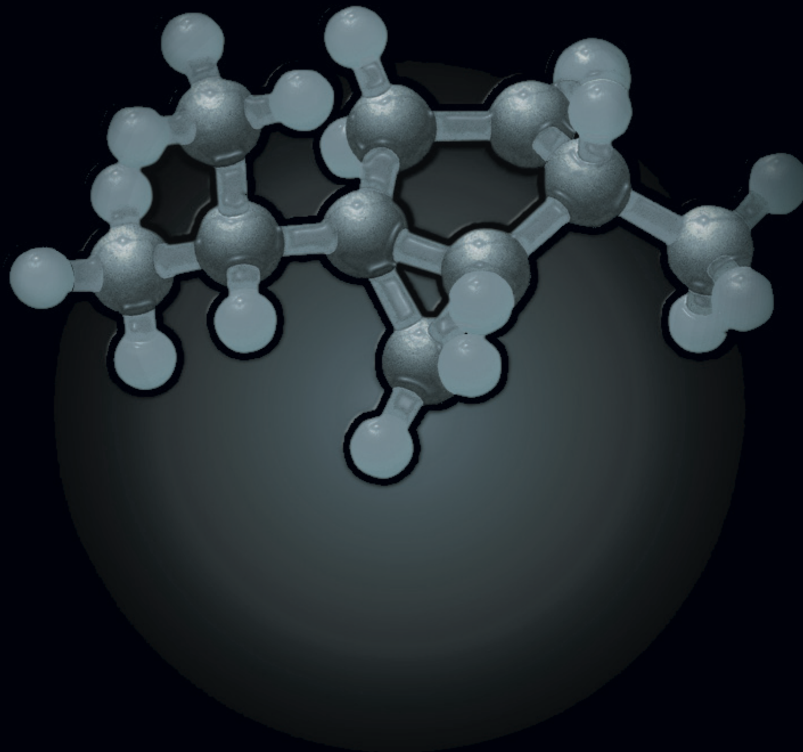

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Catalytic Oxidation Reagents

Edited by
Philip L. Fuchs

Handbook of Reagents
for Organic Synthesis

Catalytic Oxidation Reagents

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Catalytic Oxidation Reagents

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Philip L. Fuchs
Purdue University, West Lafayette, IN, USA

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I dedicate this handbook to our family's matriarch, my wife Diane, our two sons Devin and Sean, their wives Stefanie and Celeste, and their children, Dylan and Sadie, respectively.

e-EROS Editorial Board

Contents

Preface

The eight-volume *Encyclopedia of Reagents for Organic Synthesis* (*EROS*), authored and edited by experts in the field, and published in 1995, had the goal of providing an authoritative multivolume reference work describing the properties and reactions of approximately 3000 reagents. With the coming of the Internet age and the continued introduction of new reagents to the field as well as new uses for old reagents, the electronic sequel, *e-EROS*, was introduced in 2002 and now contains in excess of 4000 reagents, catalysts, and building blocks making it an extremely valuable reference work. At the request of the community, the second edition of the encyclopedia, *EROS-II*, was published in March 2009 and contains the entire collection of reagents at the time of publication in a 14-volume set.

While the comprehensive nature of *EROS* and *EROS-II* and the continually expanding *e-EROS* render them invaluable as reference works, their very size limits their practicability in a laboratory environment. For this reason, a series of inexpensive one-volume *Handbooks of Reagents for Organic Synthesis* (*HROS*), each focused on a specific subset of reagents, was introduced by the original editors of *EROS* in 1999:

Reagents, Auxiliaries, and Catalysts for C–C Bond Formation
Edited by Robert M. Coates and Scott E. Denmark

Oxidizing and Reducing Agents
Edited by Steven D. Burke and Rick L. Danheiser

Acidic and Basic Reagents
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Activating Agents and Protecting Groups
Edited by Anthony J. Pearson and William R. Roush

This series has continued over the last several years with the publication of a further series of *HROS* volumes, each edited by a current member of the *e-EROS* editorial board:

Chiral Reagents for Asymmetric Synthesis
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Reagents for High-Throughput Solid-Phase and Solution-Phase Organic Synthesis
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Reagents for Silicon-Mediated Organic Synthesis
Edited by Philip L. Fuchs

This series now continues with the present volume entitled *Catalytic Oxidation Reagents*, edited by Philip Fuchs, longstanding member of the online *e-EROS* Editorial Board. This 14th volume in the *HROS* series, like its predecessors, is intended to be an affordable, practicable compilation of reagents arranged around a central theme that it is hoped will be found at arm's reach from synthetic chemists worldwide. The reagents have been selected to give broad relevance to the volume, within the limits defined by the subject matter. We have enjoyed putting this volume together and hope that our colleagues will find it just as enjoyable and useful to read and consult.

David Crich
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Wayne State University
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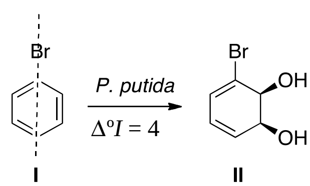
Introduction

The art/science of organic synthesis continues to evolve at an ever-increasing pace. In academia and especially in the pharmaceutical industry, chemists are paying close attention to issues related to atom economy,[1] the *E* factor (kg waste/kg product)[2] and process mass intensity (PMI = total mass in a process/mass of product).[3] The American Chemical Society Green Chemistry Institute's Pharmaceutical Roundtable has adopted PMI as the current metric for evaluating and benchmarking manufacturing processes.

Superimposed upon these important macroscopic considerations, are strategy-level factors dealing with the design and execution of efficient synthetic operations. A 2007 handbook in this series featured the use of C–H functionalization reagents[4] as a direct means of increasing structural intricacy.[5] In the last several years, the Baran group at Scripps has advanced the logic of C–H oxidative functionalization to a whole new level.[6]

Asymmetric reactions employing enantiopure catalysts acting on prochiral substrates are especially prized, since one molecule of catalyst spawns a multitude of chiral progeny. The degree of intricacy (°*I*) of a molecule is defined as the sum of the individual integer values of five component features, where *C** is the number of chiral centers, *U* is the number of prochiral unsaturations plus rings, AR is the number of aryl or heteroaryl nonhydrogen atoms, and *X* is the number of heteroatoms (eq 1).[5] One of the most striking examples of increase in intricacy is the enzymatic oxidation of monosubstituted arenes exploited so effectively by Hudlicky et al.[7] The intricacy of bromobenzene **I** is 7, which includes the ring unsaturation and the four unique olefinic prochiral centers. The enzymatic oxidation converts two of the prochiral centers to a pair of heteroatom-bearing stereocenters with concomitant enantiogenesis. Thus, diol **II** is an enantiopure substrate-bearing functionality appropriate for further manipulation at each of its resident carbon atoms.



(1)

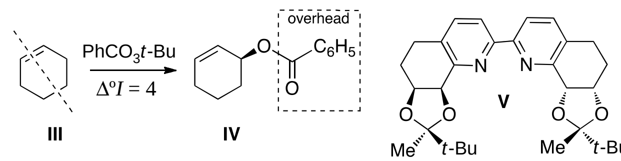
°*I* = *C** + *U* + Ar + *X* + *E*

for I °*I* = 0 + (1 + 4) + 1 + 1 + 0 = 7

for II °*I* = 2 + (1 + 4) + 0 + 3 + 1 = 11

Reactions having positive $\Delta^\circ I$ indicate creation of new molecular complexity, while reactions with $\Delta^\circ I$ equal to zero (protection/deprotection) or a negative $\Delta^\circ I$ value, signal a *status quo* or worse, *decrease of complexity*.[5] Consideration of organic transformations via the perspective of change in intricacy leads to the conclusion that oxidations are higher value-added processes than are reductions.[8] A complementary conclusion was delivered by Burns et al. in their pivotal 2009 *Angewante* review discussing redox economy in organic synthesis.[9]

The past several years have seen exponential growth in both the number of papers and complexity of substrates used in C–H functionalization. The goal of increasing molecular intricacy is well served by reactions that effect functionalization of C–H bonds, since the conversion of a C–H bond to a new heteroatom-bearing chiral center is another notable $\Delta^\circ I = 4$ process that efficiently creates enantiopure **IV** from prochiral cyclohexene **III** (eq 2).[10]



(2)

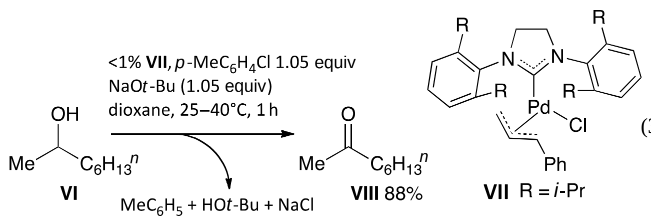
°*I* = *C** + *U* + Ar + *X* + *E*

for III °*I* = 0 + (1 + 1) + 0 + 0 + 0 = 2

for IV °*I* = 1 + (1 + 2) + 0 + 1 + 1 = 6

5% $Cu(OTf)_2$ + 5% **V**
5.25% $PhNHNH_2$, acetone, 25°C
>90% yield, 90% ee of **IV**

The continued development of catalysts capable of efficiently undergoing oxidative insertion with aryl and heteroaryl chlorides is proud testament to the creativity of many synthetic organic chemists.[11] Based on the lessons learned in designing such catalysts, it is now possible to use chlorobenzene and other inexpensive aryl chlorides as *terminal oxidants* in palladium-catalyzed room temperature oxidations of unactivated secondary alcohols. The reader is alerted to the chlorobenzene EROS entry and the seminal 2011 paper by the Navarro group[12] employing chlorotoluene (co-product toluene rather than benzene) that details optimal conditions using the commercially available NCH catalyst **VII** (eq 3).



(3)

This EROS handbook includes a pair of reagent finder tables. This format provides visual access to the handbook's contents, which may stimulate reader creativity. The first table incorporates all reagents that serve as terminal oxidants arranged by functional class subdivided by increasing molecular weight. The second reagent finder table lists specific oxidation catalysts, also arranged by reagent class subdivided by increasing molecular weight.

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Terminal Oxidants Finder

Class	Name	Structure	MW	CAS #	EROS #	Page #
Oxygen (air)	Oxygen	O_2	32	7782-44-7	ro028	454
Nitroso and Azo	Nitrosobenzene	$C_6H_5N{=}O$	107	586-96-9	rn00696[a]	[a]
	Diethyl Azodicarboxylate	$EtO_2CN{=}NCO_2Et$	174	1972-28-7	rd176[b]	[b]
	Di-*tert*-Butyl Azodicarboxylate	t-$BuO_2CN{=}NCO$$t$-Bu	230	870-50-8	rd056[c]	[c]
Peracid	Peracetic Acid	H_3CCO_3H	76	79-21-0	rp034	470
	Trifluoroperacetic Acid	F_3CCO_3H	130	359-48-8	rt254	649
	m-Cl-Perbenzoic Acid	3-$ClC_6H_4CO_3H$	173	937-14-4	rc140[d]	[d]
Hydroperoxide	Hydrogen Peroxide	HOOH	34	7722-84-1	rh040	281
	Lithium Hydroperoxide Lithium Hydroperoxide • H_2O	LiOOH LiOOH • H_2O	40 56	54637-08-0 23594-83-4	rl119	363
	tert-Butyl Hydroperoxide	t-BuOOH	90	75-91-2	rb385	96
	Urea·Hydrogen Peroxide	HOOH • $O{=}C(NH_2)_2$	94	124-43-6	rh047	295
	Sodium Percarbonate	$2Na_2CO_3 \cdot 3H_2O_2$	157	15630-89-4	rn00950[e]	[e]
	Hydroperoxide, (1*S*)-1-phenylethyl Hydroperoxide, (1*R*)-1-phenylethyl	$C_6H_5CHMeOOH$	138 138	116102-42-2 78833-98-4	rn01610	480
	Triphenylmethyl Hydroperoxide	$(C_6H_5)_3COOH$	276	4198-93-0	rt363m	667
Peroxide	*tert*-Butyl Peracetate	t-BuO_3CCH_3	132	107-71-1	rn01471	132
	Sodium Perborate	$[(HO)_2BOO]_2Na_2 \cdot 6H_2O$	154	10486-00-7	rs094[f]	[f]
	Bis(trimethylsilyl) Peroxide	TMSOOTMS	178	5796-98-5	rb219	87
	Benzenecarboperoxoic acid, 1,1-dimethylethyl ester	$C_6H_5CO_3$$t$-Bu	194	614-45-9	rn01616	20

[a] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rn00696
[b] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rd176.pub2
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[e] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rn00950
[f] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rs094.pub2

Class	Name	Structure	MW	CAS #	EROS #	Page #
	Dibenzoyl Peroxide	$C_6H_5COOOOCC_6H_5$	242	94-36-0	rd022[g]	[g]
	Bis(trimethylsilyl) Monoperoxysulfate	$TMSOOSO_3TMS$	258	23115-33-5	rb216[h]	[h]
	Bis(1-methyl-1-phenylethyl) Peroxide	$C_6H_5CMe_2OOMe_2CC_6H_5$	270	80-43-3	rn01467	77
Dihalogen	Iodine	I_2	254	7553-56-2	ri005	317
O-Halo	Sodium Hypochlorite	NaOCl	74	7681-52-9	rs084	587
	tert-Butyl Hypochlorite	*t*-BuOCl	109	507-40-4	rb388	126
	Calcium Hypochlorite	$Ca(OCl)_2$	142	7778-54-3	rc006	137
N-Halo	1-Fluoropyridinium Trifluoromethanesulfonate	$C_5H_5N–F\ O_3SCF_3$	184	108-77-0	rn00320[i]	[i]
	N-Fluoropyridinium Tetrafluoroborate	$C_5H_5N–F\ BF_4$	185	107264-09-5	rn01196	270
	1-Fluoro-2,4,6-trimethylpyridinium Tetrafluoroborate	$2,4,6\text{-}Me_3C_5H_2N–F\ BF_4$	227	109705-14-8	rn01221	274
	N-Fluoropyridinium Triflate	$C_5H_5N–F\ O_3SCF_3$	247	107263-95-6	rf012	272
	1-Fluoro-2,4,6-trimethylpyridinium Trifuoromethanesulfonate	$2,4,6\text{-}Me_3C_5H_2N–F\ O_3SCF_3$	289	107264-00-6	rn01195	274
	N-fluoro-*N*-(phenylsulfonyl)-benzenesulfonamide	$(C_6H_5SO_2)_2NF$	315	133745-75-2	rb011[j]	[j]
	1,1′-Difluoro-2,2′-bipyridinium Bis(tetrafluoroborate)	$BF_4\ F\text{-}NC_5H_4\text{-}C_5H_4N–F\ BF_4$	368	178439-26-4	rn00849	217
	Cyanamide, *N*-Chloro-*N*-(1,1-dimethylethyl)-	*t*-BuNClCN	133	502143-99-9	rn01492	94
	N-Chlorosuccinimide	$CH_2CONClCOCH_2$	134	128-09-6	rc145[k]	[k]
	Trichloroisocyanuric Acid	$(ClNC{=}O)_3$	232	87-90-1	rt209	642
	Benzenesulfonamide, *N*,*N*-Dichloro-4-methyl-	$p\text{-}MeC_6H_4SO_2NCl_2$	240	473-34-7	rn01485[l]	[l]
	N-Bromosaccharin	$(C_6H_4)CONBrSO_2$	262	35812-01-2	rn01495[m]	[m]
	N-Bromosuccinimide	$CH_2CONBrCOCH_2$	178	128-08-5	rb318[n]	[n]
	Sodium *N*-Bromo benzenesulphonamidate; Bromamine B Sodium *N*-Bromo-*p*-toluenesulphonamidate; Bromamine T	$CH_3C_6H_4SO_2NBr\ Na \bullet 3H_2O$ $C_6H_5SO_2NBr\ Na \bullet 1.5H_2O$	284 325	16917-09-2 41085-71-6	rn01612	91

[g] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rd022.pub2
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Class	Name	Structure	MW	CAS #	EROS #	Page #
	Benzenesulfonamide, *N*,*N*-Dibromo- Benzenesulfonamide, *N*,*N*-Dibromo-4-methyl-	$C_6H_5SO_2NBr_2$ $CH_3C_6H_4SO_2NBr_2$	315 329	938-05-6 21849-40-1	rn00840	188
	N-Iodosuccinimide	$CH_2CONICOCH_2$	225	516-12-1	ri038[o]	o
Oxo Compounds	Trimethylamine *N*-Oxide	$Me_3N{=}O$	75	62637-93-8	rt268	659
	Sodium Chlorite	$NaClO_2$	90	7758-19-2	rs057[p]	p
	N-Methylmorpholine *N*-Oxide	$O(CH_2CH_2)_2MeN{=}O$	117	7529-22-8	rm216	384
	Sodium Bromate	$NaBrO_3$	151	7789-38-0	rs053	583
	Potassium Permanganate	$KMnO_4$	158	7722-64-7	rp244[q]	q
	Potassium Bromate	$KBrO_3$	167	7758-01-2	rp197	502
	Molybdenum Chloride Oxide	$MoCl_2O_2$	199	13637-68-8	rn01462	407
	Sodium Periodate	$NaIO_4$	214	7790-28-5	rs095[r]	r
	Iodosylbenzene	$C_6H_5I{=}O$	220	536-80-1	ri039	338
	Periodic Acid	H_5IO_6	228	10450-60-9	rn00561[s]	s
	Iodylbenzene	$C_6H_5IO_2$	236	696-33-3	ri048[t]	t
	Peroxydisulfate (Ammonium, Sodium, Potassium)	M OSO_3OOSO_3 M	228 238 270	7727-54-0 7775-27-1 7727-21-1	ra096[u]	u
	Sodium Tungstate	$Na_2WO_4 \bullet 2H_2O$	330	13472-45-2	rn01596	411
	Iron(II) Perchlorate	$Fe(ClO_4) \bullet 6H_2O$	363	13520-69-9	ri064[v]	v
	Tetrabutylammonium Peroxydisulfate	$Bu_4N\ OSO_3OOSO_3$ NBu_4	435	88505-29-7	rn01594	615
	Potassium Monoperoxysulfate (Oxone)	$2KHSO_5 \bullet KHSO_4 \bullet K_2SO_4$	615	37222-66-5	rp246	506
Quinone	1,4-Benzoquinone	$O{=}C(CH{=}CH)_2C{=}O$	108	106-51-4	rb033	49
Aryl Halide	Chlorobenzene	C_6H_5Cl	113	108-90-7	rn01565	150
Metal (+*n*)	Iron(III) Chloride	$FeCl_3$	162	7705-08-0	ri054[w]	w

[o] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ri038.pub3

[p] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rs057

[q] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rp244.pub2

[r] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rs095.pub2

[s] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rn00561

[t] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ri048.pub2

[u] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ra096.pub2

[v] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ri064

[w] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ri054.pub2

Class	Name	Structure	MW	CAS #	EROS #	Page #
	Cerium(IV) Ammonium Nitrate	$(NH_4)_2Ce(NO_3)_6$	548	16774-21-3	rc038[x]	[x]
	Cerium(IV) Ammonium Sulfate Dihydrate	$Ce(NH_4)_4(SO_4)_4$	633	10378-47-9	rc040[y]	[y]
I(III) and I(V)	(Diacetoxyiodo)benzene	$C_6H_5I(OCOCH_3)_2$	322	3240-34-4	rd005m[z]	[z]
	Bis(2,2-dimethylpropanoato-*κ*-*O*)phenyl-iodine	$C_6H_5I(OCO\textit{t}\text{-Bu})_2$	406	57357-20-7	rn01109	69
	Phenyliodine(III) Bis(trifluoroacetate)	$C_6H_5I(OCOCF_3)_2$	430	2712-78-9	rp069[aa]	[aa]
Boron–Boron	4,4,4′,4′,5,5,5′,5′-Octamethyl-2,2′-bi-1,3,2-dioxaborolane	B_2pin_2	254	73183-34-3	rn00188	421

[x] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rc038.pub2

[y] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rc040

[z] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rd005m.pub2

[aa] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rp069.pub2

Oxidation Catalyst Finder

Class	Name	Structure	MW	CAS #	EROS #	Page #
Dioxirane	Dimethyldioxirane	$Me_2C(O—O)$	74	74087-85-7	rd329	228
	Dioxirane, methyl(trifluoromethyl)-	$CF_3MeC(O—O)$	128	115464-59-0	rm267	390
	1,2:4,5-Di-*O*-isopropylidene-*β*-D-erythrohexo-2,3-diulo-2,6-pyranose	Enantiopure Tricyclic Isopropylidine Ketone Dioxirane Precursor	258	18422-53-2	rc057[a]	[a]
	Spiro[6*H*-1,3-dioxolo[4,5-c]pyran-6,5′-oxazolidine]-3′-carboxylic acid, tetrahydro-2,2-dimethyl-2′,7-dioxo-, ethyl ester, (3a*R*,5′*S*,7a*R*)- Spiro[6*H*-1,3-dioxolo[4,5-c]pyran-6,5′-oxazolidine]-3′-carboxylic acid, tetrahydro-2,2-dimethyl-2′,7-dioxo-, 2-methyl-2-propyl ester, (3a*R*,5′*S*,7a*R*)- Spiro[6*H*-1,3-dioxolo[4,5-c]pyran-6,5′-oxazolidine]-3′-carboxylic acid, tetrahydro-2,2-dimethyl-2′,7-dioxo-, methyl ester, (3a*R*,5′*S*,7a*R*)-	Three Enantiopure Tricyclic Oxazolidine Ketone Dioxirane Precursors	301 315 343	906371-65-1 906371-64-0 319491-89-9	rn01464	604
	(*R*)-2,10-Dichloro-5*H*-dinaphtho[2,1-*g*:1,2-*i*][1,5] dioxacycloundecin-3, 6,9(7*H*)-trione	Binap Enantiopure Dioxirane Precursor	466	184034-09-1	rn00253	210
Oxo	Chromium(VI) Oxide	$Cr(=O)_3$	100	1333-82-0	rc169	157
	Selenium(IV) Oxide & *tert*-Butyl Hydroperoxide	O=Se=O	110	7446-08-4 75-91-2	rs009 (rs008)	575
	Potassium Permanganate	$KMnO_4$	158	7722-64-7	rp244[b]	[b]
	Ruthenium(VIII) Oxide	RuO_4	165	20427-56-9	rr009[c]	[c]
	Dichloro(ethoxy)oxovanadium(V)	$EtOCl_2V=O$	183	1801-77-0	rd117	213

[a] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rc057

[b] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rp244.pub2

[c] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rr009.pub2

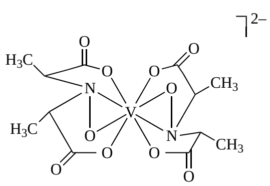
Class	Name	Structure	MW	CAS #	EROS #	Page #
	1-Piperidinyloxy, 4-methoxy-2,2,6,6-tetramethyl-4-Acetamido-2,2,6,6-tetramethyl-1-piperidinyloxy 4-Acetylamino-2,2,6,6-tetramethyl-piperidine-1-oxoammonium BF4 2,2,6,6-Tetramethylpiperidin-1-oxyl 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-(2-propyn-1-yloxy 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl	TEMPO Family	191–300	95407-69-5 14691-89-5 219543-09-6 2564-83-2 147045-24-7 2226-96-2	rn00346 ra006 rt069	2
	Molybdenum Chloride Oxide	$MoCl_2O_2$	199	13637-68-8	rn01462	407
	Chromyl Acetate	$(AcO)_2Cr(=O)_2$	202	4112-22-5	rc176	163
	Methyltrioxorhenium(VII)	$MeRe(=O)_3$	250	70197-13-6	rn00017u	396
	Rhenium(VII) Oxide	$HReO_4$ Re_2O_7	251 448	13768-11-1 1314-68-7	rn01213	541
	Osmium Tetroxide	OsO_4	254	20816-12-0	ro007	433
	Osmium Tetroxide & *tert*-Butyl Hydroperoxide	OsO_4 *t*-BuOOH	254 90	20816-12-0 75-91-2	ro008[d]	[d]
	Osmium Tetroxide & *N*-Methylmorpholine *N*-Oxide	OsO_4 NMO	254 117	20816-12-0 7529-22-8	ro009[e]	[e]
	Osmium Tetroxide & Sodium Periodate	OsO_4 $NaIO_4$	254 214	20816-12-0 7790-28-5	rs095m[f]	[f]
	Osmium Tetroxide & Potassium Ferricyanide	OsO_4 $K_3Fe(CN)_6$	254 329	20816-12-0 13746-66-2	ro010[g]	[g]
	Vanadyl Bis(acetylacetonate)	$O=V(acac)_2$	265	3153-26-2	rv003m	684
	1,2-Benziodoxol-3(1*H*)-one, 1-Hydroxy, 1-Oxide IBX and stabilized IBX	$C_6H_4IHOOO_2C$	279	61717-82-6 64297-64-9	rn00236 rn00221[h] rn01376	32
	2-Iodobenzenesulfonic Acid 2-Iodobenzenesulfonic Acid Na Salt	$C_6H_4ISO_3H$ $C_6H_4ISO_3Na$	284 306	63059-25-6 62973-69-7	rn01214	332
	Sodium Tungstate	$Na_2WO_4 \bullet 2H_2O$	330	13472-45-2	rn01596	411
	5,6,7,8-Tetrafluoro-1-hydroxy-1-oxobenziodoxol-3(1*H*)one(Tetrafluoro-IBX)	$C_6F_4IHOOO_2C$	351	954373-95-6	rn01489	618
	Tetrapropylammonium Perruthenate	$Bu_4N\ RuO_4$	351	114615-82-6	rt074	626
	Tetrabutylammonium Bis(pyrazinecarboxylato)-dioxo-vanadium(V)	Bu_4N $(O=)_2V(O_2CC_4N_2)_2$	572	251317-60-9	rn01468	609

[d] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ro008
[e] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ro009
[f] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rs095m
[g] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.ro010
[h] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rn00221

Class	Name	Structure	MW	CAS #	EROS #	Page #
	μ-Oxo-bis[tetrakis(*t*-butyl) phthalocyaninatoiron(III)]	PhthOFe-OPhth	1600	130177-29-6	rn01595	452
	Phosphotungstic Acid Phosphotungstic Acid (hydrate)	$H_3PW_{12}O_{40}$ $H_3PW_{12}O_{40} \bullet 24H_2O$	2880 3312	1343-93-7 12501-23-4	rn01615[i]	[i]
	Tetrabutylammonium dodecatungstophosphate	$(TBA)_3[PW_{12}O_{40}]$	3604	53749-37-4	rn01585	611
Metal Oxaziridine	Vanadium, bis[*N*-[(1*S*)-1-(carboxy-κO)ethyl]-*N*-(hydroxy-κO)-L-alaninato(2−)-κN,κO]-	[j]	401	12705-99-6	rn01472	681
Achiral Monodentate	Tris[4-(trifluoromethyl)phenyl]-phosphine	$P(C_6H_4CF_3\text{-p})_3$	466	13406-29-6	rn01483	677
	N,*N*′-Bis(2,4,6-trimethylphenyl)imidazol-2-ylidene Palladium(I) Allyl Chloride	NHC–PdCl(Allyl)	487	478980-04-0	rn01459	82
Achiral Bidentate	2-Pyrazinecarboxylic Acid	$C_5H_4N_2O_2$	124	98-97-5	rn01470	524
	2,3-Pyrazinedicarboxylic Acid	$C_6H_4N_2O_4$	168	89-01-0	rn01469	530
	2-Pyridinecarboxylic Acid	$C_6H_5NO_2$	123	98-98-6	rn00151	495
	4,7-Diphenyl-1,10-phenanthroline (Bathophenanthroline)	4,7-$(C_6H_5)_2$-1,10-phenanthroline	332	1662-01-7	rn01319	17
	2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline	2,9-Me_2-4,7-$(C_6H_5)_2$-1,10-phenanthroline	360	4733-39-5	rn01392	15
	Iron(II) bis(pyridine)bis(2-pyridinecarboxylato-*N*1,*kO*2)	$[C_5H_4NCO_2]_2$ $Fe(C_5H_5N)_2$	458	128391-66-2	rn00612	359
	Ruthenium(III) Complex of *cis*-Diaquabis(6,6-Dichloro-2,2-bipyridine)	*cis*-$[Ru^{II}(6,6\text{-}Cl_2bpy)_2(OH_2)_2](CF_3SO_3)_2$	885	120596-51-2	rn00594	561
Enantiopure Bidentate	(*S*)-2-(5-1*H*-Tetrazolyl)pyrrolidine (*R*)-2-(5-1*H*-Tetrazolyl)pyrrolidine	$C_4H_8NH–CN_4H$	139	33878-70-5 702700-79-6	rn00615	633
	2,2′-Bipyrrolidine, (2*S*,2′*S*)- 2,2′-Bipyrrolidine, (2*R*,2′*R*)-	$C_4H_8NH–C_4H_8NH$	140	124779-66-4 137037-20-8	rn01491	54
	1,5-Diaza-*cis*-decalin, (4a*S*,8a*S*)- 1,5-Diaza-*cis*-decalin, (4a*R*,8a*R*)-	$C_8H_{16}N_2$	140	219522-28-8 219522-27-7	rn00646	183

[i] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rn01615

[j]



Class	Name	Structure	MW	CAS #	EROS #	Page #
	(*S*)-(−)-4-(2-Methylpropyl)-2-(2-pyridyl)-2-oxazoline	C_5H_4N(*i*-Bu-oxazolinyl)	204	108915-07-7	rn00203	388
	1,2-Bis(phenylsulfinyl)ethane	$[C_6H_5S{=}OCH_2]_2$	278	6099-21-4 21461-90-5	rn00971	79
	2,2-Bis{[2-[4(*S*)-*tert*-butyl-1,3-oxazolinyl]} propane 2,2-Bis{[2-[4(*R*)-*tert*-butyl-1,3-oxazolinyl]} propane	Me_2C(*t*-Bu-oxazolinyl)$_2$	294	131833-93-7 131833-97-1	rn00090 rd346m	59
	2-Pyrrolidinemethanol, α,α-di-2-naphthalenyl-, (2*S*)- 2-Pyrrolidinemethanol, α,α-di-2-naphthalenyl-, (2*R*)- 2-Pyrrolidinemethanol, α,α-bis(3,5-dimethylphenyl)-, (2*S*)- 2-Pyrrolidinemethanol, α,α-bis(3,5-dimethylphenyl)-, (2*R*)	$C_4H_8NH–C(Ar)_2OH$	309 353	127986-84-9 130798-48-0 131180-63-7 948595-01-5	rn01486	535
	3,3,3α,3α,4,4,5,5-Octahydro-3,3,3,3-tetraisopropyl-6,6-spirobi-[6*H*-cyclopent[c]isoxazole]	tetracyclic spiro bis isoxazole	375	333972-16-0 333972-02-4 333972-03-5 927199-90-4	rn01605	415
	Palladium Sparteine Dichloride	Cl_2Pd • Sparteine	411	359796-53-5	rn01501	467
	2-Pyrrolidinemethanol, α,α-bis(3,5-dimethylphenyl)-4-(phenylmethoxy)-, (2*S*,4*R*)-	$4\text{-}BnOC_4H_7NH–C(3,5\text{-}Me_2C_6H_3)_2$	415	923985-71-1	rn01496	52
	Pyrrolidine, 3,4-bis(diphenyl-phosphino)-1-(phenylmethyl)-, (3*R*,4*R*) Pyrrolidine, 3,4-bis(diphenyl-phosphino)-1-(phenylmethyl)-, (3*S*,4*S*)-	$BnNC_4H_6[(C_6H_5)_2P]_2$	530	99135-95-2 156517-64-5	rn01502	532
	Benzeneacetamide, *N*,*N*′-(1*R*,2*R*)-1,2-cyclohexanediylbis[*N*-hydroxy-α-phenyl-Benzeneacetamide, *N*,*N*′-(1*S*,2*S*)-1,2-cyclohexanediylbis [*N*-hydroxy-α-phenyl-	$C_6H_{10}[NOHCOCH(C_6H_5)_2]_2$	535	860036-16-4 1217464-22-6	rn01291	179
	Ruthenium(III) Complex of *N*,*N*,*N*-Trimethyl-1,4,7-triazacyclononane	$Ru(Me_3tacn)(CF_3CO_2)_2OH_2]CF_3CO_2$	629	478980-00-6	rn00594	561
	Iridium, [*N*-[(1*R*,2*R*)-2-(amino-κN)-cyclohexyl]-4-methylbenzene-sulfonamidato-κN]chloro[(1,2,3,4,5-η)-1,2,3,4,5-pentamentyl-2,4,-cyclopentadien-1-yl]-, and (*S*,*S* stereoisomer)	[Cp*IrCl{(*R*,*R*)-Tscydn}] [Cp*IrCl{(*S*,*S*)-Tscydn}]	630	223247-70-9 1028632-02-1	rn01597	354
Achiral Tridentate	4,4,4-tri-*tert*-butyl-2,2:6,2-terpyridine	4-*t*-BuC_5H_2N(*t*-BuC_5H_3N)2	402	115091-29-7	rn01474	639

Class	Name	Structure	MW	CAS #	EROS #	Page #
	Manganese(2+), bis(octahydro-1,4,7-trimethyl-1*H*-1,4,7-triazonine-$\kappa N1,\kappa N4,\kappa N7$)tri-$\mu$-oxo dihexafluorophosphate(1−) (1:2)	$(MeNCC)_3Mn(O)_3$ $Mn(MeNCC)_3$ $2PF_6$	790	116633-52-4	rn01603	375
Achiral Tetradentate	Tris(2-pyridylmethyl)amine	$N(CH_2\text{-}C_5H_4N)_3$	290	16858-01-8	rn01606	670
	Manganese, chloro[[2,2′-[1,2-ethanediylbis[(nitrilo-κN)methyl-idyne]]bis[phenolato-κO]](2−)]	Salen Mn(III)	357	53177-12-1	rn01494	152
	Manganese(II) tetraphenylporphyrin	Mn(II) TPP	670	31004-82-7	rn01601	378
	Cobalt(II) tetraphenylporphyrin	Co(II) TPP	672	14172-90-8	rn01602	167
Enantiopure Tetradentate	(*R*,*R*)-*N*,*N*′-Bis(3,5-ditert-butylsalicylidene)-1,2-cyclohexanediamino manganese(III) Chloride (*S*,*S*-*N*,*N*′-Bis(3,5-ditert-butylsalicylidene)-1,2-cyclohexane-diamino manganese(III) Chloride	Salen Mn(III)Cl	635	138124-32-0 135620-04-1	rs085	600
	Cinchonan, 9,9″-[1,4-phthalazinediyl-bis(oxy)]bis[10,11-dihydro-6′-methoxy-, (8α,9*R*)-(8″α,9″*R*)- Cinchonan, 9,9″-[1,4-phthalazinediyl-bis(oxy)]bis[10,11-dihydro-6′-methoxy-, (9*S*)-(9″*S*)-	$(DHQ)_2PHAL$ $(DHQD)_2PHAL$	779	140924-50-1 140853-10-7	rn01493	483
	Titanium, bis[[(1*R*,1″*R*)-3,3″-[(1*R*,2*R*)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[2′-phenyl[1,1′-binaphthalen]-2-olato-κO]](2−)]di-μ-oxodi- Titanium, bis[[(1*R*,1″*R*)-3,3″-[(1*S*,2*S*)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[2′-phenyl[1,1′-binaphthalen]-2-olato-κO]](2−)]di-μ-oxodi-	Salen–binapTi(IV) OOTi(IV)Salen–binap	1778	357208-47-0 393573-36-9	rn01577	66
Metal–X	Ruthenium Hydroxide	$Ru(OH)_n$	152	56321-86-9	rn01593	568
	Ruthenium Trichloride	$RuCl_3$	207	10049-08-8	rr008	549
	Palladium(II) Acetate	$Pd(OAc)_2$	225	3375-31-3	rp001[k]	[k]
	Manganese(III) Acetate Manganese(III) Acetate Dihydrate	$Mn(OAc)_3$ $Mn(OAc)_3 \bullet 2H_2O$	232 268	993-02-2 19513-05-4	rm018	367
	Cerium(IV) Ammonium Nitrate	$(NH_4)_2Ce(NO_3)_6$	548	16774-21-3	rc038[l]	[l]
	Cerium(IV) Ammonium Nitrate–Sodium Bromate	$(NH_4)_2Ce(NO_3)_6$ $NaBrO_3$	548 151	16774-21-3 7789-38-0	rc039[m]	[m]

[k] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rp001.pub2

[l] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rc038.pub2

[m] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rc039

Class	Name	Structure	MW	CAS #	EROS #	Page #
	Cerium(IV) Ammonium Sulfate Dihydrate	$Ce(NH_4)_4(SO_4)_4$	633	10378-47-9	rc040[n]	[n]
	Ruthenium(0), dodecacarbonyl, triangulo	$[Ru(C{=}O)_4]_3$	639	15243-33-1	rn00582	565
	Di-μ-methoxobis(1,5-cyclooctadiene)-diiridium(I)	(1,5-COD)Ir$(OMe)_2$ Ir(1,5-COD)	663	12148-71-9	rn01167	224
	Di-μ-chlorobis(1,5-cyclooctadiene)-diiridium(I)	$(COD)_2Ir_2Cl_2$	672	12112-67-3	rd089m	195
	Iridium, Dichlorodi-μ-hydrobis [(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-	$[Cp^*IrHCl]_2$	728	84029-37-8	rn01484	357
	Di-*m*-chlorodichlorobis[(1,2,3,4,5-h)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]diiridium	$[Cp^*IrCl_2]_2$	797	12354-84-6	rn00828	202
	Vitamin B_{12}	Octahedral Co(III)	1355	68-19-9	rv023[o]	[o]
Quinone	1,4-Benzoquinone	$O{=}C(CH{=}CH)_2C{=}O$	108	106-51-4	rb033	49
	3,3,5,5-Tetra-*t*-butyldiphenoquinone	$(O{=}C(t\text{-}Bu)_2$ $(C{=}CH)_2C{=})_2$	409	2455-14-3	rn01487	630
Misc.	Benzenamine, homopolymer	$(p\text{-}C_6H_4NH)_x$	91	25233-30-1	rn01488	498
	N-Hydroxyphthalimide	$C_6H_4(C{=}O)_2NOH$	163	524-38-9	rn00598	307
	Acridinium, 10-methyl-9-(2,4,6-trimethylphenyl)-, perchlorate	2,4,6-$Me_3C_6H_2$ acridinium ClO_4	412	674783-97-2	rn01476	381
	Dispiro[2*H*-pyran-2,4-[4*H*-5,6,8b]-triazaacenaphthylene-7 (5*H*),2-[2*H*]-pyran], 1,2 ,2a,3,3,3,4,4,5,5,6,6,8,8a-tetradecahydro-1,2-dimethoxy-6,6-dimethyl-, monohydrochloride, (1*S*,2*R*,2*S*,2*R*,2a*S*,6*S*,6*S*,8a*S*)-	Enantiopure C_2-Symmetric Pentacyclic Guanidine	430	393109-20-1 393109-05-2	rn01511	257
	2-[Bis[3,5-bis(trifluoromethyl)phenyl] [(trimethylsilyl)oxy]methyl]pyrrolidine	Enantiopure C_2-Symmetric Pyrrolidine	598	848821-61-4 908303-26-4	rn00887	57
	Cinchonanium, 1,1″-[1,3-phenylenebis(methylene)]bis[9-hydroxy-, bromide(1:2), (8α,9*R*)-(8″α,9″*R*)- Cinchonanium, 1,1″-[1,3-phenylenebis(methylene)]bis[9-hydroxy-, bromide(1:2), (9*S*)-(9″*S*)-	Enantiopure C_2-Symmetric Alkaloid PTC	852	473410-07-0 479070-35-4	rn01490	478

[n] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rc040

[o] This reagent is available in the online Encyclopedia of Reagents for Organic Synthesis, DOI: 10.1002/047084289X.rv023

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Short Note on InChIs and InChIKeys

The IUPAC International Chemical Identifier (InChI™) and its compressed form, the InChIKey, are strings of letters representing organic chemical structures that allow for structure searching with a wide range of online search engines and databases such as Google and PubChem. While they are obviously an important development for online reference works, such as *Encyclopedia of Reagents for Organic Synthesis* (*e-EROS*), readers of this volume may be surprised to find printed InChI and InChIKey information for each of the reagents.

We introduced InChI and InChIKey to e-EROS in autumn 2009, including the strings in all HTML and PDF files. While we wanted to make sure that all users of *e-EROS*, the second print edition of *EROS*, and all derivative handbooks would find the same information, we appreciate that the strings will be of little use to the readers of the print editions, unless they treat them simply as reminders that *e-EROS* now offers the convenience of InChIs and InChIKeys, allowing the online users to make best use of their browsers and perform searches in a wide range of media.

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