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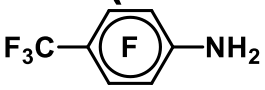
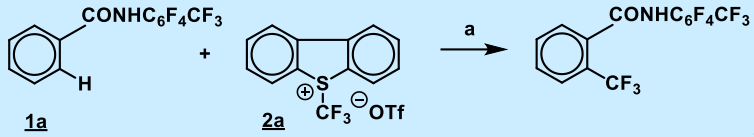
2,3,5,6-Tetrafluoro-4-(trifluoromethyl)aniline



Purity	97%
CAS Number	651-83-2
Molecular Formula	C7H2F7N
Molecular Weight	233.09

Application

1. Trifluoromethylated aromatics are considered as basic structures for medicines and agrochemicals. Although there are reports of cross-coupling synthesis between activated aromatics (halogen, boron) and CF3-forming agents using Pd/Cu catalysts, there are still few methods for directly introducing CF3 groups into aromatic C-H bonds. Selective introduction of CF3 groups at the o-position of acidic aromatic amides is achieved with a good yield through the composition of Pd-Cu catalyst + CF3-C6F4-directing group + amide additive + TFA.

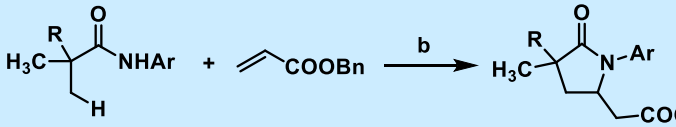


a. 1a; 0.1mmol, 2a; 0.15mmol, Pd(OAc)2 10mol%, TFA 1mmol, additive 15eq, DCE 3ml, 130℃*24hr, isolated yield, abb. NMF; N-methylformamide

No.	Aromatic substrates	additives	Cu(OAc)2	Yield(%)
2	C6H5CONHC6F4CF3	DMF 15eq	1 eq	23
3	C6H5CONHC6F4CF3	DMF 15eq	2 eq	57
6	C6H5CONHC6F4CF3	NMF 15eq	2 eq	79
3c	CH3C6H5CONHC6F4CF3	NMF 15eq	2 eq	94
3e	CH3OC6H5CONHC6F4CF3	NMF 15eq	2 eq	89

J. Am. Chem. Soc., 2012, 134, p11948-11951

2. Olefin addition to aliphatic C-H bonds was investigated using the Pd(OAc)2/ Cu(OAc)2 catalyst system and N-aryl pivalic acid/benzyl acrylate as a model. It has been found that the yield can be improved by making the aryl group electron-withdrawing.



b. substrate 0.2mmol, 0.1ml C6H5CH2OCOCH-CH2, 10mol% Pd(OAc)2, 2.0eq LiCl, 1.1eq Cu(OAc)2, 1ml DMF, N2, 120℃*12hr

No.	R	Ar	AgOAc (eq)	Yd (%)
1a	CH3	-C6H5	-	1
1b	CH3	-C6H3(NO2)2	-	47
1c	CH3	-C6F5	-	71
1d	CH3	-C6F4CF3	-	88
8a	H	-C6F5	1.1	55
9a	H	-C6F4CF3	1.1	91
10a	CH3	-C6F4CF3	1.1	94

J. Am. Che, Soc., 2010, 132, p3680-3681

Properties:

Appearance	Liquid
Boiling point, °C	185-186