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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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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/TP473-20300. 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 - 3 18 and 3 19; 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 - 3 1; nickel(+2) complexes - 31; copper(+2) complexes - 3 1; 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, 5 11, 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 25 1; 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 - 15 1, 420, and 42 1; 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?

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 Super-fund 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	C12H4C14O2	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		
Ally1 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]	C 1 0H7OOCNHCH3		N	
Carbon disulfide	cs2		S	
Carbon tetrachloride	cc14	Cl		206,282g,404g,513
Carbonyl sulfide	c o s			
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	Cl 2O2H8-xClx	Cl		
Chlorodibenzofurans	Cl 2OH8-xClx	Cl		
Chlorodibromomethane	ClBr2CH	Br,Cl		
Chlorodifluoromethane	CHClF2	Cl,F		
Chloroethane	C2H5Cl	Cl		
Chloroform	CHC13	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 for-man-tide (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) phtbalate (DEHP)	C6H4[COOCH2CH(C2H5)C4H9]2			
Endosulfan	C9H6Cl603S	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			44g,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-BenzenehexacNoride)	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-,manga.nese 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)-]	C12H7C12NO3	Cl	N	
Nitrogen mustard (2-Chloro-N-(2-cNoroethyl)-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-Nitrosonomicotine			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, and 1242)	C12ClxH10-x	Cl		70,209,351
Pentachlorobenzene	C6Cl5H	Cl		
Pentachlorophenol	C6Cl5OH	Cl		208,280,359
Peracetic acid	CH3COOOH			

Substance	Formula	Halo-gen	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]	C1		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			
set-Butyl alcohol	CH3CH2CHOHCH3			
Sevin (carbaryl)	C			
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	C	Cl	P	248
Tetrahydrofuran	CH2CH2CH2CH2O			
Thioacetamide	CH3CSNH2		S,N	
Thiourea	(NH2)2CS		S,N	

Substance	Formula	Halo-gen	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,505,5 13
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 -TrifluorobromocNoroethane	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	BrC	Br		
1 -Bromododecane	BrC12H25	Br		
1 -Butanol	CH3(CH2)3OH			101,374
1 -Dodecanol	CH3(CH2)			
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		59
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		52.315
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	Halo-gen	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			
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	NO2C 11 H22CO2H		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			
Ally1 alcohol	C3H5OH			
Alochlor				
p-Aminophenol	NH2(C6H4)OH			
Anthraquinone-Zsulfonic acid	HO3SC14H7O2			
AOX or Haloform Precursors				
Asulam				304
Azobenzenes (various)	XC6H4NNC6H4X			
Azobisformamidoacetic acid				
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		
Benzyl ethers	C6H5CH2O-R R=CH3, n-C6H13, t-C4H9, CH2)3C6H5, CH2C6H5			377
Benzyltetradecyldimethylamonium chloride	(C6H5CH2)(C14H27)(CH3)2N,Cl	Cl		
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
tButylazine			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
C 12-Betaine	(C12H25)(CH3)2NCO2		N	202,203
C 12-Amidobetaine				202

Substance	Formula	Halo-gen	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)CH2CO2I			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			
Decarnethyltetrasiloxane	(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		12,203
Doxycycline				
Dyes, unidentified				96,226,227
Eosin				
Ethambutol			N	
Ethane	2H6			
Ethanol	2H5OH			2,101,228,264,274g,329g, 74,405g
Ethylacetate	H3CO2C2H5			
Ethylenediaminetetraacetic acid	O2CCH2)4N2C2H4			8,101,342,484
2-, 3-, or 4-Ethylphenol	C2H5)C6H4OH			
Fenitrothion	C9H12NO5PS		SP	49
Fluorescein	C20H 1205			
Folicur			N	
Formamide	HC(O)NH2		N	'93
Formic Acid	HCO2H			8,90,101,163,214,251,252, 344g,416,444
Fullerenes	C60,C70, and C84			236
Fulvic acid				
Glucose	C6H11O6			18
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			
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	CH3C6H			
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	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			
n-Pentyl amine	n-C5H 11 NH2		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	427,428,5 17
Phthaldialdehyde	C6H4(CHO)2			160
Phthalan				377
Phthalic acid	C6H4(CO2H)2			160
Picoline	CH3C5H4N		N	
Piperidene	C5H10NH		N	52
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 tbiocarbamate (vernolate)	(C3H7)SC(O)(NC3H7)2		N,S	
Salicylaldehyde	C7H6O2			
Salicylic acid	C7H6O3			48,91,102,246,469
Simazine	(C2H5)Cl(NHC2H5)C3N3		N	
Sodium chloroacetate	CH3CO2Na	Cl		
Sodium dodecylbenzene sulfonate	C 12H25C6H4SO3Na		S	
Stearic acid	CH3(CH2)16CO2H			429
S tilbene	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)-NC1		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	

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	18
Aluminum (fume or dust)	Al	
Aluminum oxide	41203	
Ammonia	NH3	61g,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	21	
Chlorine dioxide	2102	
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, 243g,244g,261g,262g, 449g,459g,460g,461g, 472,501,512
Nitrogen	N2	
Oxalate ion	C2O4(2-)	
Oxygen	O2	
Ozone	O3	
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	SO4(1-)	
Sulfite	SO3(1-)	
Sulfur	S	
Sulfur oxides	SOx	449g
Sulfuric acid	H2SO4	
Thallium	Tl	
Thiocyanate	SCN(1-)	33
Thiosulfate	S2O3(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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