

# Synthesis of Triazole and Tetrazole-Functionalized Zr-Based Metal-Organic Frameworks Through Post-Synthetic Ligand Exchange

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## Materials

Name	Company	Catalog Number	Comments
2-Bromoterephthalic acid	BLD Pharm	BD5695	reagent for BDC-Triazole
Azidotrimethylsilane	Sigma Aldrich	155071	reagent for BDC-Triazole
Bis(triphenylphosphine)palladium(II) dichloride	TCI	B1667	reagent for BDC-Triazole
Copper(I) cyanide	Alfa-Aesar	12135	reagent for BDC-Tetrazole
Copper(I) iodide	Acros organics	20150	reagent for BDC-Triazole
Digital Orbital Shaker	Daihan Scientific	SHO-1D	PSE
Formic Acid	Daejung chemical	F0195	reagent for BDC-Tetrazole
Hybrid LC/Q-TOF system	Bruker BioSciences	maXis 4G	HR-MS
Lithium hydroxide monohydrate	Daejung chemical	5087-4405	reagent for BDC-Triazole
Magnesium sulfate	Samchun chemical	M1807	reagent for BDC-Triazole
Methyl alcohol	Daejung chemical	M0584	reagent for BDC-Tetrazole
N,N-Dimethylformamide	Daejung chemical	D0552	reagent for BDC-Tetrazole
Nuclear Magnetic Resonance Spectrometer-500 MHz	Bruker	AVANCE 500MHz	NMR
Polypropylene cap (22 mm, Cork-Backed Foil Lined)	Sungho Korea	22-200	material for digestion
Potassium cyanide	Alfa-Aesar	L13273	reagent for BDC-Tetrazole
PVDF Syringe filter (13 mm, 0.45 μm)	LK Lab Korea	F14-61-363	material for digestion
Scintillation vial (20 mL, borosilicate glass)	Sungho Korea	74504-20	material for digestion
Sodium azide	TCI	S0489	reagent for BDC-Tetrazole
Sodium bicarbonate	Samchun chemical	S0343	reagent for BDC-Triazole
Tetrabutylammonium fluoride (1 M THF solution)	Acros organics	20195	reagent for BDC-Triazole
Triethylamine	TCI	T0424	reagent for BDC-Triazole

Triethylamine hydrochloride	Daejung chemical	8628-4405	reagent for BDC-Tetrazole
Trimethylsilyl-acetylene	Alfa-Aesar	A12856	reagent for BDC-Triazole
Triphenylphosphine	TCI	T0519	reagent for BDC-Triazole
X RAY DIFFRACTOMETER SYSTEM	Rigaku	MiniFlex 600	PXRD
Zirconium(IV) chloride	Alfa-Aesar	12104	reagent for BDC-Tetrazole