

FLUOROBENZENE

PRODUCT IDENTIFICATION

CAS NO.	462-06-6
EINECS NO	207-321-7
FORMULA	C ₆ H ₅ F
MOL WT.	96.103
H.S. CODE	
TOXICITY	Oral rat LD50: 4399 mg/kg
SYNONYMS	Phenyl Fluoride; monofluorobenzene;
DERIVATION	
CLASSIFICATION	



PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	Colorless liquid
MELTING POINT	-41 C
BOILING POINT	85 C
SPECIFIC GRAVITY	1.024
SOLUBILITY IN WATER	Insoluble
pH	
VAPOR DENSITY	3.31
AUTOIGNITION	
REFRACTIVE INDEX	1.4650
NFPA RATINGS	Health:- ; Flammability: 3; Reactivity: 0
FLASH POINT	-15 C
STABILITY	Stable under ordinary conditions

APPLICATIONS

Fluorobenzene is used to control carbon content in steel manufacturing. It is an intermediate for pharmaceuticals, pesticides and other organic compounds.

When substituted benzene molecules undergo electrophilic substitution reactions, substituents on a benzene ring can influence the reactivity. Activating substituents that activate the benzene ring toward electrophilic attack can alter the reaction rate or products by electronically or sterically affecting the interaction of the two reactants. Deactivating substituents remove electron density from the benzene ring, making electrophilic aromatic substitution reactions slower and more difficult than benzene itself. For example, a hydroxy or methoxy substituent in phenol and anisole increases the rate of electrophilic substitution, while a nitro substituent decreases the ring's reactivity. Electron donating substituents activate the benzene ring toward electrophilic attack, and electron withdrawing substituents deactivate the ring, making it less reactive to electrophilic attack. The strongest activating substituents are the amino (-NH₂) and hydroxyl (-OH) groups.

Reactivity Effects	Activating substituents	Deactivating substituents
Strong	-NH ₂ , -NHR, -NR ₂ , -OH, -O-	-NO ₂ , -NR ₃ ⁺ , -CF ₃ , CCl ₃
Moderate	-NHCOCH ₃ , -NHCOR, -OCH ₃ , -OR	-CN, -SO ₃ H, -COOH, -COOR, -COH, -COR
Weak	-CH ₃ , -C ₂ H ₅ , -R, -C ₆ H ₅	-F, -Cl, -Br, -I

Toluene, aniline and phenol are activated aromatic compounds. Examples of deactivated

aromatic compounds are nitrobenzene, benzaldehyde and halogenated benzenes.

Activating substituents generally direct substitution to the ortho and para positions where substitutions must take place. With some exceptions, deactivating substituents direct to the meta position. Deactivating substituents which orient ortho and para- positions are the halogens (-F, -Cl, -Br, -I) and -CH₂Cl, and -CH=CHNO₂

When disubstituted benzene molecules undergo electrophilic substitution reactions, a new substituent is directed depends on the orientation of the existing substituents and their individual effects; whether the groups have cooperative or antagonistic directing effects. Ortho position is the most reactive towards electrophile due to the highest electron density ortho positions. But this increased reactivity is countervailed by steric hindrance between substituent and electrophile.

A nucleophilic substitution is a substitution reaction which the nucleophile displaces a good leaving group, such as a halide on an aromatic ring. This mechanism is called S_NAr (the two-step addition-elimination mechanism), where electron withdrawing substituents activate the ring towards nucleophilic attack. Addition-elimination reactions usually occur at sp² or sp hybridized carbon atoms, in contrast to S_N1 and S_N2 at sp³. Chloro and bromobenzene reacts with the very strong base sodium amide (NaNH₂) to give good yields of aniline. Other nucleophilic aromatic substitution mechanisms include benzyne mechanism and free radical (S_{RN}1) mechanism.

Common reactions of substituent groups on benzene ring include:

- Conversion of halogens into other various substituents
- Modifying activating substituents
- Oxidative degradation of alkyl chain
- Reduction of nitro or carbonyl substituents
- Reversibility of the aromatic sulfonation reaction

SALES SPECIFICATION

APPEARANCE	Colorless liquid
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PURITY (G.C)	99.5% min
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TRANSPORTATION

PACKING	200kgs in drum
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HAZARD CLASS	3 (Packing group II)
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UN NO.	2387
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GENERAL DESCRIPTION OF FLUORINE AND ITS COMPOUNDS

Fluorine (Symbol : F; Atomic no. 9) is a yellowish, poisonous, corrosive gas under ordinary conditions. Fluorine becomes a yellow liquid upon cooling. It is the most reactive nonmetallic element and extremely powerful oxidizing agent. Because of its extreme reactivity, fluorine does not occur uncombined in nature. Fluorine occurs widely combined in the mineral fluorspar(fluorite, the chief commercial source), cryolite and apatite. The preparation of the free element is carried out by the electrolysis of a molten mixture of hydrogen fluoride, HF, and potassium fluoride, KF in the absence of water. Fluorine can be safely stored under pressure in cylinders of stainless steel if the valves of the cylinders are free from traces of organic matter. The outstanding oxidizing properties of the elemental gas are used in some rocket fuels. The element may be used for the fluorination of organic compounds with appropriate precautions. The element is used for manufacturing various fluorides including chlorine trifluoride and cobalt(III) fluoride which are important fluorinating agents for organic compounds, sulfur(VI) fluoride used as a gaseous electrical insulator. Boron trifluoride and antimony trifluoride like hydrogen fluorides are important catalysts for alkylation reactions used to prepare organic compounds. Sodium fluoride (NaF) is used to treat dental caries and is often

used for the fluoridation of drinking water to reduce tooth decay (However, there are reports of an accompanying risk of fluoride toxicity). The element is also used for the preparation of uranium(VI) fluoride, utilized in the gaseous diffusion process of separating uranium-235 from uranium-238 (natural uranium) for reactor fuel. The importance of fluorine lies largely in its extreme ability to attract electrons and to the small size of its atoms, which can be attributed to form many stable complexes with positive ions like hexafluorosilicate(IV) and hexafluoroaluminate(III). Fluorine derivatives of hydrocarbons (compounds of carbon and hydrogen) are useful extensively as aerosol-spray propellants, refrigerants, solvents, cleansing agents for electrical and electronic components, and foaming agents in shipping-plastics manufacturing. Useful plastics with non-sticking qualities, such as polytetrafluoroethylene (known by the trade name Teflon), are readily made from unsaturated fluorocarbons. A solution of hydrogen fluoride gas in water is called hydrofluoric acid, largely consumed for cleaning metals and for polishing, frosting, and etching glass. Hydrofluoric acid is also used as a catalyst for alkylation reactions. The chemical reactions are similar to those in the sulfuric acid process, but it is possible to avoid refrigeration. (In sulfuric acid alkylation, refrigeration is necessary because of the heat generated by the reaction).