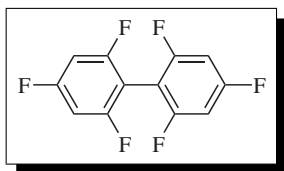


2,2',4,4',6,6'-Hexafluorobiphenyl

[41860-46-2] C₁₂H₄F₆ (MW 262.15)

InChI = 1/C12H4F6/c13-5-1-7(15)11(8(16)2-5)12-9(17)3-6(14) 4-10(12)18/h1-4H

InChIKey = GJEWKLJUCIECPJ-UHFFFAOYAY

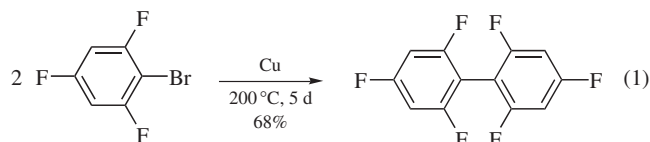
(nucleophilic fluoroarylation agent;^{1,2} can be used to prepare perfluorinated phenylene dendrimers as organic field-effect transistors and organic light-emitting diodes,¹ and for other elaborations²)

Physical Data: mp 130–132 °C.^{1–3}Solubility: soluble in toluene, tetrahydrofuran, nitrobenzene, hexane, methanol, and ethanol.^{1–3}

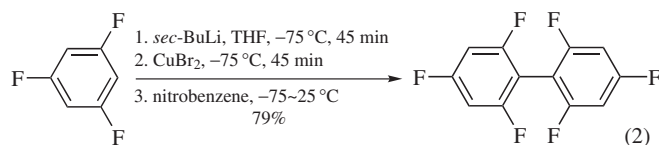
Form Supplied in: colorless needles; often prepared by Ullmann coupling reaction using 1-iodo(bromo)-2,4,6-trifluorobenzene and copper bronze,^{1,3} or using one-pot multistep reaction using 1,3,5-trifluorobenzene.²

Handling, Storage, and Precautions: 2,2',4,4',6,6'-hexafluorobiphenyl has high reactivity with strong bases such as *sec*-butyllithium; readily reacts with bromine under acidic conditions; store under anhydrous, neutral conditions; use in a fume hood.

Preparation of 2,2',4,4',6,6'-Hexafluorobiphenyl. There are two reported methods available for the preparation of 2,2',4,4',6,6'-hexafluorobiphenyl.^{1–3} The first method is the Ullmann homocoupling reaction using 1-bromo-2,4,6-trifluorobenzene (or 1-iodo-2,4,6-trifluorobenzene) and copper bronze (eq 1).^{1,3} For a typical reaction, 1-bromo-2,4,6-trifluorobenzene and an excess amount of copper bronze were heated at 200 °C in a sealed glass tube for 5 days to give 2,2',4,4',6,6'-hexafluorobiphenyl in 68% isolated yield.¹

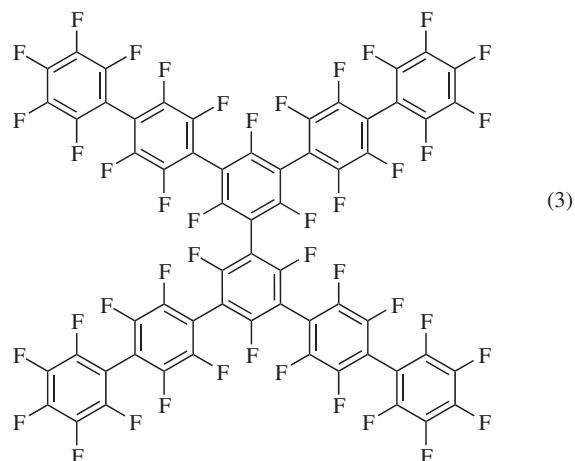
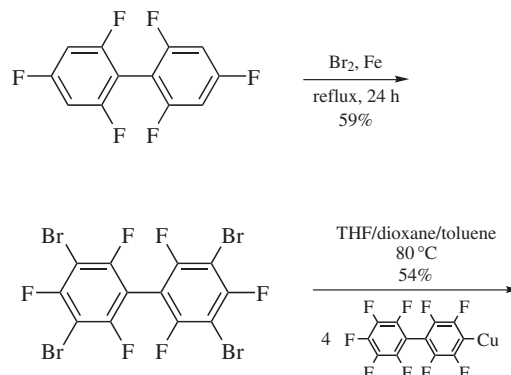


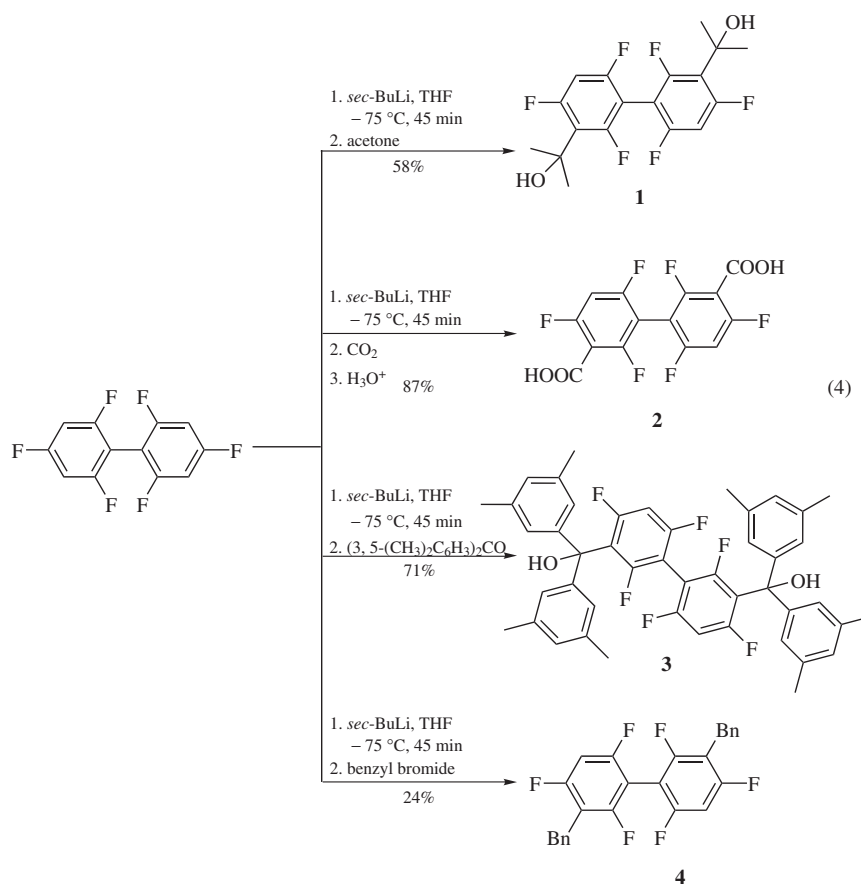
2,2',4,4',6,6'-Hexafluorobiphenyl can also be obtained using a one-pot three-step procedure from 1,3,5-trifluorobenzene by a copper-catalyzed aryl-aryl coupling reaction (eq 2).² Metallation of 1,3,5-trifluorobenzene with *sec*-butyllithium, transmetalation with copper(II) bromide, and subsequent addition of nitrobenzene gave 2,2',4,4',6,6'-hexafluorobiphenyl in 79% yield (eq 2).² Furthermore, oxidative photolysis of 1,3,5-trifluorobenzene was also able to afford 2,2',4,4',6,6'-hexafluorobiphenyl as one of the products, although the reaction yield was very low.⁴



Electrophilic Aromatic Substitution Reactions. Like other aromatic compounds, 2,2',4,4',6,6'-hexafluorobiphenyl can undergo acid-catalyzed electrophilic aromatic substitution reactions. For instance, under reflux conditions involving elemental bromine and iron particles for 24 h, 2,2',4,4',6,6'-hexafluorobiphenyl was converted to 2,2',4,4',6,6'-hexafluoro-3,3',5,5'-tetrabromobiphenyl in 59% isolated yield (eq 3).¹ The latter compound can be further converted into perfluorinated phenylene dendrimers, which are unique π -conjugated electronic materials for organic light-emitting diodes (OLEDs) (eq 3).¹

Nucleophilic Addition and Substitution Reactions. Due to the strong electron-withdrawing effect of the fluorine atoms, 2,2',4,4',6,6'-hexafluorobiphenyl readily undergoes smooth double metallation using *sec*-butyllithium to give the 3,5'-dilithiated biphenyl intermediate. The later species was trapped by ketones, carbon dioxide, and benzyl bromide to give the corresponding products **1–4** (eq 4).² This method opens the door for the further elaboration of 2,2',4,4',6,6'-hexafluorobiphenyl.





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