 14, 35, 120, 143,260, and 402; alumina - 143; carbon - 179, 184, 185, 231, 312, g453, and 473; Amborsorb - 327; or β -cyclodextrin - 5 10.

2.3 Hydrogen Peroxide and Other Oxidants

Oxygen has been the oxidant of choice in most studies, but hydrogen peroxide has been found to improve the rates of reaction with a variety of organic substrates under some conditions. This work is covered in the following:

hydrogen peroxide - 13, 22, 40, 62, 92, 102, 110, 126, 137, 170, 173, 251, 310, 330, 394, and 399;
persulfate - 130; or ozone - 17 and g436.

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. Work has appeared in the literature addressing issues related to the 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 (see Section 2.7).

2.4.1 Reactor and System Design

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

photochemical reactors - 390; photoelectrochemical system - 10; non-concentrating reactor - 137, 138, 330, 347, 421, 471, 513, 514, and 532; shallow ponds/tanks - 37, 85, and 512; parabolic trough - 52, 53, 71, 72, 134, 288, 306, and 346; kinetic modelling - 68, 214, 215, 276, 298, 301, 302, and 572; recirculating reactor - 80 and 456; fixed bed - 88, 110, 369, 415, and 530; filtration - 110; hybrid lamp/solar system - 111; equipment requirements - 197 and 421; ultrasonic reactor - 199; batch-type reactors - 228 and 229; optimization of air purification systems - 363; controlled periodic illumination - 418, 419, and 420; or falling film reactor - 521.

2.4.2 Systems Analysis

As the technology for the photocatalytic treatment of contaminated air or water has progressed, a few studies have compared the costs of sunlight and electric lamps as photon sources; others have compared the photocatalytic processes with conventional treatment methods, such as carbon adsorption or W-peroxide oxidation:

process waste water - 53, 394, and 442; photocatalysis process cost - 56, 110, 251, 364, 421, 431, 472, and 557; or photon costs from lamps and sunlight - 411 and 471.

2.5 Miscellaneous Topics

This category includes papers of interest that do not fall into the preceding headings: adsorption - 382 and 528; combined photocatalytic and biological treatment - 152, 227, 267, 268, 310, 412, 434, 435, and 476; non-aqueous solvent systems - 488 and 491; or electron microscopy of TiO_2 phases - 493.

2.6 Patents

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

catalyst formulation - 1, 149, 193, 224, 225, 280, 281, 312, 345, 400, 404, 502, and 518; photoelectrochemical system - 10 and 344; spent plating bath - 24; point-of-use water treatment system - 65; water treatment system - 85 and 456; regeneration of adsorbents - 87; metals removal from water - 118 and 281; magnetic catalyst particle - 128; oil spill treatment - 152; catalyst on inorganic fibers - 168; photocatalysis with 185 nm light for air treatment - 169; removal of chlorinated compounds from vent gas (includes scrubber) - 183; removal of air pollutants (catalyst on exterior walls of buildings) - 185 and 335; additive to enhance degradation of plastics in the environment - 190 and 291; deodorizing agents - 202, 404, 502, 503 and 518; removal of nitrogen compounds from water - 222; regenerable deodorant - 231; combined biological and photocatalytic treatment of wastewater - 267 and 268; process for killing cells or disinfection - 283, 391, and 503; photocatalyst plate material - 285; total organic carbon analyzer - 287; nitrogen and phosphorus analyzer - 451; purification of waste gases - 331; disinfecting construction materials - 333; methanol synthesis - 334 and 345; fluid purification - 391; method for preparing dialkyldipyridinium salts - 395; semiconductor modified with insoluble polyviologen derivatives - 396; moisture-resistant catalyst for ethylene oxidation - 400; or optical fiber as light source - 489.

2.7. Companies Active in the Field

The following is a list of companies that have products or services based on heterogeneous photocatalysis. The list is compiled from the best information available to the author from personal contacts and material published in the open literature.

American Energy Technologies, Inc.

Mr. Greg Peebles

P.O. Box 1865

Green Cove Springs, FL 32043

Telephone: 904-284-0552

Fax: 904-284-0006

Product(s): Stable W-transmissive polymers and glass for photoreactor construction and development and fabrication of photoreactors.

Degussa Corporation

Ms. Maria Nargiello

3500 Embassy Parkway, Suite 100

Akron, OH 44333

Telephone: 216-668-2235

Fax: 216-668-3846

Product(s): **Photocatalysts**, fumed titanium dioxide, P25 and high surface area P25.

Industrial Solar Technology

Mr. Ken May

4420 McIntyre Street

Golden, CO 80403

Telephone: 303-279-8108

Fax: 303-279-8107

-Product(s): Compound parabolic concentrators, parabolic concentrators, and glass and polymer tubes for solar reactors.

Ishihara Sangyo Kaishi, Ltd.

1-3-11, Edohori, Nishi-ku

Osaka City 550, JAPAN

Telephone: **+81-6-444-5812**

Fax: **+81-6-444-5878**

Product(s): Photocatalytic paints and papers.

IT Corporation

Mr. Richard Miller

312 Directors Drive

Knoxville, TN 37923

Telephone: 423-690-3211

Fax: 423-694-9573

Product(s): Provides technology based solutions to environmental problems, reactor design and process engineering for treatment systems, and manufactures treatment systems through its NEPCCO Equipment Division.

Kato Manufacturing Company, Ltd.
400, Iwasaki, Komaki City
Aichi Pref. 485, JAPAN
Telephone: **+81-568-72-8280** Fax: **+81-568-75-1385**
Product(s): Glassware with photocatalytic titanium dioxide coatings.

KSE, Inc.
Dr. Charles Quinlan
P.O. Box 368
Amherst, MA 01004
Telephone: 413-549-5506 Fax: 413-549-5788
Product(s): Development and manufacturing of air emission control equipment for environmental remediation, industrial emissions, and indoor air quality applications.

LightStream Photocatalytic LLC
(A Division of E. Heller & Company)
Ephraim Heller
13 11 Harbor Bay Parkway
Suite 1000
Alameda, CA 94502
Telephone: 5 10-748-690 1 Fax: 5 10-748-6902
Product(s): Photocatalytic indoor air purification systems and photocatalytic paints and coatings.

Matrix Photocatalytic, Inc.
Mr. Bob Henderson
22 Pegler Street
London, Ontario
CANADA **N5Z 2B5**
Telephone: 5 19-660-8669 Fax: 5 19-660-8525
Product(s): Develop and supply photocatalytic treatment systems for aqueous and gas phase environmental remediation and control of process emissions.

NEPCCO
Mr. John S. "Sandy" Reese
2140-100 N.E. 36th Avenue
Ocala, FL 34470
Telephone: 904-867-7482 Fax: **904-867- 1320**
Product(s): Provides photocatalytic oxidation treatment systems as stand alone units or integrated into existing treatment or manufacturing processes.

Photo-Catalytics, Inc.
Mr. Gerald Cooper
755 S. 42nd Street
Boulder, CO 80303
Telephone: **303-494-7623** Fax: **303-494-7623**

Photox

Dr. Elliot Berman

P.O. Box 15717

Kenmore Station

Boston, MA 02215

Telephone: **617-353-6407**

Fax: 617-353-6466

Product(s): Development of photocatalysts and coatings for indoor air purification and residential water treatment.

Purifics Environmental Technologies, Inc.

Mr. Brian Butters

161 Mallard Road

London, Ontario

CANADA **NOM 1Z0**

Telephone: 519-473-5788

Fax: **519-473-0934**

Product(s): Sell or lease turn-key **TiO₂** photocatalytic systems for treatment of ground water, process, and **ultra pure water**, perform laboratory and on-site treatability tests, and perform design work to integrate units into existing treatment systems.

Sachtleben Chemie

Z. Hd. Bernhard **Becker/NPP**

Dr.-Rudolf-Sachtleben - Str. 4

D-47198 Duisburg, GERMANY

Telephone: 02066-22-o

Fax: 02066-2222-00

Product(s): Photocatalysts, sulfate process titanium dioxide, Hombikat UV 100

Science Applications International

Mr. Kelly Beninga

15000 West 6th Avenue

Suite 202

Golden, CO 80401

Telephone: 303-279-5677

Fax: 303-384-0320

Product(s): Develop and fabricate low-cost photochemical reactors.

Solar Kinetics, Inc.

Mr. Bennett Howell

P.O. Box 540636

Dallas, TX 75354

Telephone: 214-556-2376

Fax: 214-869-4158

Product(s): Develop and demonstrate solar photocatalytic systems for water treatment.

Trojan Technologies

Dr. William Cairns or Mr. Rory Murphy

3020 Gore Road

London, Ontario

CANADA **N5V 4T7**

Telephone: 519-457-3400

Fax: **519-457-3030**

Product(s): Cooperative and in-house research and development of commercial **photocatalytic** systems.



United Technologies Research Center

Dr. James Freihaut

411 Silver Lane, MS 129-24

East Hartford, CT 06108

Telephone: 203-727-7328

Fax: 203-727-2 15 1

Product(s): Research and development services for photocatalytic systems.

3.0 Compounds Studied

The tables in this section have the same format as in the first report. No compounds have been removed from the tables but new compounds have been added to the second and third tables to incorporate the expanded 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 provides a convenient frame of reference for citing the application of photocatalysis to compound oxidation. 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. Again, the citation prefix "**g**" indicates a gas-phase study. The treatability of compounds not demonstrated can in many cases 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- g e n	Het. Atom	Reference
1,1,1-Trichloroethane	CCl ₃ CH ₂ Cl	Cl		43,232,275
1,1,2,2-Tetrachloroethane	CCl ₂ CHCl ₂	Cl		43,275
1,1,2-Trichloroethane	CCl ₂ CH ₂ Cl	Cl		75,384
1,1,2-Trichloro-1,2,2-trifluoroethane	CCl ₂ CF ₂ CF ₂	Cl,F		
1,1-Dichloroethane	CH ₃ CHCl ₂	Cl		75
1,1-Dimethyl hydrazine	(CH ₃) ₂ NNH ₂		N	
1,2,3-Trichloropropane	CH ₂ ClCHClCH ₂ Cl	Cl		
1,2,4-Trichlorobenzene	C ₆ H ₃ Cl ₃	cl		159,474
1,2,4-Trimethylbenzene	C ₆ H ₃ (CH ₃) ₃			
1,2-Butylene oxide	H ₂ COCHCH ₂ CH ₃			
1,2-Dibromoethane	BrCH ₂ CH ₂ Br	Br		
1,2-Dibromo-3-chloropropane (DBCP)	CH ₂ BrCHBrCH ₂ Cl	Br,Cl		
1,2-Dichlorobenzene	C ₆ H ₄ Cl ₂	Cl		
1,2-Dichloroethane	ClCH ₂ CH ₂ Cl	Cl		6,232,275
1,2-Dichloroethylene	ClHC=CHCl	Cl		
1,2-Dichloropropane	CH ₃ CHClCH ₂ Cl	cl		32
1,2-Dinitrotoluene	C ₆ H ₃ CH ₃ (NO ₂) ₂		N	
1,2-Diphenylhydrazine	C ₁₂ H ₁₂ N ₂		N	
1,2-Trans-dichloroethene	C ₂ H ₂ Cl ₂	Cl		
1,3,5-Trinitrobenzene	C ₆ H ₃ (NO ₂) ₃		N	
1,3-Butadiene	H ₂ C=CHHC=CH ₂			
1,3-Dichlorobenzene	C ₆ H ₄ Cl	Cl		
1,3-Dichloropropene	CHCl=CHCH ₂ Cl	Cl		232
1,4-Dichlorobenzene	C ₆ H ₄ Cl ₂	Cl		88,89,104,242,243,244,380
1,4-Dioxane	OCH ₂ CH ₂ OCH ₂ CH ₂			
1-Amino-2-methylantrquinone	C ₆ H ₄ [C(O)] ₂ C ₆ H ₂ NH ₂ CH ₃			
1-Bromo-4-phenyloxybenzene	p-BrC ₆ H ₄ OC ₆ H ₅	Br		
2,2,4-Trimethylpentane	(CH ₃) ₃ C ₅ H ₉			
2,3,7,8-Tetrachlorodibenzo-p-dioxin	C ₁₂ H ₄ Cl ₄ O ₂	Cl		
2,4,5-Trichlorophenoxyacetic acid	C ₆ H ₂ Cl ₃ OCH ₂ CO ₂ H	Cl		
2,4,5-TP acid (silvex)	Cl ₃ C ₆ H ₂ OCH(CH ₃)COOH	Cl		
2,4,5-Trichlorophenol	C ₆ H ₂ Cl ₃ OH	Cl		
2,4,6-Trichlorophenol	C ₆ H ₂ Cl ₃ OH	Cl		457
2,4,6-Trinitrotoluene	CH ₃ C ₆ H ₂ (NO ₂) ₃			412,500
2,4 Diaminoanisole	(NH ₂) ₂ C ₆ H ₃ OCH ₃		N	
2,4-Dichlorophenoxyacetic acid (24-D)	Cl ₂ C ₆ H ₃ OCH ₂ COOH	Cl		380,467
2,4-Diaminoanisole sulfate	(NH ₂) ₂ C ₆ H ₃ OCH ₃ .H ₂ SO ₄		N	
2,4-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	Cl		5,430,448,467,468
2,4-Dimethylphenol	(CH ₃) ₂ C ₆ H ₃ OH			

Substance	Formula	Halo- g e n	Het. Atom	Reference
2,4-Dinitrophenol	C6H3OH(NO2)2		N	
2,4-Dinitrotoluene	C6H3CH3(NO2)2			
2,4-Toluene diamine	CH3(NH2)2C6H3		N	
2,6-Dinitrotoluene	C6H3CH3(NO2)2		N	
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		91,107,175,175,176,296,423,497
2-Ethoxyethanol	H3CCH2OCH2CH2CH2OH			
2-Methoxyethanol	MeOCH2CH2OH			
2-Methylnaphthalene	C10H7CH3			
2-Nitrophenol	NO2C6H4OH		N	
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	NH2C6H4)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			328
4-Nitrobiphenyl	C6H5C6H4NO2		N	
4-Nitrophenol	NO2C6H4OH		N	140,348
5-Nitro-o-anisidine	NO2C6H3(NH2)(OCH3)		N	
Acenaphthene	C10H6(CH2)2			
Acenaphthylene	C12H8			
Acetaldehyde	CH3CHO			g404.g440

Substance	Formula	Halo- gen	Het. Atom	Reference
Acetamide	CH ₃ CNOH ₂		N	194,
Acetone	CH ₃ COCH ₃			g43.g253.g383.g384.g407. g450
Acetonitrile	CH ₃ CN		N	g43.g252.g253
Acetophenone	CH ₃ C(O)C ₆ H ₅			477
Acrolein	CH ₂ CHCHO			
Acrylamide	CH ₂ CHCONH ₂		N	
Acrylic acid	H ₂ C:CHCOOH			
Acrylonitrile	H ₂ C:CHCN		N	
Aldrin	C ₁₂ H ₈ Cl ₆	Cl		
Allyl chloride	H ₂ C=CHCH ₂ Cl	Cl		
Aniline	C ₆ H ₅ NH ₂		N	374
Anthracene	C ₆ H ₄ (CH) ₂ C ₆ H ₄			98.188
Aramite	(CH ₃) ₃ CC ₆ H ₄ OCH ₂ CH(CH ₃)- SO ₃ C ₂ H ₄ Cl	Cl	S	
Atrazine	C ₁₈ H ₁₄ ClN ₅	Cl	N	80,296,355,356,357,447,527
Benzal chloride	C ₆ H ₅ CHCl ₂	Cl		
Benzamide	C ₆ H ₅ CONH ₂		N	271,272
Benzene	C ₆ H ₆			g43,110,137,138,154,g169,200, 269,322,330,g384,414,470, 488,530
Benzidine	NH ₂ (C ₆ H ₄) ₂ NH ₂		N	
Benzoic acid	C ₆ H ₅ COOH			91,135
Benzoic trichloride	C ₆ H ₅ CCl ₃	Cl		
Benzoyl chloride	C ₆ H ₅ COCl	Cl		
Benzoyl peroxide	(C ₆ H ₅ CO) ₂ O ₂			
Benzo(a)anthracene	C ₂₂ H ₁₄			188
Benzo(a)pyrene	C ₂₀ H ₁₂			188
Benzo(b)fluoranthene	C ₂₀ H ₁₂			
Benzo(g,h,i) perylene	C ₂₂ H ₁₂			
Benzyl alcohol	C ₆ H ₅ CH ₂ OH			91.120
Benzyl chloride	C ₆ H ₅ CH ₂ Cl	Cl		
BHC (Benzenehexachloride)	C ₆ H ₆ Cl ₆	Cl		
Biphenyl	C ₆ H ₅ C ₆ H ₅			
bis(2-Chloroethoxy)methane	CH ₂ (2-ClC ₂ H ₅ O) ₂	Cl		
Bis(2-chloroethyl) ether	ClCH ₂ CH ₂ OCH ₂ CH ₂ Cl	Cl		
Bis(2-chloro-1-methylethyl) ether	[ClCH ₂ (CH ₃)CH] ₂ O	Cl		
Bis(2-ethylhexyl) adipate	(C ₇ H ₁₃) ₂ C ₄ H ₈ (CO ₂) ₂			
Bis(2-ethylhexyl)phthalate	(C ₄ H ₉ CH(CH ₂)) ₂ OOC			
Bis(chloromethyl)ether	(CH ₂ Cl)O(CH ₂ Cl)	Cl		
Bromochloromethane	BrCH ₂ Cl	Br,Cl		
Bromodichloromethane	CHCl ₂ Br	Cl,Br		
Bromoethane	C ₂ H ₅ Br	Br		

Substance	Formula	Halo- g e n	Het. Atom	Reference
Bromoform (Tribromomethane)	CHBr3	Br		235
Bromomethane (Methyl bromide)	CH3Br	Br		
Butyl acrylate	CH2:CHCOOC4H9			
Butylbenzyl phthalate	C4H9OOC6H4COOC7H7			
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	362
Carbon disulfide	cs2		S	
Carbon tetrachloride	CCl4	Cl		g43,81,82,88,164,g169,277
Carbonyl sulfide	cos			
Catechol	C6H4(OH)2			
Chloramben (Benzoic acid, 3-amino-2, 5-dichloro-)	C6H(CO2H)(NH2)Cl2	Cl	N	
Chlordane	c10H6Cl8	Cl		
Chloroacetic acid	CH2ClCOOH	Cl		40,275
Chlorobenzene	C6H5Cl	Cl		g102,322,336
Chlorobenzilnte (Benzeneacetic acid, 4-chloro-alpha-(4-chlorophenyl)-)	(C6H4Cl)2C(OH)COOC2H5	Cl		
Chlorodibentodioxins, various	c12O2H8-xClx	Cl		
Chlorodibenzofurans	c12OH8-xClx	Cl		
Chlorodibromomethane	ClBr2CH	Br,Cl		
Chlorodifluoromethane	CHClF2	Cl,F		
Chloroethane	C2H5Cl	Cl		
Chloroform	CHCl3	Cl		g43,73,81,129,219,220,232,g253, 277,278,314,315,327,364
Chloromethane	CH3Cl	Cl		g263
Chloromethyl methyl ether	C2H5ClO	Cl		
Chloroprene	H2C:CHCl:CH2	Cl		
Chlorothalonil (1,3-Benzenededicarboni- trile, 2,4,5,6-tetrachloro-)	C6Cl4(CN)2		N	
Chrysene	C18H12			
cis-1,2-Dichloroethylene	ClHC:CHCl	Cl		
cis-1,3-Dichloropropene	CHCl:CHCH2Cl	Cl		
o-,m-,p-Cresols	CH3C6H4OH			60,6 1,429
Cumene	C6H5CH(CH3)2			
Cumene hydroperoxide	C6H5C(CH3)2OOH			
Cupferron (Benzeneamine,N-hydroxy- N-nitrose ammonium salt)	C6H5N(NO)ONH4		N	
Cyclohexane	C6H12			

Substance	Formula	Halo- gen	Het. Atom	Reference
Cyclohexanone	C6H10O			
Cyclonite (RDX)	(CH2)4(NNO2)4		N	
Decabromodiphenyl oxide	(C6Br5)2O	Br		
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	265
Dicofol ,4.4'-Dichloro-alpha-trichloro-methylbenzhydroi	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	
Dimethyl phthalate	C6H4(COOCH3)2			
Dimethyl sulfate	(CH3)2SO4		S	
Dimethylcarbanyl chloride	(CH3)2NCOC1	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			35,137,138,330,477,530
Ethylene	H2C:CH2			g169,g400,g405,g518
Ethylene glycol	CH2OHCH2OH			31
Ethylene oxide	CH2CH2O			g169
Ethylene thiourea	NHCH2CH2NHCS		N,S	

Substance	Formula	Halo- gen	Het. Atom	Reference
Ethyleneimide (Aziridine)	CH ₂ NHCH ₂		N	
Fluometuron [Urea, N,N-dimethyl-N'-[3-(trifluoromethyl)phenyl]-]	C ₁₀ H ₁₁ F ₃ N ₂ O	F	N	
Fluoranthene	C ₁₆ H ₁₀			
Fluorene	C ₆ H ₄ CH ₂ C ₆ H ₄			98
Fluorotrichloromethane	CCl ₃ F	Cl,F		
Formaldehyde	HCHO			g329,354
Heptachlor/heptachlor epoxide	C ₁₀ H ₇ Cl ₇	Cl		
Heptane	CH ₃ (CH ₂) ₅ CH ₃			g368
Hexachlorobenzene	C ₆ Cl ₆	Cl		234
Hexachlorobutadiene	Cl ₂ C:CClCCl:CCl ₂	Cl		
Hexachlorocyclopentadiene	C ₅ Cl ₆	Cl		
Hexachloroethane	Cl ₃ CCCl ₃	Cl		
Hexachloronaphthalene	C ₁₀ H ₂ Cl ₆	Cl		
Hexamethylphosphoramide	[(N(CH ₃) ₂) ₃ PO		P,N	
Hexamethylene- 1,6-diisocyanate	OCN(CH ₂) ₆ NCO		N	
Hexane	CH ₃ (CH ₂) ₄ CH ₃			g43
Hydroquinone	C ₆ H ₄ (OH) ₂			467521
Indeno(1,2,3-cd)pyrene	C ₂₂ H ₁₂			
Isophorone	C(O)CHC(CH ₃)CH ₂ C(CH ₃) ₂ CH ₂			
Isopropyl alcohol	(CH ₃) ₂ CHOH			28.g46,115,143,203,235,386
Lindane (gamma-Benzenehexachloride)	C ₆ H ₆ Cl ₆	Cl		
Malachite Green	C ₂₃ H ₂₅ ClN ₂	Cl	N	
Malathion	(CH ₃ O) ₂ P(S)SCH(CO ₂ C ₂ H ₅)- CH ₂ CO ₂ C ₂ H ₅		P,S	131,177
Maleic anhydride	HC:CHC(O)OC(O)			30
Maneb (Carbamodithioic acid, 1,2-ethanediybis-,manganese complex)	(SSCNCH ₂ CH ₂ NHCSS)Mn		N,S	
Mechlorethamine	CH ₃ N(CH ₂ CH ₂ Cl) ₂	Cl	N	
Melamine	H ₂ NCNC(NH ₂)NC(NH ₂)N		N	
Methanol	CH ₃ OH			g43,53,203,g252,g253,293, 364,373,g486,498
Methoxychlor	Cl ₃ CCH(C ₆ H ₄ OCH ₃) ₂	Cl		
Methyl acrylate	CH ₂ :CHCOOCH ₃			
Methyl butyl ketone	CH ₃ COC ₄ H ₉			
Methyl ethyl ketone	CH ₃ COCH ₂ CH ₃			88,448
Methyl iodide	CH ₃ I	I		
Methyl isobutyl ketone	(CH ₃) ₂ CHCOCH ₃			
Methyl isocyanate	CH ₃ NCO		N	
Methyl methacrylate	CH ₂ :C(CH ₃)COOCH ₃			
Methyl ten-butyl ether	(CH ₃) ₃ COCH			34,g383,g334
Methylene bromide	CH ₂ Br ₂	Br		
Methylene chloride	CH ₂ Cl ₂	Cl		40,g43,232,g253

Substance	Formula	Halo- gen	Het. Atom	Reference
Methylenebis(phenylisocyanate) (MBI)	CH ₂ (C ₆ H ₄ NCO) ₂		N	
Methylhydrazine	CH ₃ NHNH ₂		N	
Michler's ketone	CO[C ₆ H ₄ N(CH ₃) ₂] ₂		N	
Mirex	C ₁₀ Cl ₁₂	Cl		
Mustard gas	S(CH ₃ CH ₂ Cl) ₂	Cl	S	121
m-Nitroaniline	NO ₂ C ₆ H ₄ NH ₂		N	
N,N-Dimethylaniline	C ₆ H ₅ N(CH ₃) ₂		N	
Naphthalene	C ₁₀ H ₈			98
Naphthylamine (alpha-, beta-)	C ₁₀ H ₇ NH ₂		N	148
Nitrilotriacetic acid	N(CH ₂ COOH) ₃		N	
Nitrobenzene	C ₆ H ₅ NO ₂		N	272,307,336,357,373
Nitrofen [Benzene, 2,4-dichloro-1-(4-nitrophenoxy)-]	C ₁₂ H ₇ Cl ₂ NO ₃	Cl	N	
Nitrogen mustard (2-Chloro-N-(2-chloroethyl)-N-methylethanamine)	(ClCH ₂ CH ₂) ₂ NCH ₃	Cl	N	
Nitroglycerin	CH ₂ NO ₃ CHNO ₃ CH ₂ NO ₃		N	317,g318.g450
Nitrophenol	NO ₂ C ₆ H ₄ OH		N	19,307
n-Butyl alcohol	CH ₃ (CH ₂) ₂ CH ₂ OH			
n-Dioctyl phthalate	(C ₈ H ₁₇ OOC) ₂ C ₆ H ₄			
N-Nitrosodiethylamine	C ₄ H ₁₀ N ₂ O		N	
N-Nitrosodimethylamine	(CH ₃) ₂ N ₂ O		N	
N-Nitrosodiphenylamine	(C ₆ H ₅) ₂ NNO		N	
N-Nitrosodi-n-butylamine	ONN(n-C ₄ H ₉) ₂		N	
N-Nitrosodi-n-propylamine	ONN(n-C ₃ H ₇) ₂		N	
N-Nitrosomethylvinylamine	ONN(CH ₃)(C ₂ H ₃)		N	
N-Niuosomorpholine	ONNC ₄ H ₈ O		N	
N-Nitrosonomicotine			N	
N-Niuosopiperidine	C ₅ H ₁₀ NHNO		N	
N-Niuoso-N-ethylurea	C(O)(NH ₂)N(NO)C ₂ H ₅		N	
N-Nitroso-N-methylurea	C(O)(NH ₂)N(NO)(CH ₃)		N	
n-Pentane	CH ₃ (CH ₂) ₃ CH ₃			
Octachloronaphthalene	C ₁₀ Cl ₈	Cl		
Octane	CH ₃ (CH ₂) ₆ CH ₃			
Oxirane	H ₂ COCH ₂			
o-Anisidine	CH ₃ OC ₆ H ₄ NH ₂		N	
o-Anisidine hydrochloride	CH ₃ OC ₆ H ₄ NH ₂ .HCl	Cl	N	
o-Nitroaniline	NO ₂ C ₆ H ₄ NH ₂		N	
o-Toluidine	CH ₃ C ₆ H ₄ NH ₂		N	
o-Toluidine hydrochloride	CH ₃ C ₆ H ₄ NH ₂ .HCl	Cl		
Parathion (DNTP)	(C ₂ H ₅ O) ₂ P(S)OC ₆ H ₄ NO ₂		P,S	
PCBs (Aroclor 1260,1254,1248, and 1242)	C ₁₂ Cl _x H _{10-x}	Cl		88,359,529 536
Pentachlorobenzene	C ₆ Cl ₅ H	Cl		
Pentachlorophenol	C ₆ Cl ₅ OH	Cl		5,52,130,277,305,306,423

Substance	Formula	Halo- gen	Het. Atom	Reference
Peracetic acid	<chem>CH3COOOH</chem>			
Phenanthrene	<chem>C14H10</chem>			
Phenol	<chem>C6H5OH</chem>			2.47.53.119.136,224,272,328. 36.g349,355,364,373,387, 15,423,429.g441,442,468, 69.566
Phenol, <i>o</i> -methyl	<chem>C7H8O</chem>			
Phosgene	<chem>COCl2</chem>	Cl		
Phthalic anhydride	<chem>C6H4(CO)2O</chem>			0
Picric acid	<chem>C6H2(NO2)3OH</chem>		N	
Polybrominatedbiphenyls	<chem>C12BrxH10-x</chem>	Br,Cl		
Propane sultone	<chem>C3H6SO2</chem>		S	
Propionaldehyde	<chem>C2H5CHO</chem>			45,246,g522
Propiolactone, beta -	<chem>C3H4O2</chem>			
Propoxur [Phenol, 2-(1-methylethoxy)- methylcarbamate]	<chem>C11H15NO3</chem>		N	96
Propylene oxide	<chem>C2H2OCHCH3</chem>			
Propylene (Propene)	<chem>C3H6</chem>			367
Propyleneimine	<chem>C3H5NH</chem>		N	
Pyrene	<chem>C16H10</chem>			
p-Anisidine	<chem>C7H7NO</chem>		N	
p-Chloro-m-cresol	<chem>C6H4ClOH</chem>	Cl		
p-Cresidine	<chem>C7H9NO</chem>		N	
p-Nitrosodiphenylamine	<chem>(C6H5)2NNO</chem>		N	
p-Phenylenediamine	<chem>C6H4(NH2)2</chem>		N	
Quinoline	<chem>C9H7N</chem>		N	
Quinone	<chem>C6H4O2</chem>			
Quintozene (Pentachloronitrobenzene)	<chem>C6Cl5NO2</chem>	Cl	N	
Safrole	<chem>C9H8O2</chem>			
sec-Butyl alcohol	<chem>C4H9OH</chem>			
Sevin (carbaryl)	<chem>C10H7O2N</chem>			
Sodium Alizarinsulfonate	<chem>C14H9O6S2Na</chem>		N,S	
Styrene	<chem>C8H8</chem>			176
Styrene oxide	<chem>C8H8O</chem>			
Terephthalic acid	<chem>C6H4(COOH)2</chem>			
tert-Butyl alcohol	<chem>(CH3)3COH</chem>			34
tert-Butylformate	<chem>(CH3)3COC(O)H</chem>			34,
Tetrachloroethylene	<chem>C2Cl4</chem>	Cl		g4,88,g183,g195,217,232,g253
Tetrachlorvinphos	<chem>C10HCl4O4P</chem>	Cl	P	
Tetrahydrofuran	<chem>C4H8O</chem>			73
Thioacetamide	<chem>CH3CSNH2</chem>		S,N	
Thiourea	<chem>(NH2)2CS</chem>		S,N	

Substance	Formula	Halo- g e n	Het. Atom	Reference
Toluene	C ₆ H ₅ CH ₃			g16.g43.66,110.137.138.g169, g195.269,270.g329.330.336, g403.448.470,530
Toluene diisocyanate	CH ₃ C ₆ H ₃ (NCO) ₂		N	
Total xylenes	C ₆ H ₄ (CH ₃) ₂			
Toxaphene	C ₁₀ H ₁₀ Cl ₈	Cl		
Triaziquone	C ₁₂ H ₁₃ N ₃ O ₂		N	
Trichlorfon	(CH ₃ O) ₂ P(O)CH(OH)CCl ₃	Cl	P	
Trichloroethylene	CHCl:CCl ₂	Cl		g4.g11,40.g43.167.g174.g183, g195.g196.g198,217.232.239, 240.g252.g253,269,270,288, 327,346.g384.g445,448.g494, g485.g496,523,532
Triethylamine	N(C ₂ H ₅) ₃		N	
Trifluralin	F ₃ C(NO ₂) ₂ C ₆ H ₂ N(C ₃ H ₇) ₂	F	N	
Tnnitrophenylmethylnitramine	(NO ₂) ₃ C ₆ H ₂ N(NO ₂)CH ₃		N	
Tris(2,3-dibromopropyl) phosphate	(CH ₂ BrCHBrCH ₂ O) ₃ PO	Br	P	
Urethane (ethyl carbamate)	CO(NH ₂)OC ₂ H ₅		N	
Vinyl acetate	CH ₃ COOCH:CH ₂			
Vinyl bromide	CH ₂ CHBr	Br		
Vinyl chloride	CH ₂ :CHCl	Cl		g43
Vinylidene chloride	CH ₂ :CCl ₂	Cl		
Xylene (mixed isomers)	C ₆ H ₄ (CH ₃) ₂			110,137.138,269,313.330,g403, 470,530
Zineb	Zn(CS ₂ NHCH ₂) 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	Cl ₃ CCH ₂ Cl	Cl		275
1,1,1-Trifluoro-2,2,2-trichloroethane	F ₃ CCCL ₃	F,Cl		
1,1,1-Trifluorobromochloroethane	C ₂ H ₂ F ₃ ClBr	F		
1,1-Difluoro-1,2,2-trichloroethane	ClF ₂ CCCl ₂	F,Cl		
1,1-Difluoro-1,2-dichloroethane	F ₂ ClCClH ₂	F,Cl		
1,1-Difluoroethylene	C ₂ H ₂ CF ₂	F		
1,2-Dimethoxybenzene	(CH ₃ O) ₂ C ₆ H ₄			172
1,2-Bis(2-chloroethoxy)ethane	(ClC ₂ H ₄) ₂ C ₂ H ₄	Cl		106
1,2,4,5-Tetramethylbenzene	(CH ₃) ₄ C ₆ H ₂			113
1,3-Diphenylisobenzofuran	(C ₆ H ₅) ₂ C ₆ H ₂ OC ₆ H ₄			
1-Benzylnicotinamide	(C ₆ H ₅)CH ₂ (C ₅ H ₃ N)C(O)NH ₂		N	133
1-Bromodecane	BrC ₁₀ H ₂₁	Br		
1-Bromododecane	BrC ₁₂ H ₂₅	Br		
1-Butanol	CH ₃ (CH ₂) ₃ OH			
1-Dodecanol	CH ₃ (CH ₂) ₁₁ OH			
1-Hexene	C ₆ H ₁₂			
1-(Methoxyphenyl)-2-propanol	(CH ₃ OC ₆ H ₄)(CH ₃)CHOH			15
1-Propanol	n-C ₃ H ₇ OH			245,246,247
2,3-, 2,4- or 3,4-Difluorophenol	F ₂ C ₆ H ₃ OH	F		129
Tris-(2,4-dichlorophenoxy)ethylphosphite	C ₂ H ₅ P[OC ₆ H ₃ Cl ₂] ₃	Cl	P	
2,6-Dichlorophenol	C ₆ H ₃ Cl ₂ OH	Cl		
2,7-Dichlorodibenzo-p-dioxin	Cl ₂ C ₁₂ H ₆ O ₂	Cl		
2-, 3-, 4-Fluorophenol	F ₃ C ₆ H ₄ OH	F		129
2-Chlorodibenzo-p-dioxin	ClC ₁₂ H ₇ O ₂	Cl		
2-Chloroethylmethylsulfide	ClCH ₂ CH ₂ SCH ₃	Cl	S	
2,3-Benzofuran	C ₈ H ₆ O			
2,3- and 2,5-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	Cl		
2,5-Dinitrophenol	(NO ₂) ₂ C ₆ H ₃ OH	Cl	N	
2,6-Dichloroindophenol	C ₈ H ₂ N(OH)Cl ₂			
2,5-Furandimethanol	C ₄ H ₂ O(CH ₂ OH) ₂			388
2-Chloroaniline	ClC ₆ H ₄ NH ₂	Cl	N	525
2-Coumaranone	C ₈ H ₆ O ₂			
2-Furoic Acid	(CH ₂) ₃ CHOCO ₂ H			
2-Hydroxypyridine	HOC ₅ H ₄ N		N	271
2-Hydroxytetrahydropyran	HOC ₅ H ₉ O			59
2-Naphthol	C ₁₀ H ₇ OH			
3,3,3-Trifluoropropene	CH ₂ CHCF ₃			
3,3'-Dichlorobiphenyl	(ClC ₆ H ₄) ₂	Cl		

Substance	Formula	Halo- gen	Het. Atom	Reference
3,4-Chlorophenol	3,4-Cl ₂ C ₆ H ₃ OH	Cl		
3-Chlorophenol	m-ClC ₆ H ₄ OH	Cl		175.296,497
3-Chlorosalicylic acid	C ₇ H ₅ ClO ₃	Cl		
4-Bromophenol	BrC ₆ H ₄ OH	Br		328
4-t-Butyltoluene	p-(t-C ₄ H ₉)C ₆ H ₄ CH ₃			
4-Chloro-3-nitro-benzotrifluoride	C ₆ HCl(NO ₂)F ₃	F,Cl	N	
4-Chlorophenol	ClC ₆ H ₄ OH	Cl		108,140,141,142,172,173,175,277, 279,296,298,303,328,394, 443,g444,481,484,485,497, 512,513,514,521
4-Chlorophenylisocyanate	ClC ₆ H ₄ NCO	Cl	N	375
4-Fluorophenol	FC ₆ H ₄ OH	F		328
4-Hydroxyacetophenone	HOC ₆ H ₄ C(O)CH ₃			328
4-Hydroxybenzyl Alcohol	p-HO(C ₆ H ₄)CH ₂ OH			386
4-Iodophenol	IC ₆ H ₄ OH	I		328
4-Methoxyphenol	CH ₃ C ₆ H ₄ OH			328
4-Nitroaniline	NO ₂ C ₆ H ₄ NH ₂		N	442
4-Nitrocatechol	(NO ₂)C ₆ H ₃ (OH) ₂		N	
4-Niuophenylethylphosphinate	(NO ₂)C ₆ H ₄ (C ₂ H ₅)PO ₂		N,P	
4-Nitrophenylisopropylphosphinate			N,P	
4-nitrophenyldiethylphosphate			N,P	
4-Thiophenyl- 1 -butanol	C ₆ H ₅ S(CH ₂) ₄ OH		S	
4-Trifluoromethylphenol	CF ₃ C ₆ H ₄ OH	F		328
5-Fluorouracil	FC ₄ H(NH) ₂ (O) ₂	F		12
5-Hydroxypentanoic acid	HO(CH ₂) ₄ CO ₂ H			
12-phenyldodecanesulfonate, Sodium Salt	C ₆ H ₅ (CH ₂) ₁₂ SO ₃ H			
Acenaphthene	C ₁₀ H ₁₆ (CH ₂) ₂			98,188
Acetic Acid	CH ₃ CO ₂ H			52,203,210,212,275,354,g416, g417
Acetophenone	CH ₃ COC ₆ H ₅			
Acetylene	C ₂ H ₂			236,254
Acid orange 7	Na ₂ O ₃ SC ₆ H ₄ N ₂ C ₁₀ H ₆ OH		N,S	480,482,483
Adipic acid	C ₅ H ₁₁ CO ₂ H			147
Aldicarb	CH ₃ SC(CH ₃) ₂ CHN(O)C(O)NHCH ₃		N,S	5
p-alkylphenol (various)	R(C ₆ H ₄)OH			
Allyl alcohol	C ₃ H ₅ OH			
Alochlor				
p-Aminophenol	NH ₂ (C ₆ H ₄)OH		N	74,79,101
Anthraquinone-2-sulfonic acid	HO ₃ SC ₁₄ H ₇ O ₂		S	227
AOX or Haloform Precursors				248,249,434,435
Asulam				
Azobenzenes (various)	XC ₆ H ₄ NNC ₆ H ₄ X		N	103
Azobisformamidoaceuc acid			N	490

Substance	Formula	Halo- g e n	Het. Atom	Reference
Bacteria/Algae/Virus				15,55,123,124,125,126,g139,189, 216,283,284,333,365,391,401, 437,503,505,507
Benzaldehyde	C ₆ H ₅ C(O)H			476
Benzophenone	(C ₆ H ₅) ₂ CO			323
Benzoquinone	C ₆ H ₄ O ₂			272,385,387
Benzyl dodecyl dimethyl ammonium chloride	(C ₆ H ₅ CH ₂)(C ₁₂ H ₂₅)(CH ₃) ₂ N,Cl	Cl	N	161,533
Benzyl tetradecyl dimethyl ammonium chloride	(C ₆ H ₅ CH ₂)(C ₁₄ H ₂₇)(CH ₃) ₂ N,Cl	Cl	N	158,160
Biomass				187
Bipthalate	(C ₆ H ₄)(CO ₂ H)(CO ₂) ⁽⁻¹⁾			
Bromobutene	BrC ₆ H ₅	Br		336
Butane	C ₄ H ₁₀			
But-2-ene, trans	C ₄ H ₈			g181
Butyl alcohol	n-C ₄ H ₉ OH			53
Butylamine	n-C ₄ H ₉ NH ₂		N	75
t-Butylazine			N	296,393
Butadiene	C ₄ H ₆			g329
Butyric acid	C ₃ H ₇ CO ₂ H			135,354
Carbetamide			N	54
Carbon dioxide (reduction)	202			166,186,191,282,334,438,460
Carbon monoxide	30			g264,g405,g452
Carbon tetrabromide	CBr ₄	Br		
Catechol	C ₆ H ₄ (OH) ₂			521
Cetyl dimethyl benzyl ammonium chloride	(C ₁₈ H ₃₇)(CH ₃) ₂ N,Cl		N	200,370
Cetyl pyridinium chloride	(C ₁₈ H ₃₇)(C ₅ H ₅ N),Cl		N	370
Chloroacetaldehyde	ClCH ₂ COH	Cl		275
Chlorobenzoic acids, o-, m-, or p-	Cl(C ₆ H ₄)CO ₂ H	Cl		g3
Chlorofluorocarbons, various		F,C		
Chloral hydrate	Cl ₃ CO(OH) ₂	Cl		275,534
Chloranil, o- and p-	C ₆ Cl ₄ O ₂	Cl		
Chloroethyl ammonium chloride	ClH ₃ N,Cl	Cl	N	
Chlorpyrifos		Cl	S,N	127
Ciba Orange RI				528
Coal or Carbon				567
Color and/or COD (in wastewater)				13,100,103,251,332,434,435, 159,465
Congo Red	C ₃₂ H ₂₂ O ₆ N ₆ S ₂ Na ₂			
Cresol violet	C ₁₆ H ₈ NO(NH ₂),Cl		N	
Creosote phenolics				464
Cyanuric acid	C ₃ N ₃ (OH) ₃		N	
Cyclododecanol	C ₁₂ H ₂₃ OH			120
Cyclohexane	C ₆ H ₁₂			g368,g508
Cyclohexanedicarboxylic Acids	C ₆ H ₁₀ (CO ₂ H) ₂			

Substance	Formula	Halo- g e n	Her. Atom	Reference
Cyclohexanol	C ₆ H ₁₁ OH			120,442
Cyclohexene	C ₆ H ₁₀			
Cyclohexene oxide	C ₆ H ₁₀ O			
Cyclophosphamide	OPONHC ₃ H ₆ [N(C ₂ H ₄ Cl) ₂]		N	
Cinnamyl alcohol	C ₆ H ₄ C ₂ H ₂ OH			
DDT	(ClC ₆ H ₄) ₂ CHCCl ₃	Cl		
Decalin	C ₁₀ H ₁₈			
Decamethylteuasiloxane	(CH ₃) ₁₀ Si ₄ O ₃		Si	3361
Decanoic acid	C ₉ H ₁₉ CO ₂ H			
Decanol	HOC ₁₀ H ₂₁			
Desipramine	(C ₆ H ₄) ₂ (CH ₂) ₂ N(CH ₂) ₃ NHCH ₃			
Dibenzo-p-dioxines, various		Cl		536,555
Dibromomethane	CH ₂ Br ₂	Br		
Dichloroacetic acid	Cl ₂ CHCO ₂ H	Cl		40,52,167,256,275,277,392
Dichloroacetyl Chloride	Cl ₂ CHCOCl	Cl		3239,g240
Dimethylamme	CH ₃) ₂ NH		N	364
Dimethylsulfide	(CH ₃) ₂ S		S	3361,g363
Dimethyl-2,2-dichlorovinyl phosphate	CH ₃) ₂ (Cl ₂ CCH)PO ₄	Cl	P	177
Diphenylmethane	C ₆ H ₅) ₂ CH ₂			
Diphenylsulfide	(C ₆ H ₅) ₂ S		S	
Direct blue 1	(Na ₂ O ₃ S)C ₁₆ H ₆ (NH ₂)(OH)- (OCH ₃) ₂ N ₂) ₂		N,S	480
Dodecane	C ₁₂ H ₂₆			
Dodecyl sulfate	C ₁₂ H ₂₅) ₂ SO ₄			
Dodecylbenzenesulfonate	(C ₁₂ H ₂₅)C ₆ H ₄ SO ₃ (-1)		S	160,161,533
Dodecyldecaoxyethylenephosphates			P	162
Dodecylpyridinium chloride	(C ₁₂ H ₂₅)C ₅ H ₅ NH ₂ Cl	Cl		23,156,158
Doxycycline				
Eosin				
Ethambutol			N	261
Ethane	C ₂ H ₆			3487,488
Ethanol	C ₂ H ₅ OH			28,g43,122,194,203,g450, 154
Ethylacetate	CH ₃ CO ₂ C ₂ H ₅			
Ethylenediaminetetraacetic acid	(O ₂ CCH ₂) ₄ N ₂ C ₂ H ₄			259,373
2-, 3-, or 4-Ethylphenol	(C ₂ H ₅)C ₆ H ₄ OH			177
Fenitiothion	C ₉ H ₁₂ NO ₅ PS		P	
Fluorescein	C ₂₀ H ₁₂ O ₅			
Folicur			N	491
Formic Acid	HCO ₂ H			2,80,117,135,223,233,275,354, 373,418,419,420
Fullerenes	C ₆₀ , C ₇₀ , and C ₈₄			207,208,408
Fulvic acid				177,573

Substance	Formula	Halo- g e n	Het. Atom	Reference
Glycerol	C3H5(OH)3			
HCFC or HFC		Cl,F		g455
Heparin				54
Hexafluorobenzene	C6F6	F		308
Hexafluoropropene	CF2CFCF3	F		113
Hexanol	C6H13OH			120
Humic Acids				132.170.250.332,479
Hydroxybenzoic acid (various)	HOC6H4(OH)CO2H			
Hydroxycarboxylic acids, alpha	RCH(OH)CO2H			
Hydroxyethylcellulose				
Indole	C8H6NH		N	g361
Isobutane	C4H10			86
Isobutanol	CH3CH(CH3)CH2OH			
Isobutene	C4H8			
Isobutyric Acid	CH3CH(CH3)CO2H			
Isoprene	CH2C(CH3)CHCH2			g192
Isorsorbide dinitrate	C6O2H8(ONO2)2		N	
Iso-octane	(CH3)2CH(CH2)4CH3			g43.g253
L-Lysine	NH2(CH2)4CH(NH2)CO2H			
Lactic acid	C3H6O3			163
Kraft lignin				187,337,434,435
Maleic acid	HO2CCHCHCO2H			135
Malonic acid	CH2(CO2H)2			135,147,259
Methane	CH4			g487,488
Methanethiol	CH3SH			g504
Methylcyclohexane	CH3C6H11			g368
Methyl orange	Na.O3SC6H4N2C6H4N(CH3)2		N,S	77,78,301
Methyl viologen	(CH3C5H4N)2.Cl2	Cl	N	g60,301,501
Methylene blue	(CH3)2NC6H3NSC6H3N(CH3)2.Cl	Cl	N,S	17,39,324,463,475
Methylvinylketone	CH3COC2H3			
Monuron	ClC6H4NHCON(CH3)2	Cl	N	g0,375
m-Phenoxytoluene	m-C6H5O-C6H4CH3			
N,N,N',N'-Tetraethyloxonine			N	179
Naphthol	C10H7OH			
Nile Blue A	C16NO(NH2)N(C2H5)2.SO4		N,S	179
Nitrocellulose			N	12
p-Nitrotoluenesulfonic acid	(CH3)(NO2)C6H3SO3H		N,S	310
Nitrotoluene, various	NO2C6H4CH3		N	
Nonylphenoethoxylate	C9H17C6H4OC2H5			
Oil/Petroleum				44.152,153,200,320
Oxalic acid	C2O4H2			135,147,259,273,275,354
Pendimethalin				351
Pentafluorophenol	C6F5OH			308

Substance	Formula	Halo- g e n	Het. Atom	Reference
n-Pentyl amine	n-C5H11NH2		N	
Permethrin				161
Phenosafranin	C6H5N2C12H4(NH2(CH3)2		N	39
Picoline	CH3C5H4N		N	
Piperidene	C5H10NH		N	75
Polyethoxylene Alkyl Ethers	R2(OC2H4)n			156,432
Polyethylene	(CH2CH2)n			291
Polypropylene	[(CH3)CHCH2]n			291
Polyvinylalcohol	(C2H3OH)n			213,292
Proline	C4H8NCO2H		N	
Prometon				
Prometryn				
Propane	C3H8			g487
Propionic acid	C2H5CO2H			
Propylene glycol dinitrate	CH3CH(NO3)CH2(NO3)		N	257
Propyne	CH3CCH			
Propyzamide			N	473
Pyridine	C5H5N		N	75.g195.27 1.g402
Pyrocatechol	o-C6H4(OH)2			
Pyrrole	C4H5N		N	g361
Reactive Dyes				299
Red Dye 79			N,S	
Resorcinol	C6H6O2			101
Rhodamine B	CH3OC(O)(C6H4)C13H6O(NH2)2		N	
Rhodamine 6G	C2H5OC(O)C6H4C13H4(CH3)2- [N(C2H5)]2.Cl	Cl	N	297
Rhodamine 6ZH				237
Rose Bengal	Na2.O2CC6Cl4C13H2O14O2	Cl		393
S-Dodecyl thioether carboxylates			S	157
S-Ethyl-N,N-dipropyl thiocarbamate (EPTC)	(C2H5)SC(O)N(C3H7)2		N,S	478
S-Ethyl-N,N-diisopropylthiocarbamate (Butylate)	(C2H5)SC(O)N(i-C3H7)2		N,S	478
S-Ethyl-4-hexahydro-1-H-azepine-1- carbothionate (molinate)			N,S	478
S-Propyl-N-cyclohexyl thiocarbamate (cycloate)	(C3H7)SC(O)NH(C6H11)		N,S	478
S-Propyl-N,N-dipropyl thiocarbamate (vemolate)	(C3H7)SC(O)(NC3H7)2		N,S	478
Salicylic acid	C7H6O3			7,92,95,97,99,221,302,373,376, 448,454,466.52 1,524
Simazine	(C2H5)Cl(NHC2H5)C3N3			
Sodium chloroacetate	CH3CO2Na	Cl		

Substance	Formula	Halo- g e n	Het. Atom	Reference
Sodium dodecylbenzene sulfonate	$C_{12}H_{25}C_6H_4SO_3Na$		S	
Stilbene	$C_{16}H_{14}$			
Succinic acid	$C_4H_6O_4$			35.147,163
Sucrose	$C_{12}H_{22}O_{11}$			
Sulfones	$RS(O)_2R'$		S	139
Tetrachlorvinphos	$C_2HCl_3CH_2(2,4,5-Cl_3C_6H_2)(CH_3)PO_4$	Cl	P	118
Tetrafluoroethylene	C_2F_4	F		
Tetralin	$C_{10}H_{12}$			
Tetramethylenediamine	$NH_2(CH_2)_4NH_2$		N	
Tetrabutylammonium phosphate	$[(n-C_4H_9)_4N]_4.PO_4$		P	
Theophylline	$C_7H_8N_4O_2.H_2O$		N	
Thioethers	RSR'		S	121
Thiobencarb				322.336
Thymine	$C_5H_6N_2O_2$		N	
Thionine	$3\ C_12NS(NH_2)_2O_2CCH_3$		S,N	19
p-Toluenesulfonic acid	$CH_3(C_6H_4)SO_3H$		S	50.62
s-Triazines			N	274
Trichloroacetic acid	Cl_3CCO_2H	Cl		10.275
Trietazine			N	
Triethanolamine	$N(CH_2CH_2OH)_3$		N	433
Trifluoroacetic acid	CF_3CO_2H	F		238
Trihydrazmotriazine			N	490
Trihydroxybenzene	$(HO)_3C_6H_3$			
Trimethylamine	$(CH_3)_3N$		N	
Trinitrophenol	$(NO_2)_3C_6H_2OH$			
Triphenylacetic acid	$(C_6H_5)_3CCO_2H$			
Umbelliferone	$C_9H_6O_3$			

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	
Aluminum (fume or dust)	Al	
Aluminum oxide	Al ₂ O ₃	
Ammonia	NH ₃	364,492,518
Ammonium nitrate (soln)	NH₄NO₃	58
Ammonium sulfate (soln)	(NH₄)₂SO₄	
Antimony	Sb	
Arsenic	As	
Asbestos	Mg,Si	
Azide ion	N ₃ ⁻	
Barium	Ba	
Beryllium	Be	
Bismuth	Bi	
Boron	B	
Cadmium	Cd	221,371,372,373
Chlorine	Cl	
Chlorine dioxide	ClO ₂	
Chromium	Cr	71,72,106,134,255,371,372,373
Cobalt	co	
Copper	cu	109,117,165,166,221,371,372,373, 498
Cyanide and Complexes	CN(-1) and M(CN)_x	3,9,106,178,262,377,378,379,540,545,571
Cyanite ion	CNO(-1)	57
Gold	Au	57,115,373
Halide ion	X ⁽⁻¹⁾ , X = F, Cl, Br, or I	292,398,542
Hydrazine	H₂NNH₂	
Hydrogen sulfide	H₂S	338,539,562,570
Hypophosphorus acid	H₂PO₂	24,163,282
Iron	Fe	154
Lead	Pb	272
Manganese	Mn	
Mercury	Hg	3,22,137,1373,377,379, 162,499
Molybdenum	Mo	
Nickel	Ni	109,371,372,373
Nitrates/nitrites	NO₃(-1),NO₂(-1)	294,295

Substance/Element	Formula/Symbol	Reference
Nitrogen oxides	NOX	g179,g180,g181,g182,g409, g410,g453
Nitrogen	N2	461
Oxalate ion	C2O4(2-)	
Oxygen	O2	
Ozone	O3	g436
Palladium	Pd	
Phosphorus		
Platinum	Pt	37 1,372,373
Radium	Ra	
Radon	Rn	
Rhodium	Rh	
Selenium	Se	
Silicon	Si	
Silver	Ag	25,78,92,155,294,37 1,373
Strontium	Sr	
Sulfate radical	SO4(1-)	
Sulfite		114,294,54 1
Sulfur		
Sulfur dioxide	so2	
Sulfuric acid	H2SO4	
Thallium	Tl	
Thiocyanate	SCN(1-)	59,540
Thiosulfate	S2O3(2-)	
Thorium	th	
Tin	Sn	
Tritium	H,(T)	
Tungsten	W	
Vanadium	V	
Zinc	zn	

4.0 Conclusions

The level of activity in this field continues to grow at a rapid rate. The potential to develop new methods for solving environmental problems is the primary driving force for the R&D activity. However, the patents that have been awarded and the increase in research activity in areas such as water and air disinfection, odor control, indoor air quality, and consumer products indicate that the technology has a broader commercial potential. Recent work reflects the increased interest in applying photocatalytic processes to the treatment of contaminated gas streams. More attention is also 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. This can be an aid in developing an understanding of the chemical mechanisms of the processes and is necessary to insure that potentially harmful substances are not left in the processed stream. Still, relatively few studies include mass balances for the reactions. Kinetic models that can be used to size treatment systems are also relatively 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. The high level of activity in this field is likely to continue -- it remains to be seen how widespread the applications may be.

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TiO₂, other semiconductor, solar, nonaqueous, application.

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TiO₂, other semiconductor, modified **TiO₂**.
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TiO₂, nonaqueous, modified **TiO₂**.
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TiO₂, oxidant, **reductant**, aqueous phase, mechanism.
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TiO₂, gas phase, modified **TiO₂**, application, IAQ, adsorbent, immobilized **TiO₂**.
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TiO₂, metallized **TiO₂**, disinfection, aqueous phase, modified **TiO₂**, process efficiency, immobilized **TiO₂**.
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TiO₂, gas phase, modified **TiO₂**, immobilized **TiO₂**, adsorbent.
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TiO₂, gas phase, modified **TiO₂**, mechanism.

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 TiO_2 , metallized TiO_2 , aqueous phase, modified TiO_2 , immobilized TiO_2 .
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 TiO_2 , aqueous phase, modified TiO_2 .
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 TiO_2 , aqueous phase, biotreatment.
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TiO₂, aqueous phase other semiconductors.

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TiO₂, aqueous phase, modified **TiO₂**.

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TiO₂, reactor, engineering, aqueous phase, process efficiency.

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TiO₂, engineering, reactor, modeling, aqueous phase, process efficiency, mechanism.

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TiO₂, engineering, reactor, aqueous phase, process efficiency.

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TiO₂, other semiconductor, aqueous phase, modified **TiO₂**, mechanism.

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TiO₂, other semiconductor, oxidant, aqueous phase, mechanism.

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TiO₂, aqueous phase, mechanism.

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TiO₂, aqueous phase, process efficiency.

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TiO₂, aqueous phase, mechanism.

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TiO₂, aqueous phase, adsorption.

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TiO₂, engineering, reactor, modeling, aqueous phase, cost.

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TiO₂, aqueous phase, application.

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TiO₂, aqueous phase, application, engineering.
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TiO₂, engineering, aqueous phase, application.
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TiO₂, other semiconductor, oxidant' gas phase, mechanism.
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Microbial, **TiO₂**, disinfection, aqueous phase, modified **TiO₂**.
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TiO₂, reductant, nonaqueous.
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TiO₂, gas phase, modified **TiO₂**.
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TiO₂, aqueous phase, mechanism.

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TiO_2 , aqueous phase, mechanism.

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TiO_2 , gas phase, mechanism.

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TiO_2 , gas phase, mechanism.

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TiO_2 , modified TiO_2 .

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TiO_2 , reactor, solar, pesticide, aqueous phase, immobilized TiO_2 , application.

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TiO_2 , other semiconductor, metallized TiO_2 , aqueous phase, modified TiO_2 .

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TiO_2 , aqueous phase, modified TiO_2 , immobilized TiO_2 .

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TiO_2 , gas phase, application, oxidant.

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TiO_2 , aqueous phase, application.

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 TiO_2 , metallized TiO_2 , gas phase, modified TiO_2 , immobilized TiO_2 , adsorbent, adsorption, carbon monoxide.
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 TiO_2 , gas phase, modified TiO_2 , application, immobilized TiO_2 , adsorbent.
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 TiO_2 , other semiconductor, gas phase, mechanism.
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 TiO_2 , aqueous phase, anion inhibition.
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 TiO_2 , aqueous phase, anion inhibition.
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TiO₂, reductant, aqueous phase, application, metal removal.
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TiO₂, reductant, aqueous phase, modified **TiO₂**.
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aqueous phase, application, **TiO₂**.
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TiO₂, aqueous phase, application, reactor.
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TiO₂, modeling, aqueous phase, modified **TiO₂**, process efficiency, aerogel.
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TiO₂, metallized **TiO₂**, pesticide, aqueous phase.
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TiO₂, aqueous phase.
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TiO₂, aqueous phase, mechanism.
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aqueous phase, **TiO₂**, engineering, process efficiency, reactor, solar.
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TiO₂, engineering, reactor, solar, aqueous phase, immobilized **TiO₂**.
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TiO₂, engineering, reactor, gas phase, application, cost, competing technologies.

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TiO₂, pesticide, aqueous phase, immobilized **TiO₂**, adsorbent.

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TiO₂, metallized **TiO₂**, aqueous phase, immobilized **TiO₂**.

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5.2. Key Words Used in the Bibliography

adsorbent	metal removal
adsorption	metallized TiO_2
anion inhibition	modeling
application	modified TiO_2
aqueous phase	nonaqueous
biotreatment	other semiconductor
catalyst characterization	oxidant
catalyst reactivation	pesticide
cost	photocatalysis
disinfection	process efficiency
engineering	reactor
gas phase	reductant
IAQ	solar
immobilized TiO_2	TiO_2
mechanism	

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