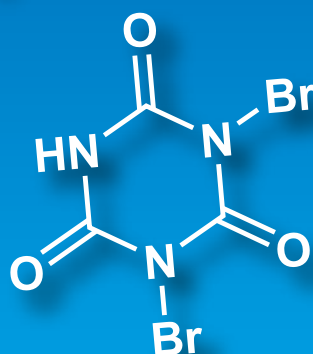
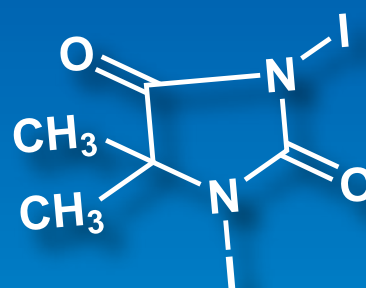
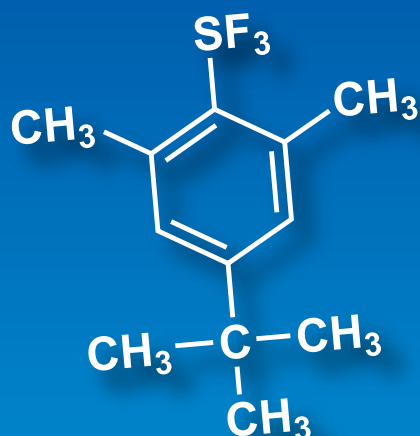


Halogenation Reagents



Fluorinating Agents

Chlorinating Agents

Brominating Agents

Iodinating Agents

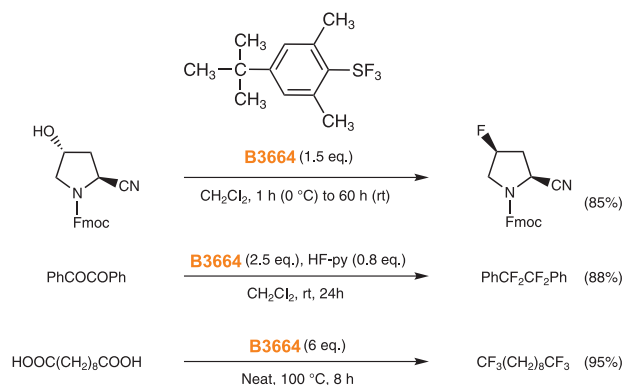
Halogenation Reagents

Halogenation is a basic and fundamental transformation in organic chemistry, and halogenated compounds are of extreme importance as building blocks in organic synthesis.

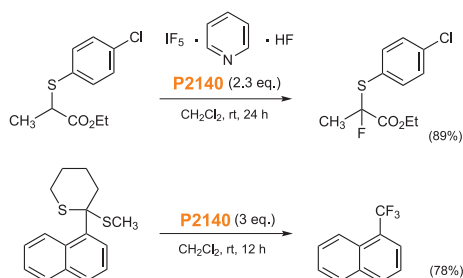
The development of modern coupling reactions, such as the Suzuki-Miyaura and Mizoroki-Heck reactions, have greatly increased the demand for halogenated compounds as starting materials.

On the other hand, introduction of fluorine into a certain position of bioactive compound such as a pharmaceutical and an agricultural chemical may remarkably reduce the toxicity of the compound, or improve the efficiency of medicine. This is due to the structurally mimic and blocking effect characterized by fluorine. In response to this situation, a number of novel halogenation reagents have been developed.

4-*tert*-Butyl-2,6-dimethylphenylsulfur trifluoride (FLUOLEAD™) [B3664] is introduced as below: B3664 is a novel nucleophilic fluorinating agent which was first reported by Umemoto *et al.*¹⁾ Differing from other existing fluorinating agents, such as DAST, B3664 is a crystalline solid with high thermal stability and less fuming character, which makes it easier to handle. B3664 fluorinates a hydroxyl or carbonyl group to afford the corresponding fluorinated compounds in good yields.¹⁾

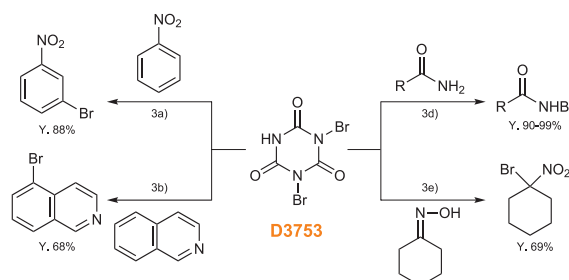


IF₅-Pyridine-HF (Hara Reagent) [P2140] is also a novel fluorinating agent which was first reported by Hara *et al.*²⁾ P2140 is a crystalline solid reagent with air stability and non-hygroscopicity, and can be used as an alternative reagent to IF₅ which is an unstable liquid in air. P2140 can be applied to various fluorination reactions of sulfides as follows.

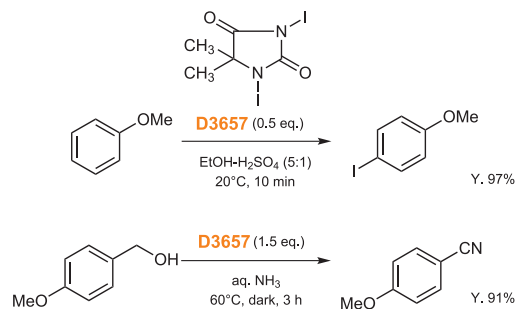


Dibromoisocyanuric acid (DBI) [D3753] which was first reported by Gottardi, is a mild and highly effective brominating agent,^{3a,b,c)} and has

superior brominating ability when compared with *N*-bromosuccinimide (NBS), which is frequently used in organic synthesis. For instance, nitrobenzene was converted to 3-bromonitrobenzene in 88% yield with D3753 in conc. sulfuric acid in 5 min at 20 °C,^{3a)} however, in only 70% yield with NBS in 50% sulfuric acid in 3 h at 85 °C. Thus D3753 has been widely used as an effective brominating agent.^{3d,f)}



1,3-Diiodo-5,5'-dimethylhydantoin (DIH) [D3657], which was first reported by Orazi, is a useful iodinating agent.^{4a)} D3657 has higher reactivity and selectivity than molecular iodine or *N*-iodosuccinimide (NIS), which are frequently used for iodination reactions. D3657 reacts smoothly at room temperature with aromatic compounds in the presence of sulfuric acid to give the corresponding iodinate in a high regioselectivity and a high yield.^{4b)} And primary alcohols, and primary, secondary, and tertiary amines can be easily and efficiently converted into the corresponding nitriles in aqueous ammonia using D3657.^{4c)} In addition, dimethylhydantoin, which is formed after the reaction, can easily be removed by aqueous extraction.



TCI offers a variety of halogenation reagents other than the two items above. All the products are listed below.

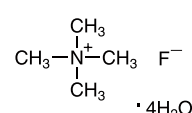
References

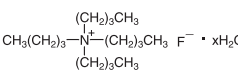
- 1) T. Umemoto, R. P. Singh, Y. Xu, N. Saito, *J. Am. Chem. Soc.* **2010**, *132*, 18199.
- 2) S. Hara, M. Mono, R. Umemura, C. Fuse, *Tetrahedron* **2012**, *68*, 10145.
- 3) a) W. Gottardi, *Monatsh. Chem.* **1968**, *99*, 815.
b) W. D. Brown, A. H. Gouliaev, *Synthesis* **2002**, 83.
c) S. C. Virgil, in *Encyclopedia of Reagents for Organic Synthesis*, ed. by L. A. Paquette, John Wiley & Sons, Chichester, **2001**, pp. 1560-1561.
d) Z. P. Demko, M. Bartsch, K. B. Sharpless, *Org. Lett.* **2000**, *2*, 2221.
e) T. R. Walters, W. W. Zajac Jr., J. M. Woods, *J. Org. Chem.* **1991**, *56*, 316.
- 4) a) O. O. Orazi, R. A. Corral, H. E. Bertorello, *J. Org. Chem.* **1965**, *30*, 1101.
b) V. K. Chaikovskii, V. D. Filimonov, A. A. Funk, V. I. Skorokhodov, V. D. Ogorodnikov, *Russ. J. Org. Chem.* **2007**, *43*, 1291.
c) S. Iida, H. Togo, *Tetrahedron* **2007**, *63*, 8274.

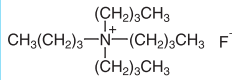
Fluorinating Agents

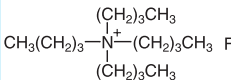
Nucleophilic Fluorinating Agents

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KHF₂
Potassium Hydrogenfluoride
CAS RN: 7789-29-9

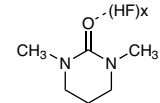
T2754 5g 25g

Tetramethylammonium Fluoride Tetrahydrate
CAS RN: 17787-40-5

T1037 25g 100g

Tetrabutylammonium Fluoride Hydrate
CAS RN: 22206-57-1

T1339 25g 100g 500g

Tetrabutylammonium Fluoride (70-75% in Water)
CAS RN: 429-41-4

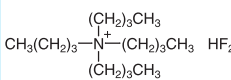
T1338 25mL 100mL 500mL

Tetrabutylammonium Fluoride (ca. 1mol/L in Tetrahydrofuran)
CAS RN: 429-41-4

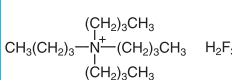
T2022 10g
 $(\text{CH}_3\text{CH}_2)_3\text{N} \cdot 3\text{HF}$
Triethylamine Trihydrofluoride
CAS RN: 73602-61-6

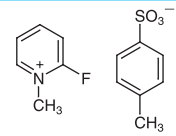
D5272 1g 5g

DMPU-HF Reagent (HF 65%)
CAS RN: 287966-55-6

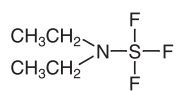
T2026 10g
 $(\text{CH}_3\text{CH}_2)_4\text{N}^+ \text{F}^- \cdot 3\text{HF}$
Tetraethylammonium Fluoride Trihydrofluoride
CAS RN: 42539-97-9

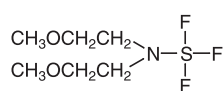
T2027 10g
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CAS RN: 145826-81-9


T1295 5g 25g

Tetrabutylammonium Bifluoride
CAS RN: 23868-34-0

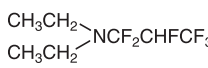
T1635 5g 25g

Tetrabutylammonium Dihydrogen Trifluoride
CAS RN: 99337-56-1

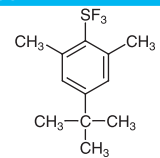
F0225 5g 25g

2-Fluoro-1-methylpyridinium p-Toluenesulfonate
CAS RN: 58086-67-2

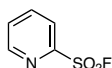
D1868 5g 25g 100g

DAST
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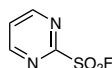
B2440 5g 25g

Bis(2-methoxyethyl)-aminosulfur Trifluoride
CAS RN: 202289-38-1

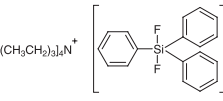
M1573 1g 5g

Morph-DAST
CAS RN: 51010-74-3

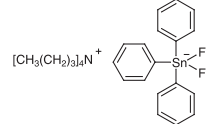
H0598 25g 100g

Ishikawa's Reagent
CAS RN: 309-88-6

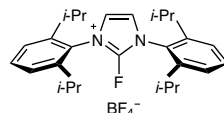
B3664 1g 5g

FLUOLEAD™
CAS RN: 947725-04-4

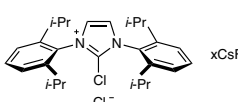
P2398 5g

PyFluor
CAS RN: 878376-35-3

P2465 1g 5g

Pyrimidine-2-sulfonyl Fluoride
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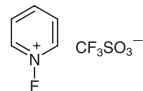
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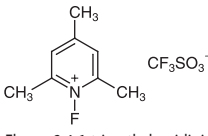
T1592 1g 5g

Tetrabutylammonium Difluorotriphenylstannate
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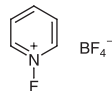
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AlkylFluor™
CAS RN: 2043361-32-4

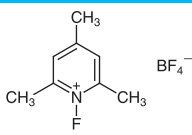
P2420 1g 5g

PhenoFluor™ Mix
CAS RN: 1648825-53-9

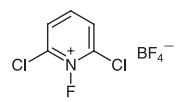
Electrophilic Fluorinating Agents

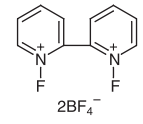
F0327 5g 25g

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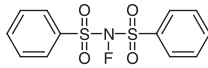
F0328 5g 25g

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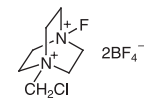
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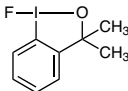
F0346 5g

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

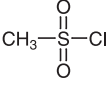
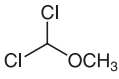
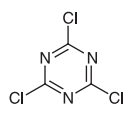
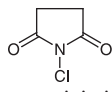
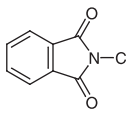
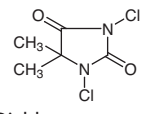
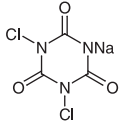
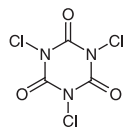
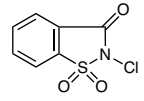
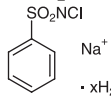
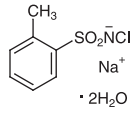
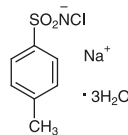
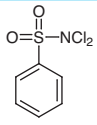
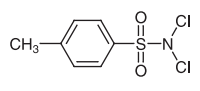
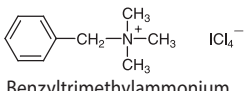
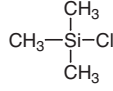
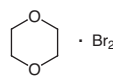
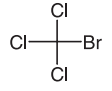
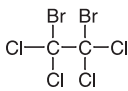
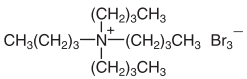
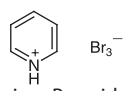
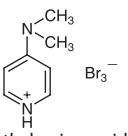
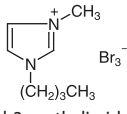
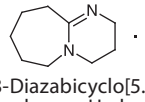
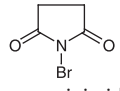
D3812 1g 5g 25g 100g

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CAS RN: 178439-26-4

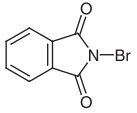
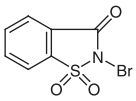
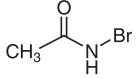
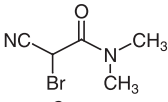
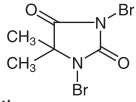
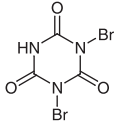
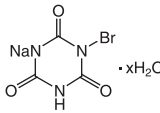
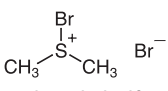
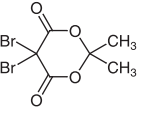
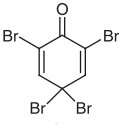
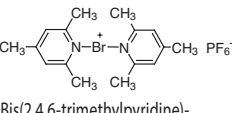
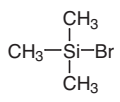
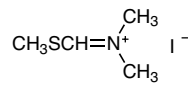
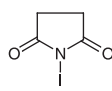
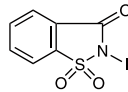
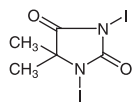
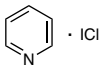
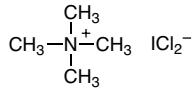
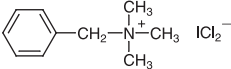
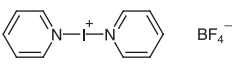
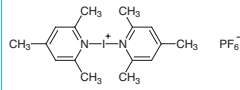
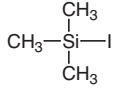
F0335 5g 25g

N-Fluorobenzenesulfonimide
CAS RN: 133745-75-2

F0358 5g 25g 100g

F-TEDA-BF₄
CAS RN: 140681-55-6

F0957 1g

1-Fluoro-3,3-dimethyl-1,2-benzodioxole
CAS RN: 1391728-13-4

Chlorinating Agents

Chlorinating Agents		T2040 500mL  Thionyl Chloride CAS RN: 7719-09-7	T2048 500mL  Thionyl Chloride (ca. 1mol/L in Dichloromethane) CAS RN: 7719-09-7	M0094 25g 500g  Methanesulfonyl Chloride CAS RN: 124-63-0
		T0611 5g 25g $\text{CCl}_3\text{SO}_2\text{Cl}$ Trichloromethanesulfonyl Chloride CAS RN: 2547-61-7	H0362 25g $(\text{CH}_3)_3\text{COCl}$ tert-Butyl Hypochlorite CAS RN: 507-40-4	D1645 25g 250g  Dichloromethyl Methyl Ether CAS RN: 4885-02-3
C0460 25g 500g  Cyanuric Chloride CAS RN: 108-77-0	C0291 25g 100g 500g  N-Chlorosuccinimide (= NCS) CAS RN: 128-09-6	C0802 25g 500g  N-Chlorophthalimide CAS RN: 3481-09-2	D1783 25g 100g 500g  1,3-Dichloro-5,5-dimethylhydantoin CAS RN: 118-52-5	D1003 25g 500g  Sodium Dichloroisocyanurate CAS RN: 2893-78-9
T0620 25g 500g  Trichloroisocyanuric Acid CAS RN: 87-90-1	C1674 5g 25g  N-Chlorosaccharin CAS RN: 14070-51-0	C0075 25g 500g  Chloramine B Hydrate CAS RN: 304655-80-9	C1374 25g  o-Chloramine T Dihydrate CAS RN: 110076-44-3	C0076 25g 500g  Chloramine T Trihydrate CAS RN: 7080-50-4
D0317 5g 25g  Dichloramine B CAS RN: 473-29-0	D0318 25g 500g  Dichloramine T CAS RN: 473-34-7	B1543 5g  Benzyltrimethylammonium Tetrachloriodate CAS RN: 121309-88-4	C0306 25mL 100mL 500mL  Trimethylsilyl Chloride CAS RN: 75-77-4	
Brominating Agents		B2414 90g 500g Br_2 Bromine CAS RN: 7726-95-6	B2719 5g 25g  Bromine - 1,4-Dioxane Complex CAS RN: 15481-39-7	B0662 25g 500g  Bromotrichloromethane CAS RN: 75-62-7
		D1987 25g  1,1,2,2-tetrachloroethane CAS RN: 630-25-1	T0038 25g 100g 500g CBr_4 Carbon Tetrabromide CAS RN: 558-13-4	T1284 25g 100g 500g  Tetrabutylammonium Tribromide CAS RN: 38932-80-8
P0825 25g 100g 500g  Pyridinium Bromide Perbromide CAS RN: 39416-48-3	D1787 5g 25g  4-Dimethylaminopyridinium Bromide Perbromide CAS RN: 92976-81-3	B3596 5g  1-Butyl-3-methylimidazolium Tribromide CAS RN: 820965-08-0	D3976 5g  1,8-Diazabicyclo[5.4.0]-7-undecene Hydrogen Tribromide CAS RN: 138666-59-8	B0656 25g 100g 500g  N-Bromosuccinimide (= NBS) CAS RN: 128-08-5

B1697 5g 25g  N-Bromophthalimide CAS RN: 2439-85-2	B2152 5g 25g  N-Bromosaccharin CAS RN: 35812-01-2	B0530 5g 25g  N-Bromoacetamide CAS RN: 79-15-2	B1016 1g  2-Bromo-2-cyano- N,N-dimethylacetamide CAS RN: 15430-62-3	D1265 25g 500g  1,3-Dibromo- 5,5-dimethylhydantoin CAS RN: 77-48-5
D3753 5g 25g  Dibromoisocyanuric Acid (= DBI) CAS RN: 15114-43-9	B2148 25g  Monosodium Bromoisocyanurate Hydrate CAS RN: 164918-61-0	B2553 100mL BBr ₃ Boron Tribromide (17% in Dichloromethane, ca. 1mol/L) CAS RN: 10294-33-4	B4417 100mL BBr ₃ Boron Tribromide (29% in Heptane, ca. 1mol/L) CAS RN: 10294-33-4	P1743 300g PBr ₃ Phosphorus Tribromide CAS RN: 7789-60-8
B3311 5g 25g  Bromodimethylsulfonium Bromide CAS RN: 50450-21-0	D1710 5g 25g  5,5-Dibromomeldrum's Acid CAS RN: 66131-14-4	T1235 5g 25g  2,4,4,6-Tetrabromo- 2,5-cyclohexadienone CAS RN: 20244-61-5	B2358 1g 5g  Bis(2,4,6-trimethylpyridine)- bromonium Hexafluorophosphate CAS RN: 188944-77-6	B1087 5mL 25mL 250mL  Trimethylsilyl Bromide CAS RN: 2857-97-8
<h2 style="margin: 0;">Iodinating Agents</h2>				
C1190 1g 5g ICH ₂ CH ₂ Cl 1-Chloro-2-iodoethane CAS RN: 624-70-4	D4340 5g 25g  N,N-Dimethyl-N-(methyl- sulfanylmethylene)- ammonium iodide CAS RN: 29085-13-0	I0074 5g 25g 100g  N-Iodosuccinimide (= NIS) CAS RN: 516-12-1	I0784 5g  N-Iodosaccharin CAS RN: 86340-94-5	D3657 5g 25g  1,3-Diiodo-5,5- dimethylhydantoin (= DIH) CAS RN: 2232-12-4
P2086 1g 5g  Pyridine Iodine Monochloride CAS RN: 6443-90-9	T2717 5g  Tetramethylammonium Dichloriodate CAS RN: 1838-41-1	B1604 5g 25g  Benzyltrimethylammonium Dichloriodate CAS RN: 114971-52-7	B2539 1g  Bis(pyridine)iodonium Tetrafluoroborate CAS RN: 15656-28-7	B2359 1g 5g  Bis(2,4,6-trimethylpyridine)- iodonium Hexafluorophosphate CAS RN: 113119-46-3
I0308 5g 25g  Trimethylsilyl Iodide CAS RN: 16029-98-4				

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