MOF_Synthesis_Quiz_Clean

July 25, 2021

1 Welcome to the MOF Synthesis prediction quiz!

Human against machine: Who is better in predicting MOF synthesis conditions? Hint: Our machine learning models find MOF synthesis prediction rather challenging, so give your best to beat them! Please check the MOFs on the following pages and tell us your educated guesses.

Short tutorial: Go through this jupyter notebook and follow the instructions. Please always use **"Shift+Enter" to run each code cell**, or click all "run cell" buttons (triangles). In the end you will receive a file, which you can send to us for analysis.

2 Getting started

We first need to import and install some libraries that are needed later. Afterwards, please upload the zip file with the MOF data that we provided for you.

Instructions: Please klick at the grey code cells, press "Shift+Enter", and wait for the each cell to finish processing.

[1]:
```
pip install py3Dmol
```

```
Collecting py3Dmol
  Downloading py3Dmol-0.9.2-py2.py3-none-any.whl (6.2 kB)
Installing collected packages: py3Dmol
Successfully installed py3Dmol-0.9.2
WARNING: You are using pip version 20.3.3; however, version 21.2.1 is
available.
You should consider upgrading via the '/home/pascal/anaconda3/bin/python -m pip
install --upgrade pip' command.
Note: you may need to restart the kernel to use updated packages.
```

[2]:
```
pip install ase
```

```
Collecting ase
  Downloading ase-3.22.0-py3-none-any.whl (2.2 MB)
```

```
     |                | 2.2 MB 3.5 MB/s eta 0:00:01
Requirement already satisfied: numpy>=1.15.0 in
/home/pascal/anaconda3/lib/python3.6/site-packages (from ase) (1.19.5)
Requirement already satisfied: scipy>=1.1.0 in
/home/pascal/anaconda3/lib/python3.6/site-packages (from ase) (1.4.1)
Collecting matplotlib>=3.1.0
  Downloading matplotlib-3.3.4-cp36-cp36m-manylinux1_x86_64.whl (11.5 MB)
     |                | 11.5 MB 16.4 MB/s eta 0:00:01
Requirement already satisfied: kiwisolver>=1.0.1 in
/home/pascal/anaconda3/lib/python3.6/site-packages (from matplotlib>=3.1.0->ase)
(1.2.0)
Requirement already satisfied: pyparsing!=2.0.4,!=2.1.2,!=2.1.6,>=2.0.3 in
/home/pascal/anaconda3/lib/python3.6/site-packages (from matplotlib>=3.1.0->ase)
(2.4.7)
Requirement already satisfied: cycler>=0.10 in
/home/pascal/anaconda3/lib/python3.6/site-packages (from matplotlib>=3.1.0->ase)
(0.10.0)
Requirement already satisfied: pillow>=6.2.0 in
/home/pascal/anaconda3/lib/python3.6/site-packages (from matplotlib>=3.1.0->ase)
(6.2.1)
Requirement already satisfied: python-dateutil>=2.1 in
/home/pascal/anaconda3/lib/python3.6/site-packages (from matplotlib>=3.1.0->ase)
(2.8.1)
Requirement already satisfied: six in /home/pascal/anaconda3/lib/python3.6/site-
packages (from cycler>=0.10->matplotlib>=3.1.0->ase) (1.15.0)
Installing collected packages: matplotlib, ase
  Attempting uninstall: matplotlib
    Found existing installation: matplotlib 3.0.2
    Uninstalling matplotlib-3.0.2:
      Successfully uninstalled matplotlib-3.0.2
Successfully installed ase-3.22.0 matplotlib-3.3.4
WARNING: You are using pip version 20.3.3; however, version 21.2.1 is
available.
You should consider upgrading via the '/home/pascal/anaconda3/bin/python -m pip
install --upgrade pip' command.
Note: you may need to restart the kernel to use updated packages.
```

[4]:
```
import os
import sys
import ase
import numpy as np
import matplotlib.pyplot as plt
from IPython.display import Image
try:
    from google.colab import files
except:
```

```
    pass
```

Instructions: In the following cell, please press "Shift+Enter" as usual and then upload the data.zip file.

[ ]:
```
if os.path.exists("data.zip"):
  os.system("rm data.zip")
uploaded = files.upload()
```

Instructions: In the next cell, your uploaded data will be processed. If this works without error, you are ready for the synthesis prediction!

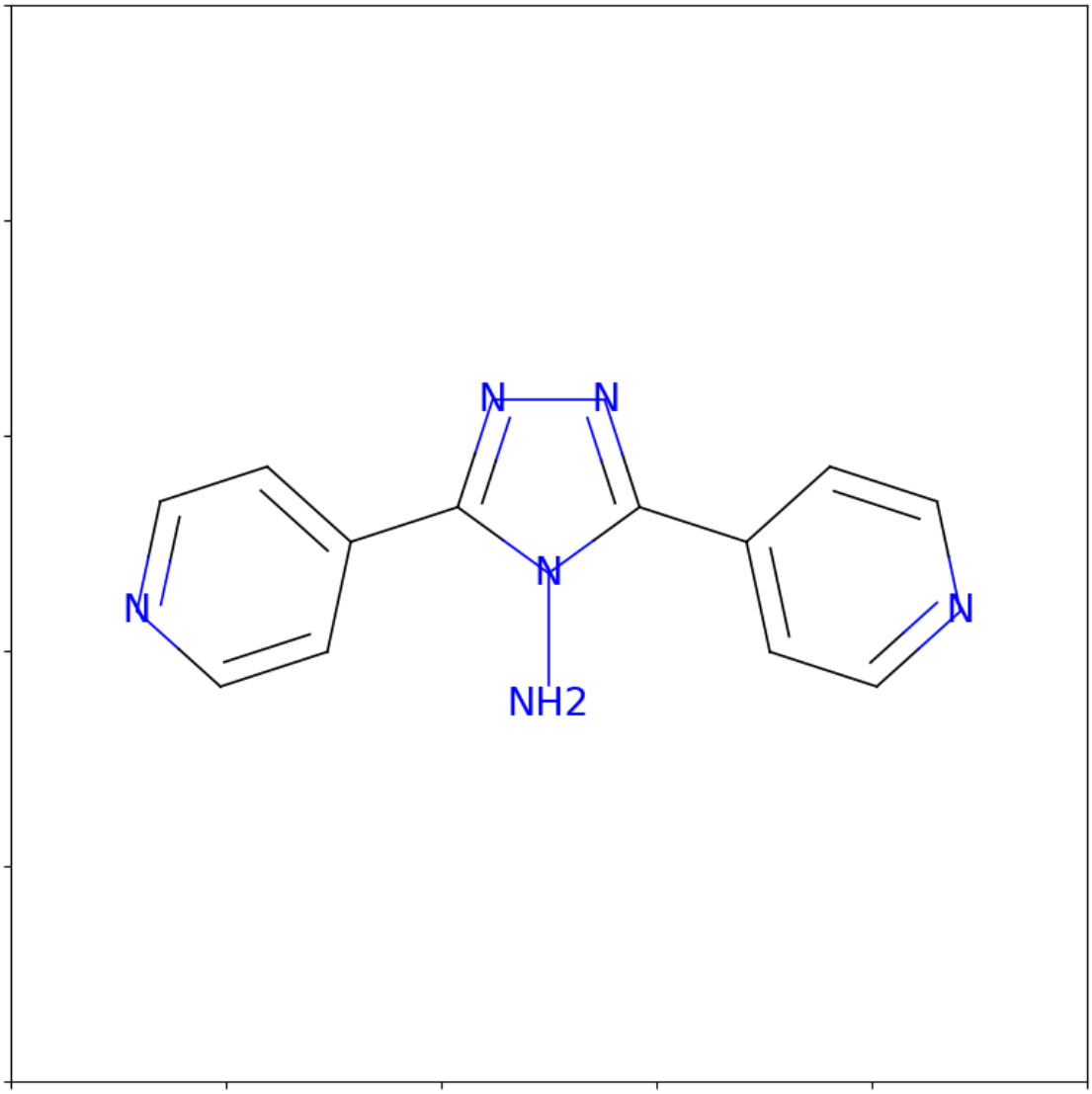
[5]:
```
# let's unzip the provided file
if os.path.exists("data.zip"):
  os.system("unzip data.zip")
else:
  print("Please upload the data.zip file first")

os.system("mv ./data/nutils.py .")
import nutils
import importlib
importlib.reload(nutils)
results =  {}
```

MOF 1

Here is the linker:

[6]:
```
Image('./WOPHIU01_cleansingle_linker1.png')
```

[6]:



The metal center of this MOF is ``Zn''. The oxidation state of the metel is ``2''

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[7]:
```
nutils.viewer('./WOPHIU01_clean.cif')
```

[8]:
```
temperature_mof_1_Celsius  = 135.0 #@param {type:'number'}
time_mof_1_hours  =  48#@param {type:'number'}
```

```
first_solvent_mof_1 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_1 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_1 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_1 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_1 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_1_mol_per_liter  =  0.01#@param {type:'number'}
concentration_first_linker_mof_1_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_second_linker_mof_1_mol_per_liter  =  0.050#@param {type:'number'}
are_you_sure_about_your_selction_mof_1 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_1 =  "not  sure about the stoichiometry␣
↪ratio between the linkers" #@param {type:'string'}
results['mof_1'] = {}
results['mof_1']['temperature']=temperature_mof_1_Celsius
results['mof_1']['time']=time_mof_1_hours
results['mof_1']['solvent1']=first_solvent_mof_1
```

```
results['mof_1']['solvent2']=second_solvent_mof_1
results['mof_1']['solvent3']=third_solvent_mof_1
results['mof_1']['additive']=additive_mof_1
results['mof_1']['counter']=counter_ion_mof_1
results['mof_1']['metal']=concentration_metal_mof_1_mol_per_liter
results['mof_1']['linker1']=concentration_first_linker_mof_1_mol_per_liter
results['mof_1']['linker2']=concentration_second_linker_mof_1_mol_per_liter
results['mof_1']['surely']=are_you_sure_about_your_selction_mof_1
results['mof_1']['additional']=what_makes_you_so_sure_or_unsure_mof_1
```

[9]:
```
nutils.print_choice(temperature_mof_1_Celsius, time_mof_1_hours,␣
↪first_solvent_mof_1,second_solvent_mof_1,third_solvent_mof_1 ,␣
↪counter_ion_mof_1, concentration_metal_mof_1_mol_per_liter,␣
↪concentration_first_linker_mof_1_mol_per_liter,concentration_second_linker_mof_1_mol_per_li
↪, additive_mof_1,are_you_sure_about_your_selction_mof_1,␣
↪what_makes_you_so_sure_or_unsure_mof_1 )
```

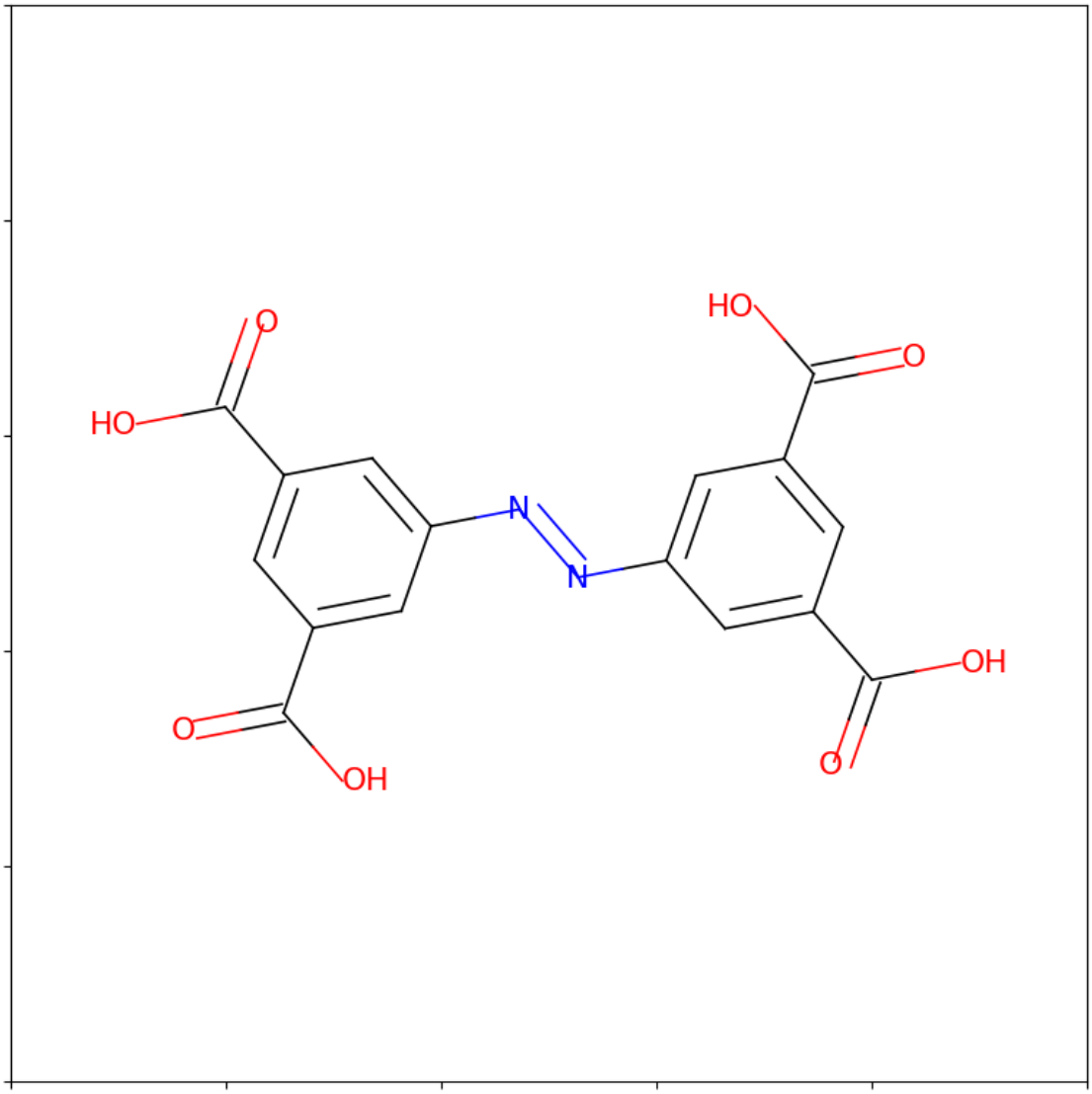
```
Thanks for your input
Your selection was:
Temperature: 135.0
Time: 48
Solvent1: N,N-diethylformamide (DEF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.01
First_Linker_Concentration: 0.025
Second_Linker_Concentration: 0.05
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: not  sure about the stoichiometry ratio between
the linkers
```

```
# MOF 2
```

Here is the linker:

[10]:
```
Image('./RIDCEN_chargedsingle_linker0.png')
```

[10]:



The metal center of this MOF is ``In''. The oxidation state of the metel is ``3''

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[11]:
```
nutils.viewer('./RIDCEN_charged.cif')
```

[12]:
```
temperature_mof_2_Celsius  = 170 #@param {type:'number'}
time_mof_2_hours  =  72#@param {type:'number'}
```

```
first_solvent_mof_2 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_2 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_2 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_2 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_2 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_2_mol_per_liter  =  0.025#@param {type:'number'}
concentration_first_linker_mof_2_mol_per_liter  =  0.015#@param {type:'number'}
concentration_second_linker_mof_2_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_2 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_2 =  'The concentration of the In and the␣
↪ligand + here the addition of an acid modulator could play an important role␣
↪during crystallization' #@param {type:'string'}
results['mof_2'] = {}
results['mof_2']['temperature']=temperature_mof_2_Celsius
results['mof_2']['time']=time_mof_2_hours
```

```
results['mof_2']['solvent1']=first_solvent_mof_2
results['mof_2']['solvent2']=second_solvent_mof_2
results['mof_2']['solvent3']=third_solvent_mof_2
results['mof_2']['additive']=additive_mof_2
results['mof_2']['counter']=counter_ion_mof_2
results['mof_2']['metal']=concentration_metal_mof_2_mol_per_liter
results['mof_2']['linker1']=concentration_first_linker_mof_2_mol_per_liter
results['mof_2']['linker2']=concentration_second_linker_mof_2_mol_per_liter
results['mof_2']['surely']=are_you_sure_about_your_selction_mof_2
results['mof_2']['additional']=what_makes_you_so_sure_or_unsure_mof_2
```

[13]:
```
nutils.print_choice(temperature_mof_2_Celsius, time_mof_2_hours,␣
↪first_solvent_mof_2,second_solvent_mof_2,third_solvent_mof_2 ,␣
↪counter_ion_mof_2, concentration_metal_mof_2_mol_per_liter,␣
↪concentration_first_linker_mof_2_mol_per_liter,concentration_second_linker_mof_2_mol_per_li
↪, additive_mof_2,are_you_sure_about_your_selction_mof_2,␣
↪what_makes_you_so_sure_or_unsure_mof_2 )
```

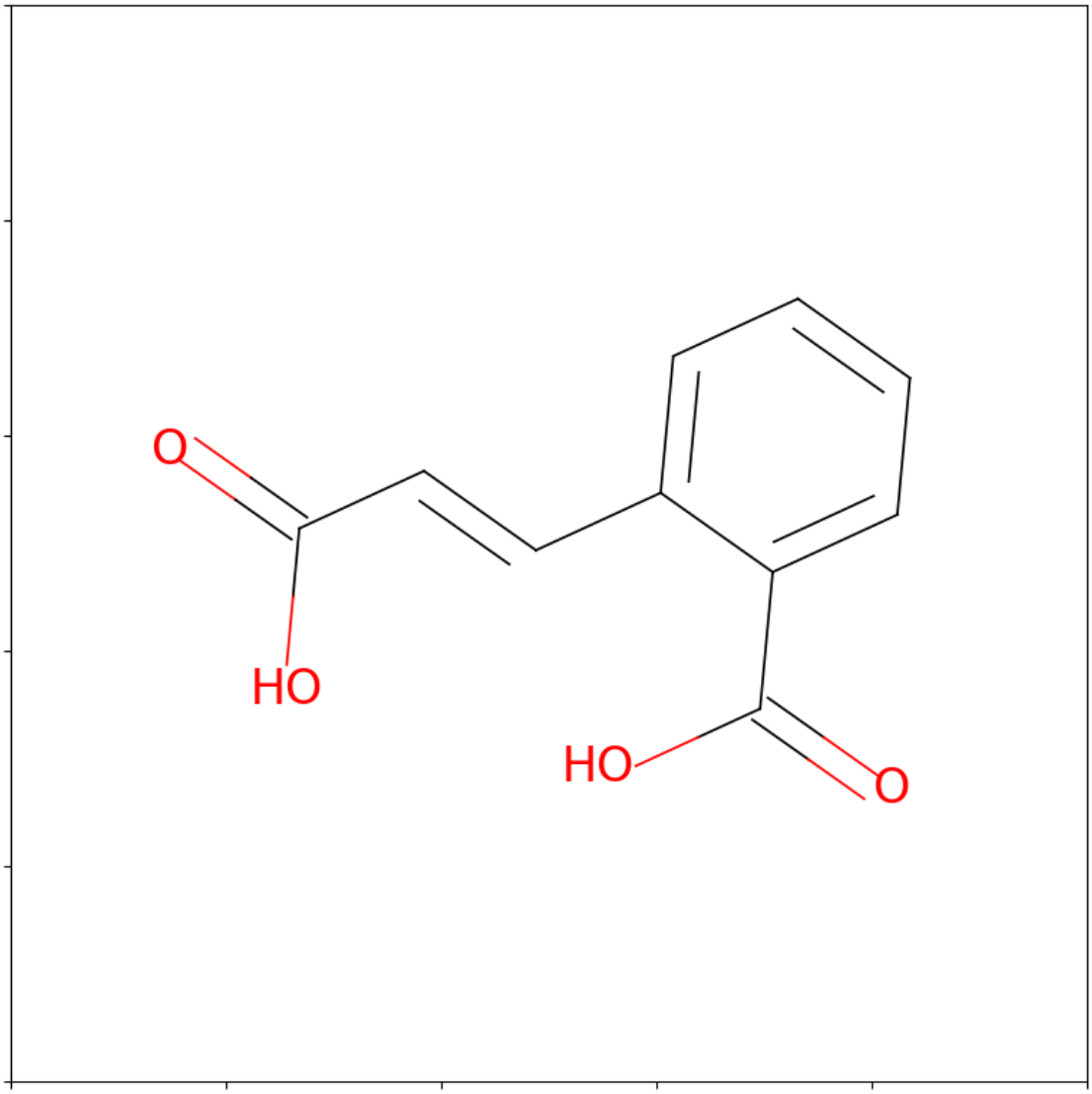
```
Thanks for your input
Your selection was:
Temperature: 170
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.025
First_Linker_Concentration: 0.015
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: The concentration of the In and the ligand + here
the addition of an acid modulator could play an important role during
crystallization
```

```
# MOF 3
```

Here is the linker:

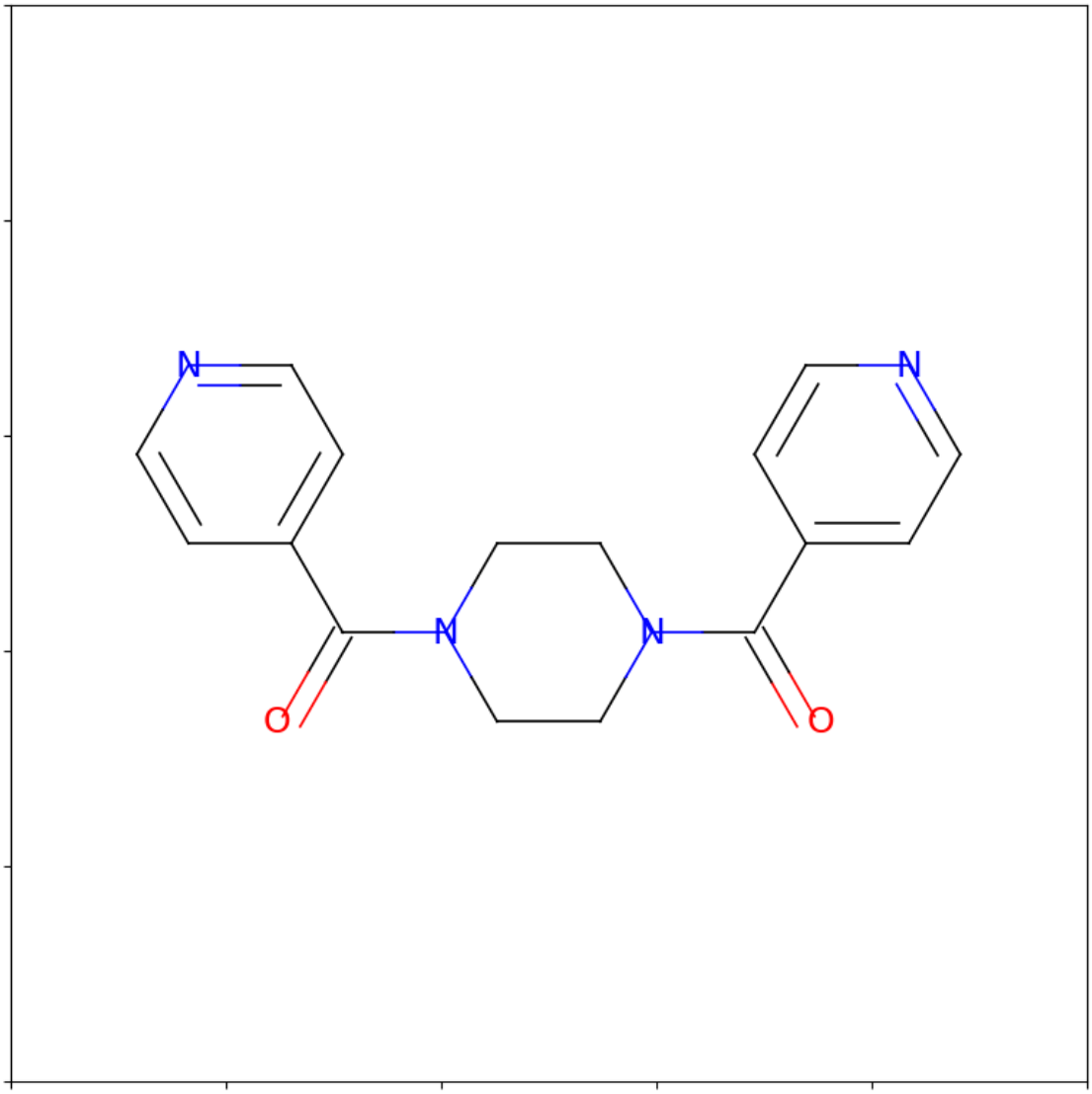
[14]:
```
Image('./AJINOY_cleansingle_linker0.png')
```

[14]:



[15]:
```
Image('./AJINOY_cleansingle_linker3.png')
```

[15]:



The metal center of this MOF is ``Cu''. The oxidation state of the metel is ``2''

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[16]:
```
nutils.viewer('./AJINOY_clean.cif')
```

[17]:
```
temperature_mof_3_Celsius  = 130.0 #@param {type:'number'}
time_mof_3_hours  = 48 #@param {type:'number'}
```

```
first_solvent_mof_3 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_3 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_3 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_3 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_3 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_3_mol_per_liter  =  0.025#@param {type:'number'}
concentration_first_linker_mof_3_mol_per_liter  =  0.025#@param {type:'number'}
concentration_second_linker_mof_3_mol_per_liter  =  0.05#@param {type:'number'}
are_you_sure_about_your_selction_mof_3 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_3 =  'Stoichiometry between the linkers␣
↪and the overall concentration of the reagents' #@param {type:'string'}
results['mof_3'] = {}
results['mof_3']['temperature']=temperature_mof_3_Celsius
results['mof_3']['time']=time_mof_3_hours
results['mof_3']['solvent1']=first_solvent_mof_3
```

```
results['mof_3']['solvent2']=second_solvent_mof_3
results['mof_3']['solvent3']=third_solvent_mof_3
results['mof_3']['additive']=additive_mof_3
results['mof_3']['counter']=counter_ion_mof_3
results['mof_3']['metal']=concentration_metal_mof_3_mol_per_liter
results['mof_3']['linker1']=concentration_first_linker_mof_3_mol_per_liter
results['mof_3']['linker2']=concentration_second_linker_mof_3_mol_per_liter
results['mof_3']['surely']=are_you_sure_about_your_selction_mof_3
results['mof_3']['additional']=what_makes_you_so_sure_or_unsure_mof_3
```

[18]:
```
nutils.print_choice(temperature_mof_3_Celsius, time_mof_3_hours,␣
↪first_solvent_mof_3,second_solvent_mof_3,third_solvent_mof_3 ,␣
↪counter_ion_mof_3, concentration_metal_mof_3_mol_per_liter,␣
↪concentration_first_linker_mof_3_mol_per_liter,concentration_second_linker_mof_3_mol_per_li
↪, additive_mof_3,are_you_sure_about_your_selction_mof_3,␣
↪what_makes_you_so_sure_or_unsure_mof_3 )
```

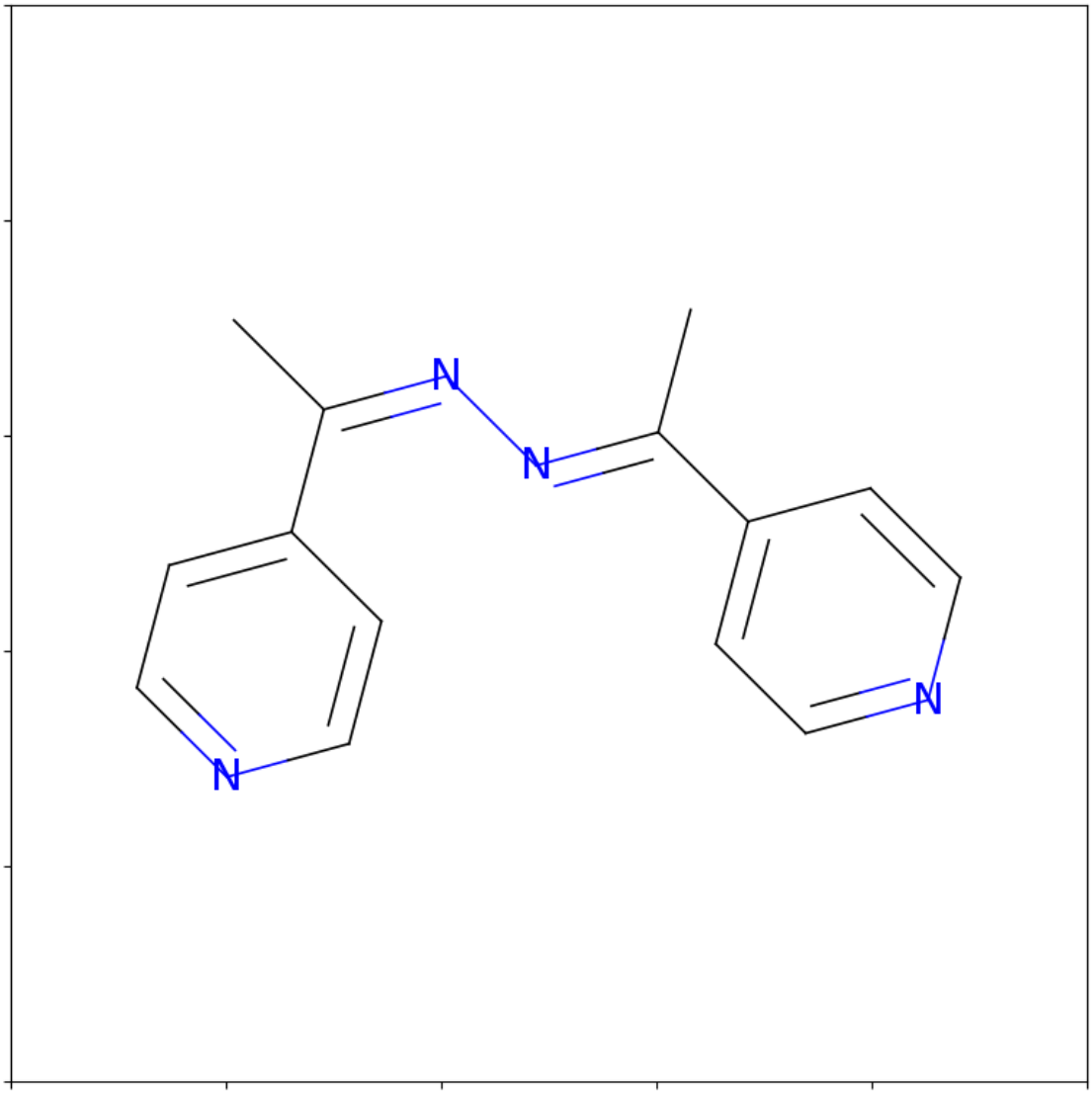
```
Thanks for your input
Your selection was:
Temperature: 130.0
Time: 48
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.025
First_Linker_Concentration: 0.025
Second_Linker_Concentration: 0.05
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Stoichiometry between the linkers and the overall
concentration of the reagents
```

```
# MOF 4
```

Here is the linker:

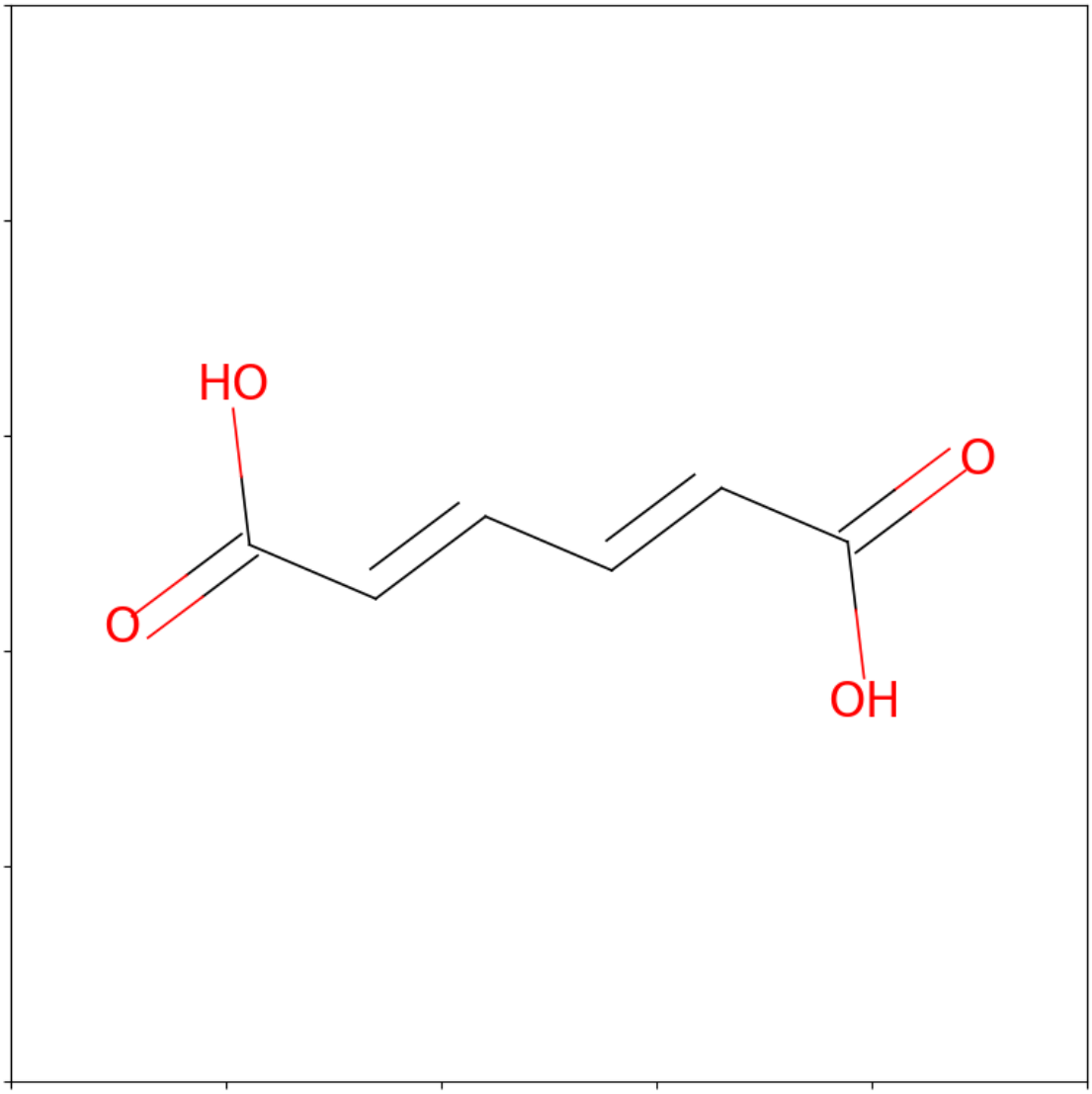
[19]:
```
Image('./QIVZEC_cleansingle_linker0.png')
```

[19]:



[20]:
```
Image('./QIVZEC_cleansingle_linker1.png')
```

[20]:



The metal center of this MOF is ``Zn''. The oxidation state of the metel is ``2''

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[21]:
```
nutils.viewer('./QIVZEC_clean.cif')
```

[22]:
```
temperature_mof_4_Celsius  = 150 #@param {type:'number'}
time_mof_4_hours  =  72#@param {type:'number'}
```

```
first_solvent_mof_4 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_4 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_4 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_4 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_4 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_4_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_first_linker_mof_4_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_4_mol_per_liter  = 0.03 #@param {type:'number'}
are_you_sure_about_your_selction_mof_4 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_4 =  'Stoichiometry between the linkers␣
↪and the overall concentration of the reagents' #@param {type:'string'}
results['mof_4'] = {}
results['mof_4']['temperature']=temperature_mof_4_Celsius
results['mof_4']['time']=time_mof_4_hours
results['mof_4']['solvent1']=first_solvent_mof_4
```

```
results['mof_4']['solvent2']=second_solvent_mof_4
results['mof_4']['solvent3']=third_solvent_mof_4
results['mof_4']['additive']=additive_mof_4
results['mof_4']['counter']=counter_ion_mof_4
results['mof_4']['metal']=concentration_metal_mof_4_mol_per_liter
results['mof_4']['linker1']=concentration_first_linker_mof_4_mol_per_liter
results['mof_4']['linker2']=concentration_second_linker_mof_4_mol_per_liter
results['mof_4']['surely']=are_you_sure_about_your_selction_mof_4
results['mof_4']['additional']=what_makes_you_so_sure_or_unsure_mof_4
```

[23]:
```
nutils.print_choice(temperature_mof_4_Celsius, time_mof_4_hours,␣
↪first_solvent_mof_4,second_solvent_mof_4,third_solvent_mof_4 ,␣
↪counter_ion_mof_4, concentration_metal_mof_4_mol_per_liter,␣
↪concentration_first_linker_mof_4_mol_per_liter,concentration_second_linker_mof_4_mol_per_li
↪, additive_mof_4,are_you_sure_about_your_selction_mof_4,␣
↪what_makes_you_so_sure_or_unsure_mof_4 )
```

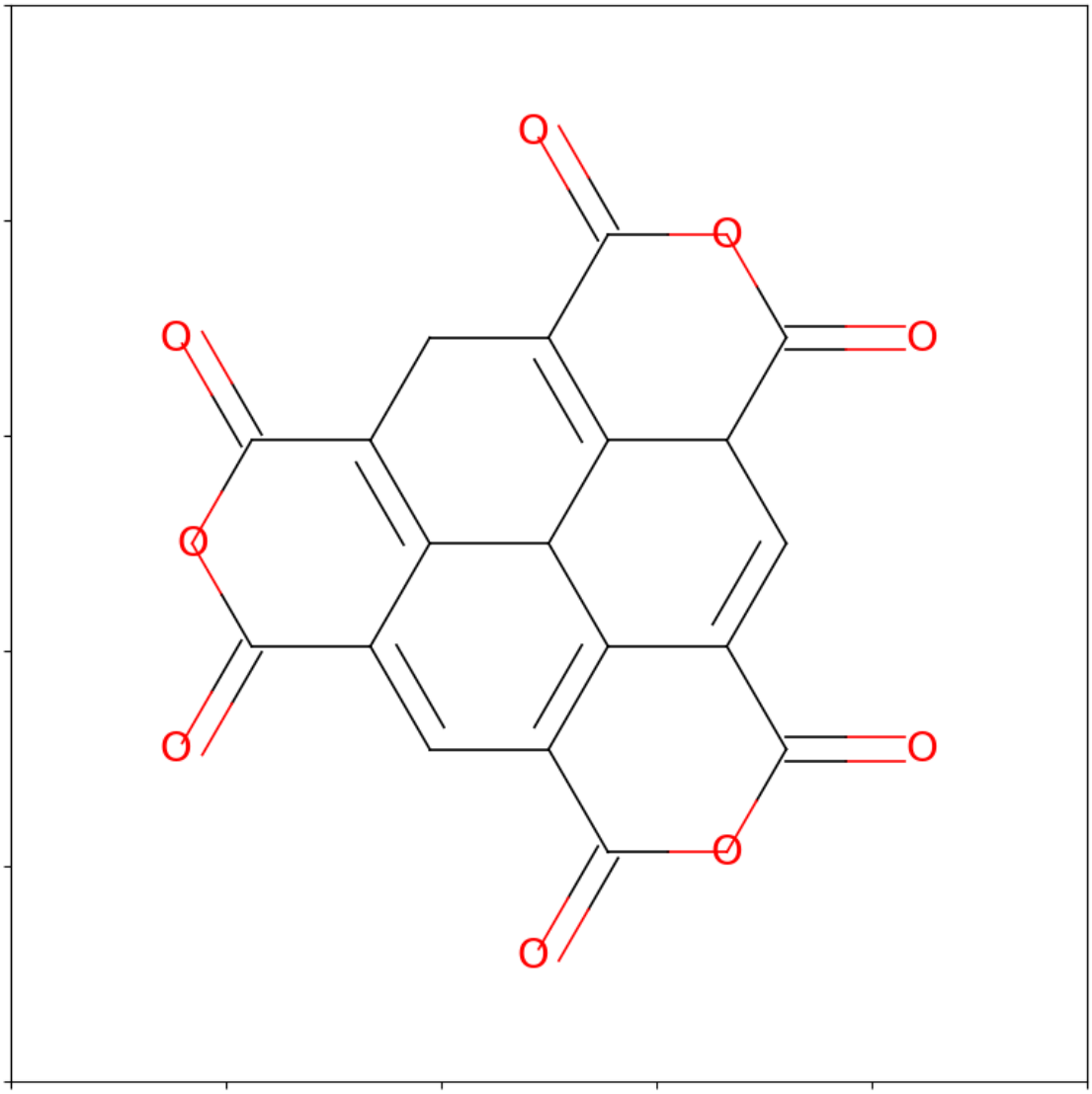
```
Thanks for your input
Your selection was:
Temperature: 150
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.025
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.03
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Stoichiometry between the linkers and the overall
concentration of the reagents
```

```
# MOF 5
```

Here is the linker:

[24]:
```
Image('./LIKGUJ_cleansingle_linker0.png')
```

[24]:



The metal center of this MOF is ``Cu''. The oxidation state of the metel is ``2''

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[25]:
```
nutils.viewer('./LIKGUJ_clean.cif')
```

[26]:
```
temperature_mof_5_Celsius  = 11 #@param {type:'number'}
time_mof_5_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_5 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_5 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_5 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_5 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_5 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_5_mol_per_liter  =  0.050#@param {type:'number'}
concentration_first_linker_mof_5_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_second_linker_mof_5_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_5 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_5 =  'This MOF is far from the ones that␣
↪we are use to synthesise, which are mainly based on carboxyl, imidazole and␣
↪pyridine type linkers. I would say that the crystallization conditions are␣
↪good enough to obtain the material, but with high uncertainities about the␣
↪crystal size obtained at the end of the reaction' #@param {type:'string'}
results['mof_5'] = {}
```

```
results['mof_5']['temperature']=temperature_mof_5_Celsius
results['mof_5']['time']=time_mof_5_hours
results['mof_5']['solvent1']=first_solvent_mof_5
results['mof_5']['solvent2']=second_solvent_mof_5
results['mof_5']['solvent3']=third_solvent_mof_5
results['mof_5']['additive']=additive_mof_5
results['mof_5']['counter']=counter_ion_mof_5
results['mof_5']['metal']=concentration_metal_mof_5_mol_per_liter
results['mof_5']['linker1']=concentration_first_linker_mof_5_mol_per_liter
results['mof_5']['linker2']=concentration_second_linker_mof_5_mol_per_liter
results['mof_5']['surely']=are_you_sure_about_your_selction_mof_5
results['mof_5']['additional']=what_makes_you_so_sure_or_unsure_mof_5
```

[27]:
```
nutils.print_choice(temperature_mof_5_Celsius, time_mof_5_hours,␣
↪first_solvent_mof_5,second_solvent_mof_5,third_solvent_mof_5 ,␣
↪counter_ion_mof_5, concentration_metal_mof_5_mol_per_liter,␣
↪concentration_first_linker_mof_5_mol_per_liter,concentration_second_linker_mof_5_mol_per_li
↪, additive_mof_5,are_you_sure_about_your_selction_mof_5,␣
↪what_makes_you_so_sure_or_unsure_mof_5 )
```

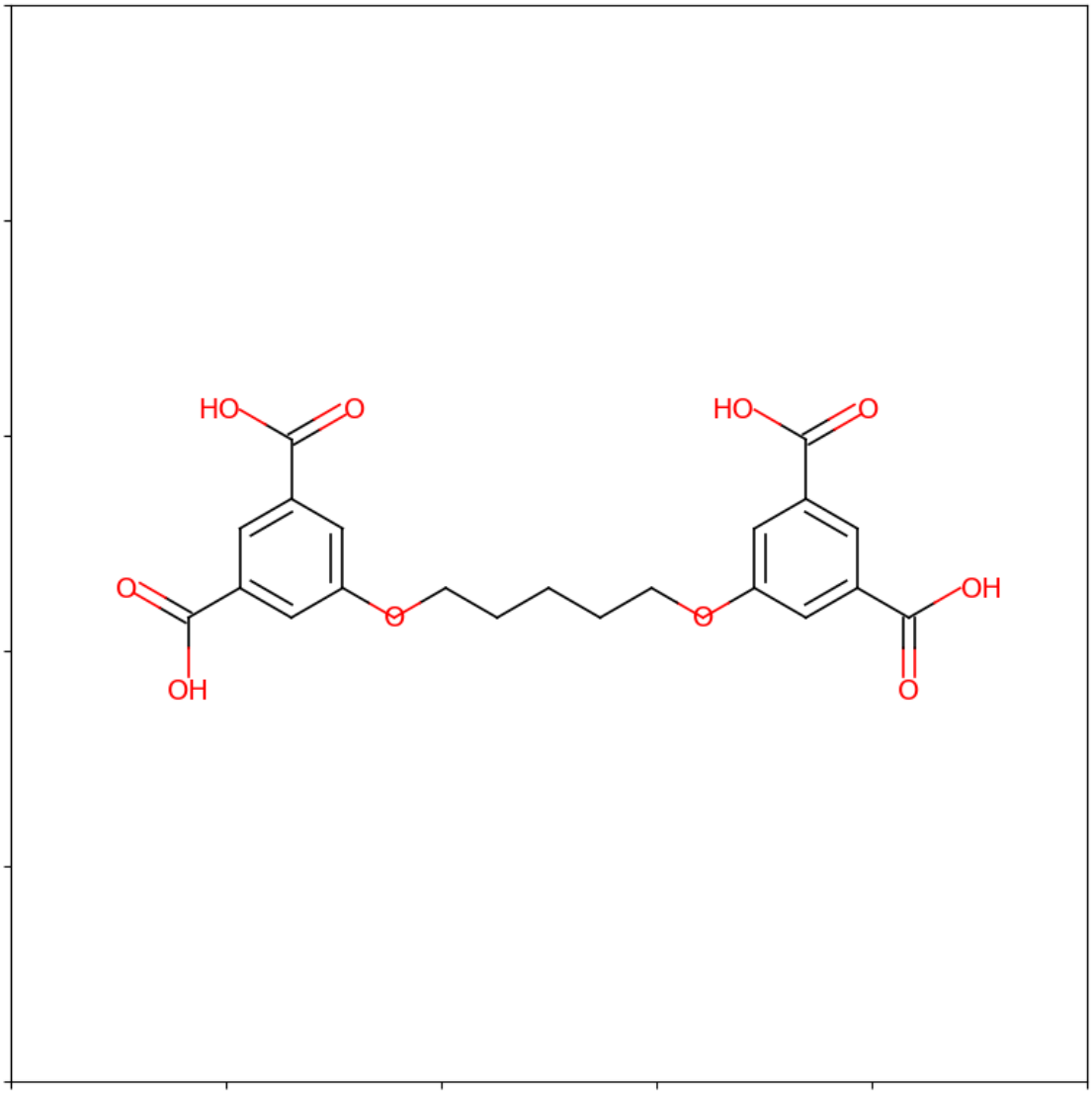
```
Thanks for your input
Your selection was:
Temperature: 11
Time: 72.0
Solvent1: N,N-diethylformamide (DEF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.05
First_Linker_Concentration: 0.025
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: This MOF is far from the ones that we are use to
synthesise, which are mainly based on carboxyl, imidazole and pyridine type
linkers. I would say that the crystallization conditions are good enough to
obtain the material, but with high uncertainities about the crystal size
obtained at the end of the reaction
```

```
# MOF 6
```

Here is the linker:

[28]:
```
Image('./XULDOZ_cleansingle_linker0.png')
```

[28]:



The metal center of this MOF is ``Co''. The oxidation state of the metel is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[29]:
```
nutils.viewer('./XULDOZ_clean.cif')
```

[30]:
```
temperature_mof_6_Celsius  = 135 #@param {type:'number'}
time_mof_6_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_6 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_6 = 'acetonitrile' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_6 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_6 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_6 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_6_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_first_linker_mof_6_mol_per_liter  =  0.045#@param {type:'number'}
concentration_second_linker_mof_6_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_6 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_6 =  ';Mainly the Metal:Linker molar␣
↪stoichiometry' #@param {type:'string'}
results['mof_6'] = {}
results['mof_6']['temperature']=temperature_mof_6_Celsius
results['mof_6']['time']=time_mof_6_hours
results['mof_6']['solvent1']=first_solvent_mof_6
```

```
results['mof_6']['solvent2']=second_solvent_mof_6
results['mof_6']['solvent3']=third_solvent_mof_6
results['mof_6']['additive']=additive_mof_6
results['mof_6']['counter']=counter_ion_mof_6
results['mof_6']['metal']=concentration_metal_mof_6_mol_per_liter
results['mof_6']['linker1']=concentration_first_linker_mof_6_mol_per_liter
results['mof_6']['linker2']=concentration_second_linker_mof_6_mol_per_liter
results['mof_6']['surely']=are_you_sure_about_your_selction_mof_6
results['mof_6']['additional']=what_makes_you_so_sure_or_unsure_mof_6
```

[31]:
```
nutils.print_choice(temperature_mof_6_Celsius, time_mof_6_hours,␣
↪first_solvent_mof_6,second_solvent_mof_6,third_solvent_mof_6 ,␣
↪counter_ion_mof_6, concentration_metal_mof_6_mol_per_liter,␣
↪concentration_first_linker_mof_6_mol_per_liter,concentration_second_linker_mof_6_mol_per_li
↪, additive_mof_6,are_you_sure_about_your_selction_mof_6,␣
↪what_makes_you_so_sure_or_unsure_mof_6 )
```

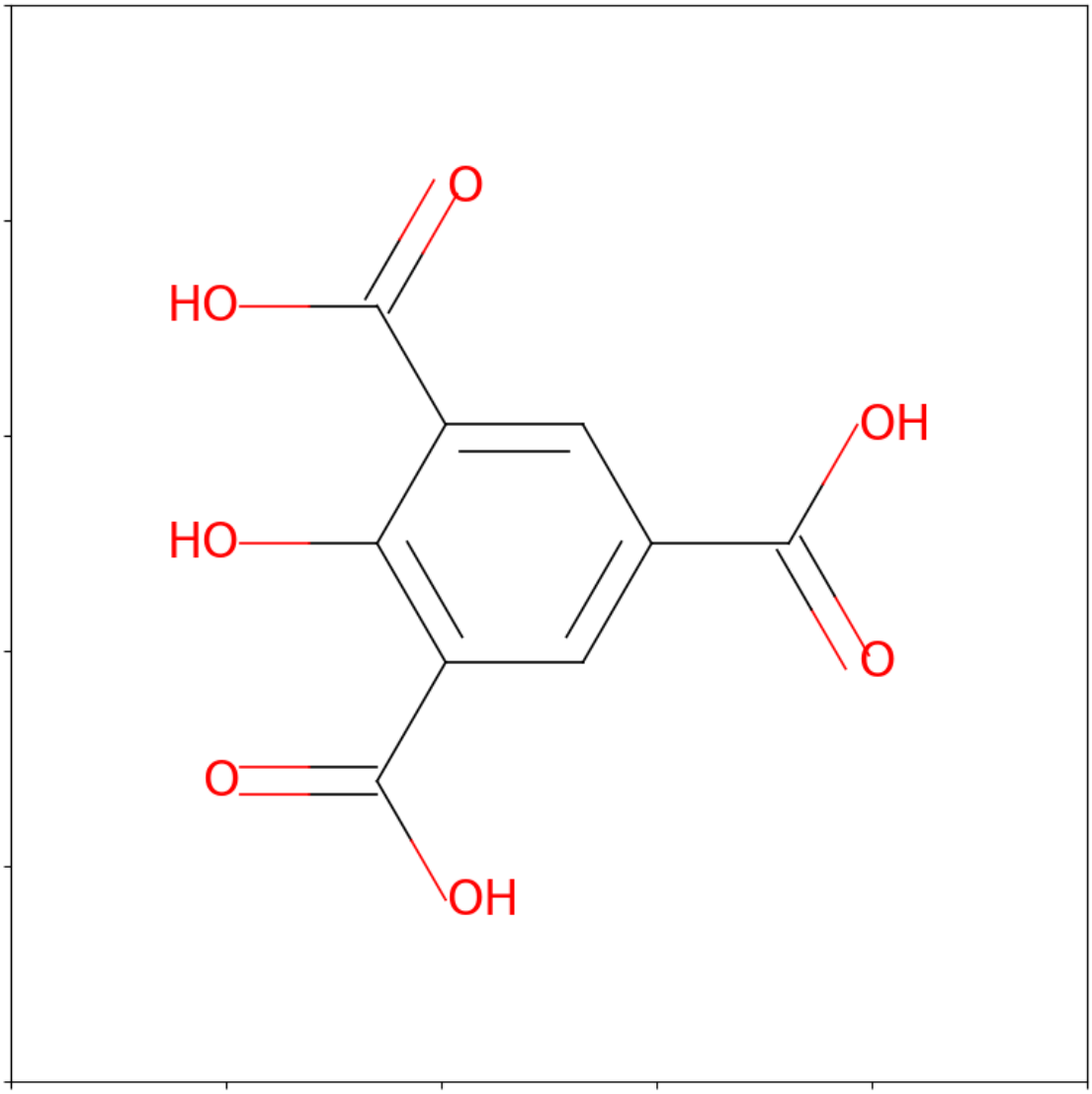
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: acetonitrile
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.025
First_Linker_Concentration: 0.045
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: ;Mainly the Metal:Linker molar stoichiometry
```

```
# MOF 7
```

Here is the linker:

[32]:
```
Image('./HAFSOZ_cleansingle_linker0.png')
```

[32]:



The metal center of this MOF is ``Zn''. The oxidation state of the metel is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[33]:
```
nutils.viewer('./HAFSOZ_clean.cif')
```

[34]:
```
temperature_mof_7_Celsius  = 110 #@param {type:'number'}
time_mof_7_hours  = 48 #@param {type:'number'}
```

```
first_solvent_mof_7 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_7 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_7 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_7 = 'base' #@param ['no additive', 'acid', 'base']
counter_ion_mof_7 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_7_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_first_linker_mof_7_mol_per_liter  = 0.040 #@param {type:'number'}
concentration_second_linker_mof_7_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_7 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_7 =  'Not sure about the overall␣
↪conditions, I have suggested a tentative ones based on the metal, linker and␣
↪structure information' #@param {type:'string'}
results['mof_7'] = {}
results['mof_7']['temperature']=temperature_mof_7_Celsius
results['mof_7']['time']=time_mof_7_hours
```

```
results['mof_7']['solvent1']=first_solvent_mof_7
results['mof_7']['solvent2']=second_solvent_mof_7
results['mof_7']['solvent3']=third_solvent_mof_7
results['mof_7']['additive']=additive_mof_7
results['mof_7']['counter']=counter_ion_mof_7
results['mof_7']['metal']=concentration_metal_mof_7_mol_per_liter
results['mof_7']['linker1']=concentration_first_linker_mof_7_mol_per_liter
results['mof_7']['linker2']=concentration_second_linker_mof_7_mol_per_liter
results['mof_7']['surely']=are_you_sure_about_your_selction_mof_7
results['mof_7']['additional']=what_makes_you_so_sure_or_unsure_mof_7
```

[35]:
```
nutils.print_choice(temperature_mof_7_Celsius, time_mof_7_hours,␣
↪first_solvent_mof_7,second_solvent_mof_7,third_solvent_mof_7 ,␣
↪counter_ion_mof_7, concentration_metal_mof_7_mol_per_liter,␣
↪concentration_first_linker_mof_7_mol_per_liter,concentration_second_linker_mof_7_mol_per_li
↪, additive_mof_7,are_you_sure_about_your_selction_mof_7,␣
↪what_makes_you_so_sure_or_unsure_mof_7 )
```

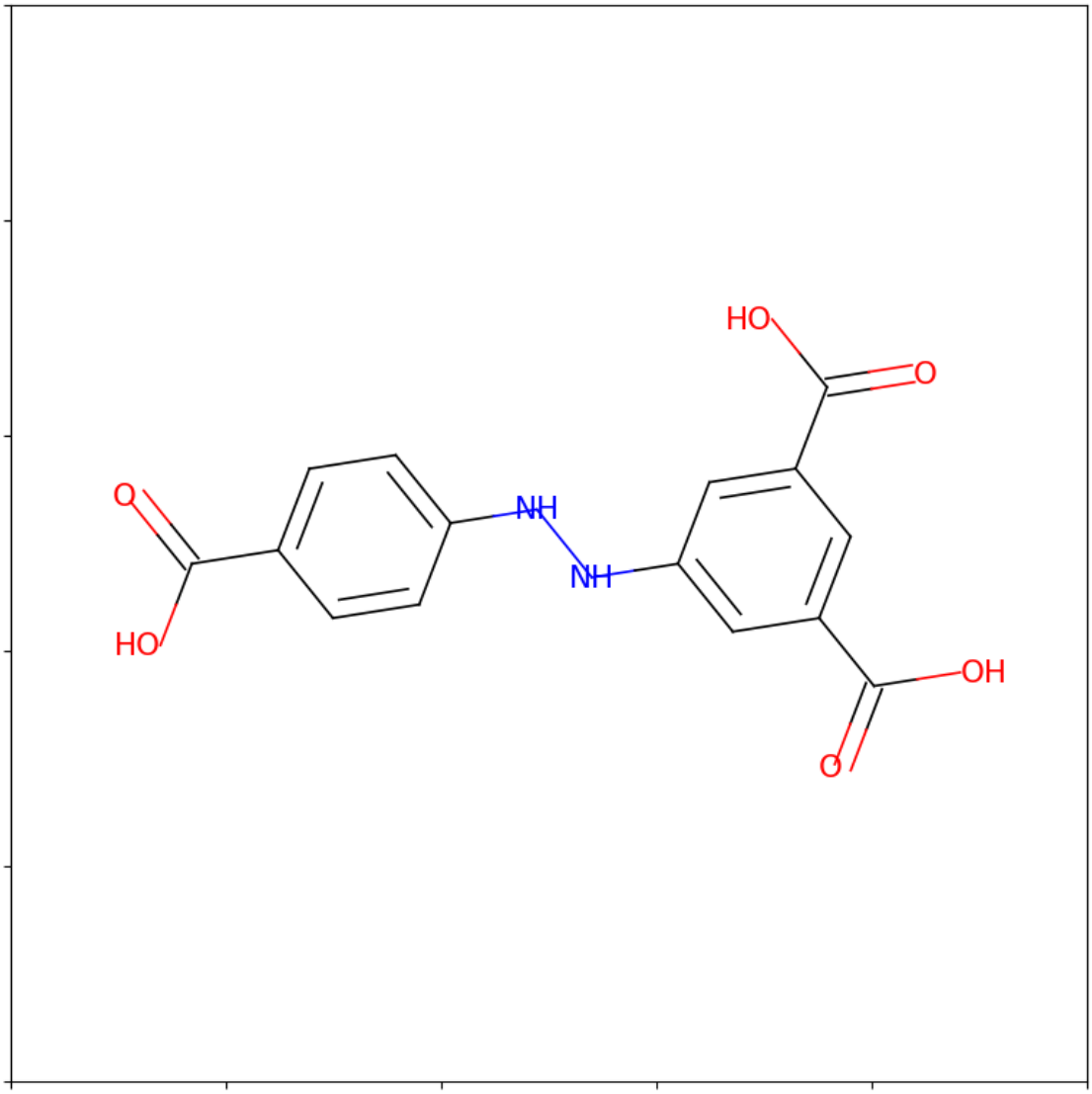
```
Thanks for your input
Your selection was:
Temperature: 110
Time: 48
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.025
First_Linker_Concentration: 0.04
Second_Linker_Concentration: 0.0
Additive: base
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the overall conditions, I have
suggested a tentative ones based on the metal, linker and structure information
```

```
# MOF 8
```

Here is the linker:

[36]:
```
Image('./INOVEN_cleansingle_linker0.png')
```

[36]:



The metal center of this MOF is ``Gd''. The oxidation state of the metel is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[37]:
```
nutils.viewer('./INOVEN_clean.cif')
```

[38]:
```
temperature_mof_8_Celsius  = 150 #@param {type:'number'}
time_mof_8_hours  = 48 #@param {type:'number'}
```

```
first_solvent_mof_8 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
 ↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
 ↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
 ↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
 ↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
 ↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
 ↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_8 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
third_solvent_mof_8 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
additive_mof_8 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_8 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
 ↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
 ↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
 ↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
 ↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
 ↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_8_mol_per_liter  = 0.020 #@param {type:'number'}
concentration_first_linker_mof_8_mol_per_liter  = 0.045 #@param {type:'number'}
concentration_second_linker_mof_8_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_8 = 'yes' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_8 =  'Relatively sure about the␣
 ↪crystallization of the MOF, not so sure if the overall concentration and␣
 ↪metal/linker ratios are the best ones to obtain single crystals' #@param␣
 ↪{type:'string'}
results['mof_8'] = {}
results['mof_8']['temperature']=temperature_mof_8_Celsius
```

```
results['mof_8']['time']=time_mof_8_hours
results['mof_8']['solvent1']=first_solvent_mof_8
results['mof_8']['solvent2']=second_solvent_mof_8
results['mof_8']['solvent3']=third_solvent_mof_8
results['mof_8']['additive']=additive_mof_8
results['mof_8']['counter']=counter_ion_mof_8
results['mof_8']['metal']=concentration_metal_mof_8_mol_per_liter
results['mof_8']['linker1']=concentration_first_linker_mof_8_mol_per_liter
results['mof_8']['linker2']=concentration_second_linker_mof_8_mol_per_liter
results['mof_8']['surely']=are_you_sure_about_your_selction_mof_8
results['mof_8']['additional']=what_makes_you_so_sure_or_unsure_mof_8
```

[39]:
```
nutils.print_choice(temperature_mof_8_Celsius, time_mof_8_hours,␣
↪first_solvent_mof_8,second_solvent_mof_8,third_solvent_mof_8 ,␣
↪counter_ion_mof_8, concentration_metal_mof_8_mol_per_liter,␣
↪concentration_first_linker_mof_8_mol_per_liter,concentration_second_linker_mof_8_mol_per_li
↪, additive_mof_8,are_you_sure_about_your_selction_mof_8,␣
↪what_makes_you_so_sure_or_unsure_mof_8 )
```

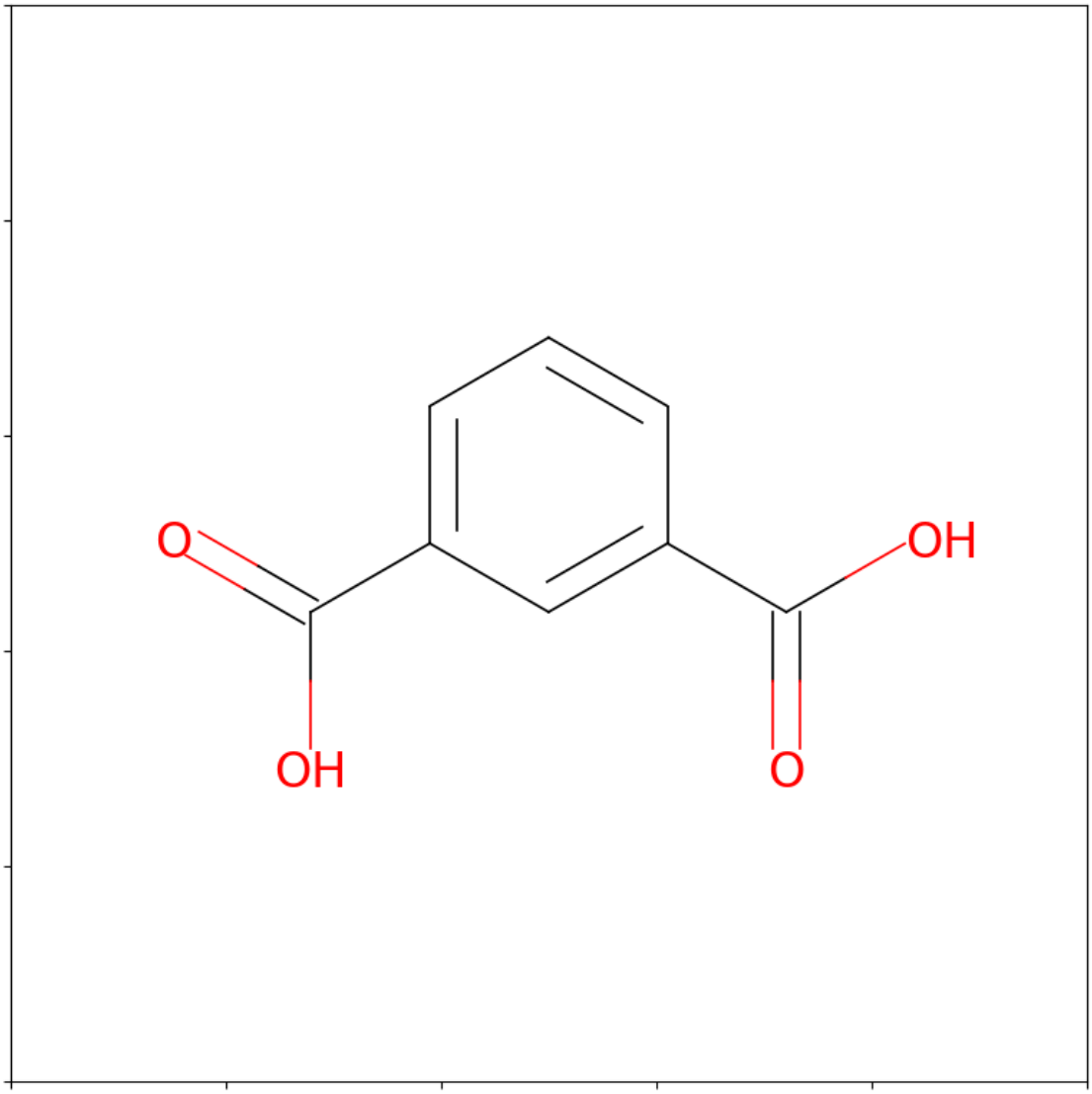
```
Thanks for your input
Your selection was:
Temperature: 150
Time: 48
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.02
First_Linker_Concentration: 0.045
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: yes
What_Makes_You_So_Sure/Unsure: Relatively sure about the crystallization of the
MOF, not so sure if the overall concentration and metal/linker ratios are the
best ones to obtain single crystals
```

```
# MOF 9
```

Here is the linker:

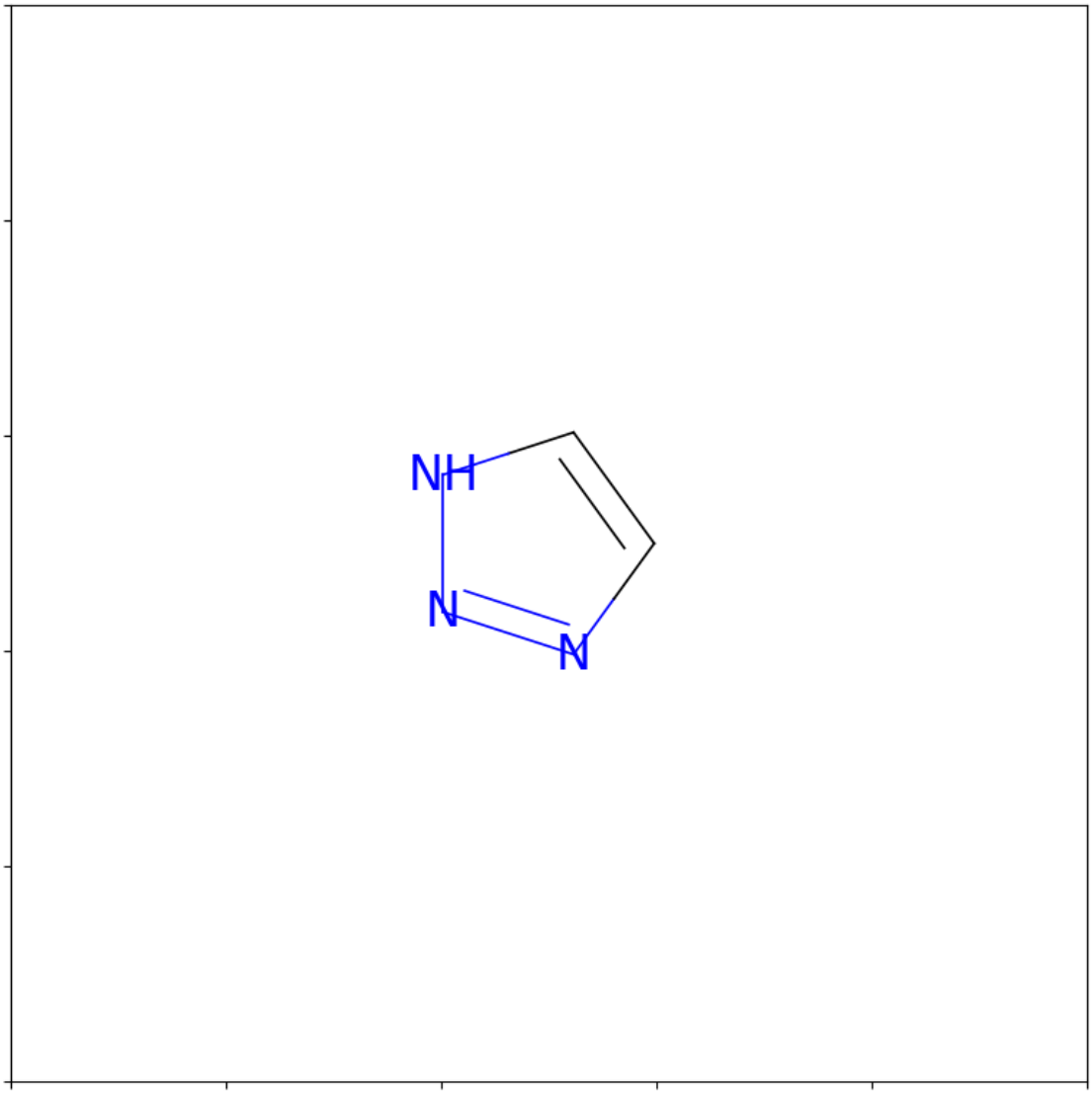
[40]:
```
Image('./COVYIX_cleansingle_linker0.png')
```

[40]:



[41]:
```
Image('./COVYIX_cleansingle_linker1.png')
```

[41]:



The metal center of this MOF is Cu``.The oxidation state of the metel is''2".

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[42]:
```
nutils.viewer('./COVYIX_clean.cif')
```

[43]:
```
temperature_mof_9_Celsius  = 135 #@param {type:'number'}
time_mof_9_hours  = 48 #@param {type:'number'}
```

```
first_solvent_mof_9 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_9 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_9 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_9 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_9 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_9_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_first_linker_mof_9_mol_per_liter  =  0.05#@param {type:'number'}
concentration_second_linker_mof_9_mol_per_liter  = 0.15 #@param {type:'number'}
are_you_sure_about_your_selction_mof_9 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_9 =  'Not sure about the overall␣
↪conditions' #@param {type:'string'}
results['mof_9'] = {}
results['mof_9']['temperature']=temperature_mof_9_Celsius
results['mof_9']['time']=time_mof_9_hours
results['mof_9']['solvent1']=first_solvent_mof_9
```

```
results['mof_9']['solvent2']=second_solvent_mof_9
results['mof_9']['solvent3']=third_solvent_mof_9
results['mof_9']['additive']=additive_mof_9
results['mof_9']['counter']=counter_ion_mof_9
results['mof_9']['metal']=concentration_metal_mof_9_mol_per_liter
results['mof_9']['linker1']=concentration_first_linker_mof_9_mol_per_liter
results['mof_9']['linker2']=concentration_second_linker_mof_9_mol_per_liter
results['mof_9']['surely']=are_you_sure_about_your_selction_mof_9
results['mof_9']['additional']=what_makes_you_so_sure_or_unsure_mof_9
```

[44]:
```
nutils.print_choice(temperature_mof_9_Celsius, time_mof_9_hours,␣
↪first_solvent_mof_9,second_solvent_mof_9,third_solvent_mof_9 ,␣
↪counter_ion_mof_9, concentration_metal_mof_9_mol_per_liter,␣
↪concentration_first_linker_mof_9_mol_per_liter,concentration_second_linker_mof_9_mol_per_li
↪, additive_mof_9,are_you_sure_about_your_selction_mof_9,␣
↪what_makes_you_so_sure_or_unsure_mof_9 )
```

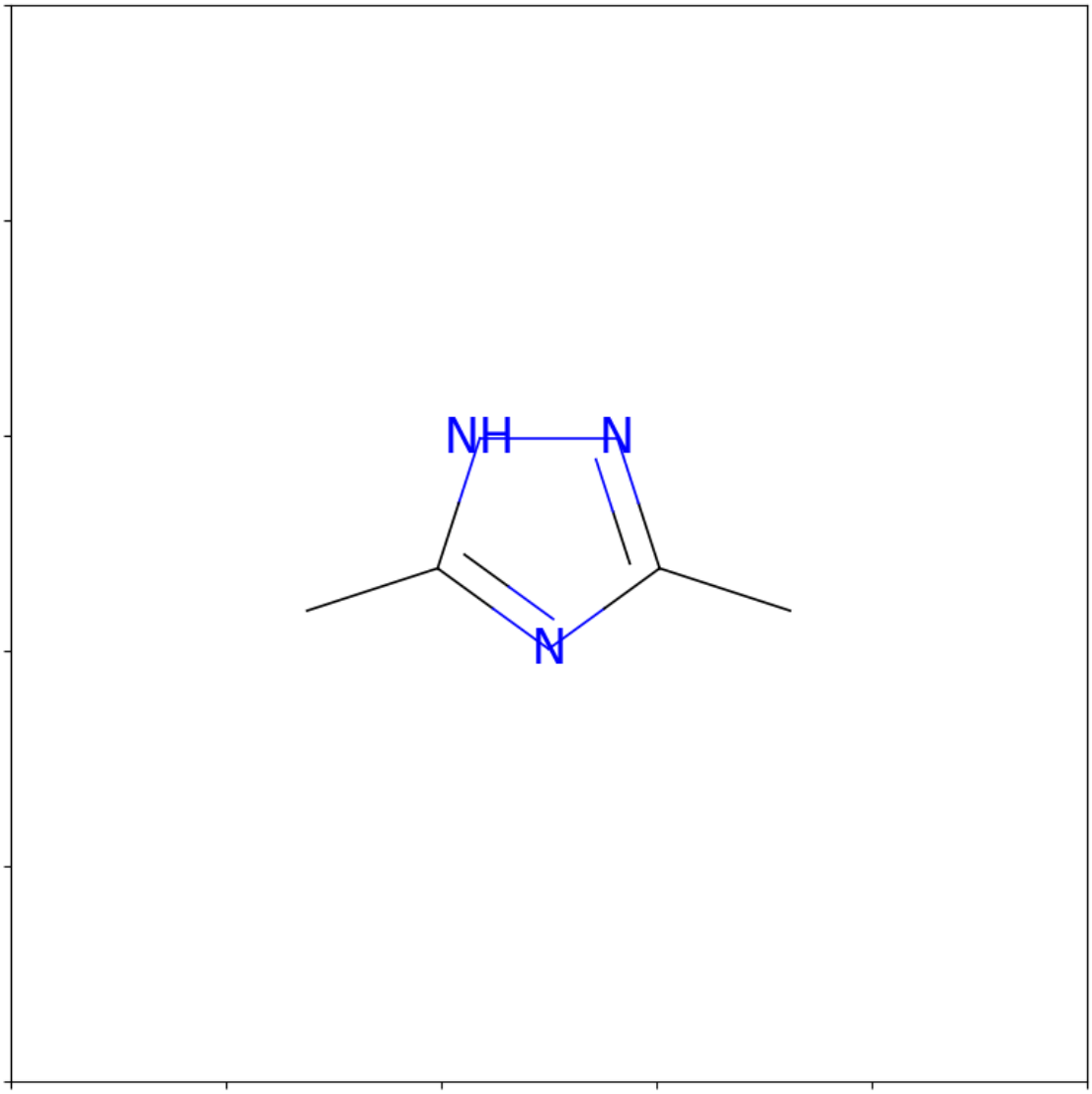
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 48
Solvent1: ethanol
Solvent2: N,N-diethylformamide (DEF)
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.025
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.15
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the overall conditions
```

```
# MOF 10
```

Here is the linker:

[45]:
```
Image('./RUFZID_cleansingle_linker0.png')
```

[45]:



The metal center of this MOF is ``Cu''. The oxidation state of the metel is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[46]:
```
nutils.viewer('./RUFZID_clean.cif')
```

[47]:
```
temperature_mof_10_Celsius  = 135 #@param {type:'number'}
time_mof_10_hours  = 48 #@param {type:'number'}
```

```
first_solvent_mof_10 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
 ↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
 ↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
 ↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
 ↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
 ↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
 ↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_10 = 'ethanol' #@param ["None", "1-butanol",␣
 ↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
 ↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
 ↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
 ↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
 ↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
 ↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_10 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
additive_mof_10 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_10 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
 ↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
 ↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
 ↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
 ↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
 ↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_10_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_10_mol_per_liter  = 0.35 #@param {type:'number'}
concentration_second_linker_mof_10_mol_per_liter  = 0.05 #@param {type:'number'}
are_you_sure_about_your_selction_mof_10 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_10 =  'A linker is missing, therephtalic␣
 ↪acid' #@param {type:'string'}
results['mof_10'] = {}
results['mof_10']['temperature']=temperature_mof_10_Celsius
results['mof_10']['time']=time_mof_10_hours
results['mof_10']['solvent1']=first_solvent_mof_10
```

```
results['mof_10']['solvent2']=second_solvent_mof_10
results['mof_10']['solvent3']=third_solvent_mof_10
results['mof_10']['additive']=additive_mof_10
results['mof_10']['counter']=counter_ion_mof_10
results['mof_10']['metal']=concentration_metal_mof_10_mol_per_liter
results['mof_10']['linker1']=concentration_first_linker_mof_10_mol_per_liter
results['mof_10']['linker2']=concentration_second_linker_mof_10_mol_per_liter
results['mof_10']['surely']=are_you_sure_about_your_selction_mof_10
results['mof_10']['additional']=what_makes_you_so_sure_or_unsure_mof_10
```

[48]:
```
nutils.print_choice(temperature_mof_10_Celsius, time_mof_10_hours,␣
↪first_solvent_mof_10,second_solvent_mof_10,third_solvent_mof_10 ,␣
↪counter_ion_mof_10, concentration_metal_mof_10_mol_per_liter,␣
↪concentration_first_linker_mof_10_mol_per_liter,concentration_second_linker_mof_10_mol_per_
↪, additive_mof_10,are_you_sure_about_your_selction_mof_10,␣
↪what_makes_you_so_sure_or_unsure_mof_10 )
```

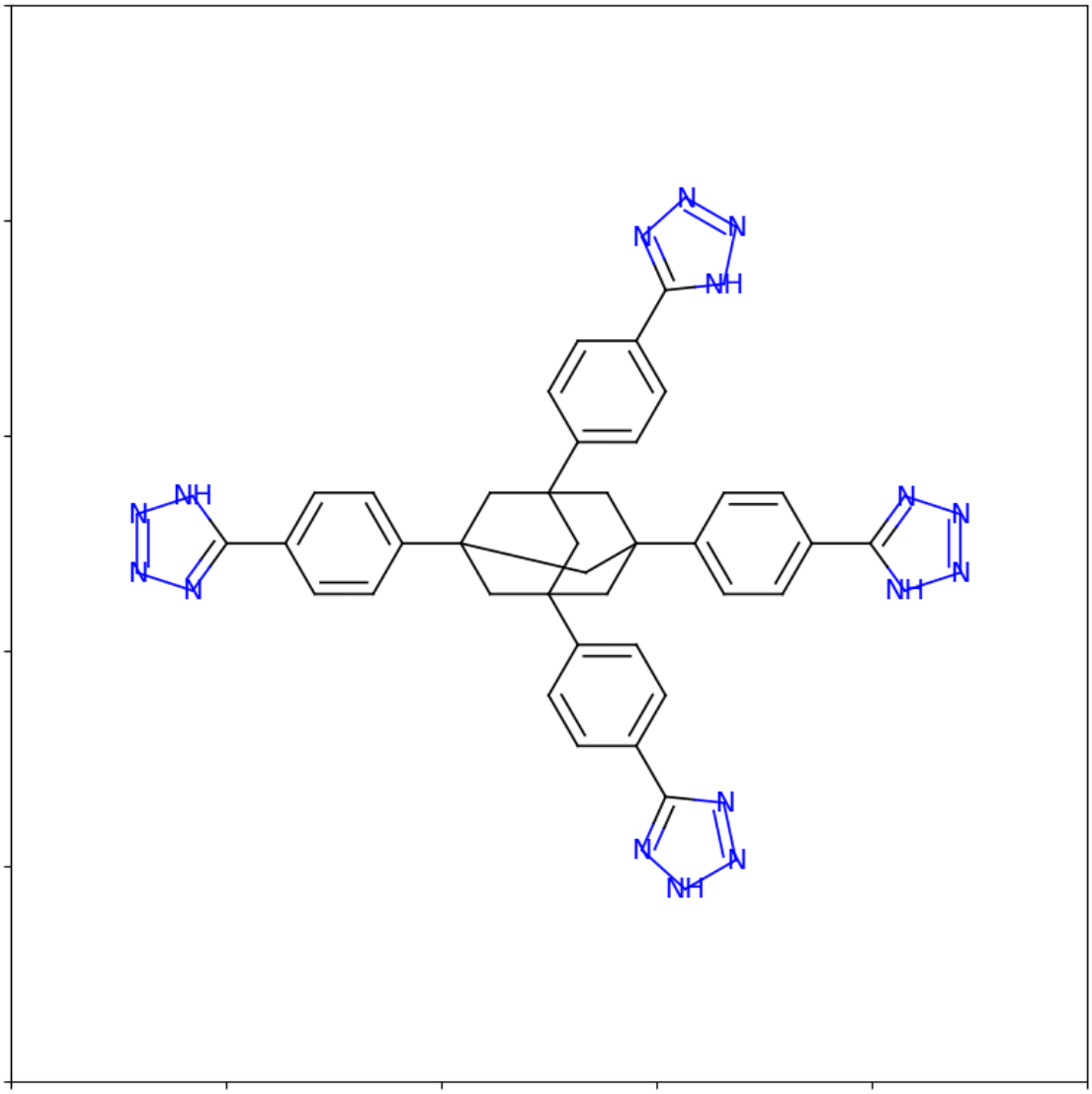
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 48
Solvent1: N,N-diethylformamide (DEF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.35
Second_Linker_Concentration: 0.05
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: A linker is missing, therephtalic acid
```

```
# MOF 11
```

Here is the linker:

[49]:
```
Image('./LELROL_cleansingle_linker0.png')
```

[49]:



The metal center of this MOF is ``Mn''. The oxidation state of the metel is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[50]:
```
nutils.viewer('./LELROL_clean.cif')
```

[51]:
```
temperature_mof_11_Celsius  = 135 #@param {type:'number'}
time_mof_11_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_11 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_11 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_11 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_11 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_11 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_11_mol_per_liter  =  0.025#@param {type:'number'}
concentration_first_linker_mof_11_mol_per_liter  =  0.05#@param {type:'number'}
concentration_second_linker_mof_11_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_11 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_11 =  'Not used to working with triazolate␣
↪like linkers' #@param {type:'string'}
results['mof_11'] = {}
results['mof_11']['temperature']=temperature_mof_11_Celsius
results['mof_11']['time']=time_mof_11_hours
results['mof_11']['solvent1']=first_solvent_mof_11
```

```
results['mof_11']['solvent2']=second_solvent_mof_11
results['mof_11']['solvent3']=third_solvent_mof_11
results['mof_11']['additive']=additive_mof_11
results['mof_11']['counter']=counter_ion_mof_11
results['mof_11']['metal']=concentration_metal_mof_11_mol_per_liter
results['mof_11']['linker1']=concentration_first_linker_mof_11_mol_per_liter
results['mof_11']['linker2']=concentration_second_linker_mof_11_mol_per_liter
results['mof_11']['surely']=are_you_sure_about_your_selction_mof_11
results['mof_11']['additional']=what_makes_you_so_sure_or_unsure_mof_11
```

[52]:
```
nutils.print_choice(temperature_mof_11_Celsius, time_mof_11_hours,␣
↪first_solvent_mof_11,second_solvent_mof_11,third_solvent_mof_11 ,␣
↪counter_ion_mof_11, concentration_metal_mof_11_mol_per_liter,␣
↪concentration_first_linker_mof_11_mol_per_liter,concentration_second_linker_mof_11_mol_per_
↪, additive_mof_11,are_you_sure_about_your_selction_mof_11,␣
↪what_makes_you_so_sure_or_unsure_mof_11 )
```

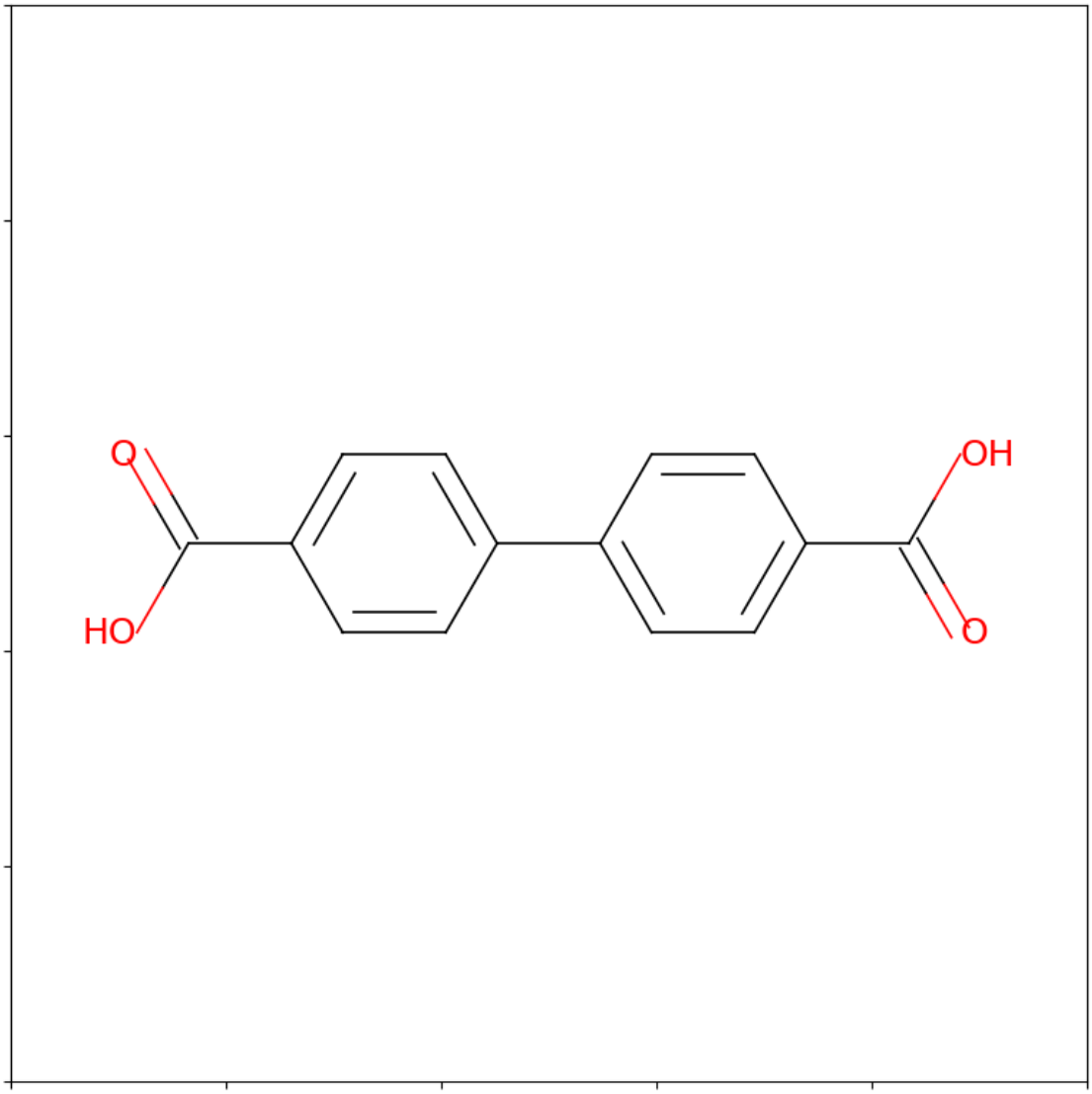
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.025
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to working with triazolate like linkers
```

```
# MOF 12
```

Here is the linker:

[53]:
```
Image('./GAJVIY_chargedsingle_linker0.png')
```

[53]:



The metal center of this MOF is ``Zn''. The oxidation state of the metel is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[54]:
```
nutils.viewer('./GAJVIY_charged.cif')
```

[55]:
```
temperature_mof_12_Celsius  = 135 #@param {type:'number'}
time_mof_12_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_12 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_12 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_12 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_12 = 'base' #@param ['no additive', 'acid', 'base']
counter_ion_mof_12 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_12_mol_per_liter  =  0.05 #@param {type:'number'}
concentration_first_linker_mof_12_mol_per_liter  =  0.075#@param {type:'number'}
concentration_second_linker_mof_12_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_12 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_12 =  'sure about the crystallization, not␣
↪sure about the quality of the single crystals' #@param {type:'string'}
results['mof_12'] = {}
results['mof_12']['temperature']=temperature_mof_12_Celsius
results['mof_12']['time']=time_mof_12_hours
results['mof_12']['solvent1']=first_solvent_mof_12
```

```
results['mof_12']['solvent2']=second_solvent_mof_12
results['mof_12']['solvent3']=third_solvent_mof_12
results['mof_12']['additive']=additive_mof_12
results['mof_12']['counter']=counter_ion_mof_12
results['mof_12']['metal']=concentration_metal_mof_12_mol_per_liter
results['mof_12']['linker1']=concentration_first_linker_mof_12_mol_per_liter
results['mof_12']['linker2']=concentration_second_linker_mof_12_mol_per_liter
#results['mof_12']['linker']=concentration_linker_mof_12_mol_per_liter
results['mof_12']['surely']=are_you_sure_about_your_selction_mof_12
results['mof_12']['additional']=what_makes_you_so_sure_or_unsure_mof_12
```

[56]:
```
nutils.print_choice(temperature_mof_12_Celsius, time_mof_12_hours,␣
↪first_solvent_mof_12,second_solvent_mof_12,third_solvent_mof_12 ,␣
↪counter_ion_mof_12, concentration_metal_mof_12_mol_per_liter,␣
↪concentration_first_linker_mof_12_mol_per_liter,concentration_second_linker_mof_12_mol_per_
↪, additive_mof_12,are_you_sure_about_your_selction_mof_12,␣
↪what_makes_you_so_sure_or_unsure_mof_12 )
```

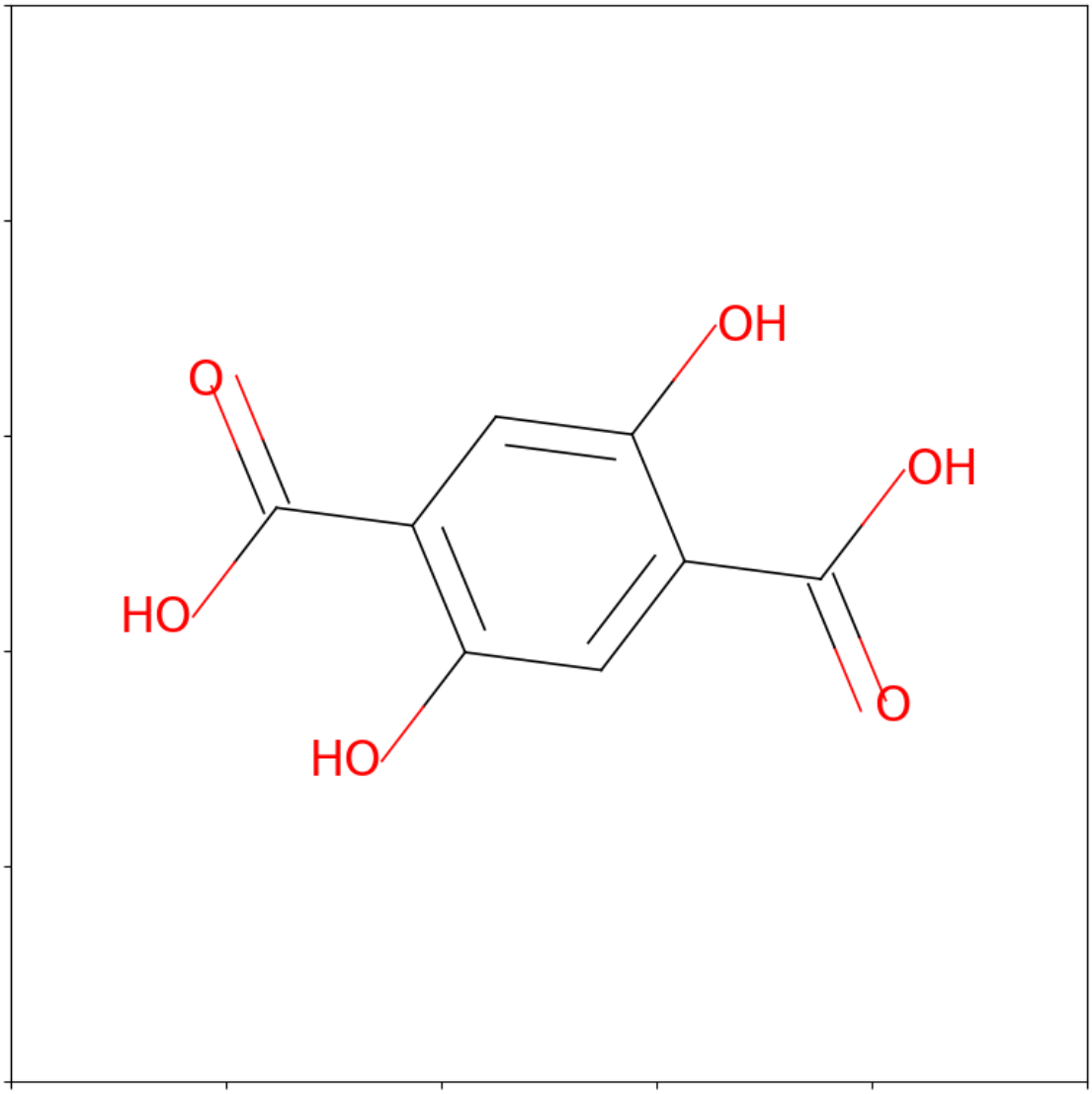
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.0
Additive: base
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: sure about the crystallization, not sure about
the quality of the single crystals
```

```
# MOF 13
```

Here is the linker:

[57]:
```
Image('./LENKIA_cleansingle_linker0.png')
```

[57]:



The metal center of this MOF is ``Cu''. The oxidation state of the metel is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[58]:
```
nutils.viewer('./LENKIA_clean.cif')
```

[59]:
```
temperature_mof_13_Celsius  = 135 #@param {type:'number'}
time_mof_13_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_13 = 'tetrahydrofuran (THF)' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_13 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_13 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_13 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_13 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_13_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_13_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_13_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_13 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_13 =  'Pretty sure about the␣
↪crystallization, but not about the quality of the crystals' #@param {type:
↪'string'}
results['mof_13'] = {}
results['mof_13']['temperature']=temperature_mof_13_Celsius
results['mof_13']['time']=time_mof_13_hours
```

```
results['mof_13']['solvent1']=first_solvent_mof_13
results['mof_13']['solvent2']=second_solvent_mof_13
results['mof_13']['solvent3']=third_solvent_mof_13
results['mof_13']['additive']=additive_mof_13
results['mof_13']['counter']=counter_ion_mof_13
results['mof_13']['metal']=concentration_metal_mof_13_mol_per_liter
results['mof_13']['linker1']=concentration_first_linker_mof_13_mol_per_liter
results['mof_13']['linker2']=concentration_second_linker_mof_13_mol_per_liter
results['mof_13']['surely']=are_you_sure_about_your_selction_mof_13
results['mof_13']['additional']=what_makes_you_so_sure_or_unsure_mof_13
```

[60]:
```
nutils.print_choice(temperature_mof_13_Celsius, time_mof_13_hours,␣
↪first_solvent_mof_13,second_solvent_mof_13,third_solvent_mof_13 ,␣
↪counter_ion_mof_13, concentration_metal_mof_13_mol_per_liter,␣
↪concentration_first_linker_mof_13_mol_per_liter,concentration_second_linker_mof_13_mol_per_
↪, additive_mof_13,are_you_sure_about_your_selction_mof_13,␣
↪what_makes_you_so_sure_or_unsure_mof_13 )
```

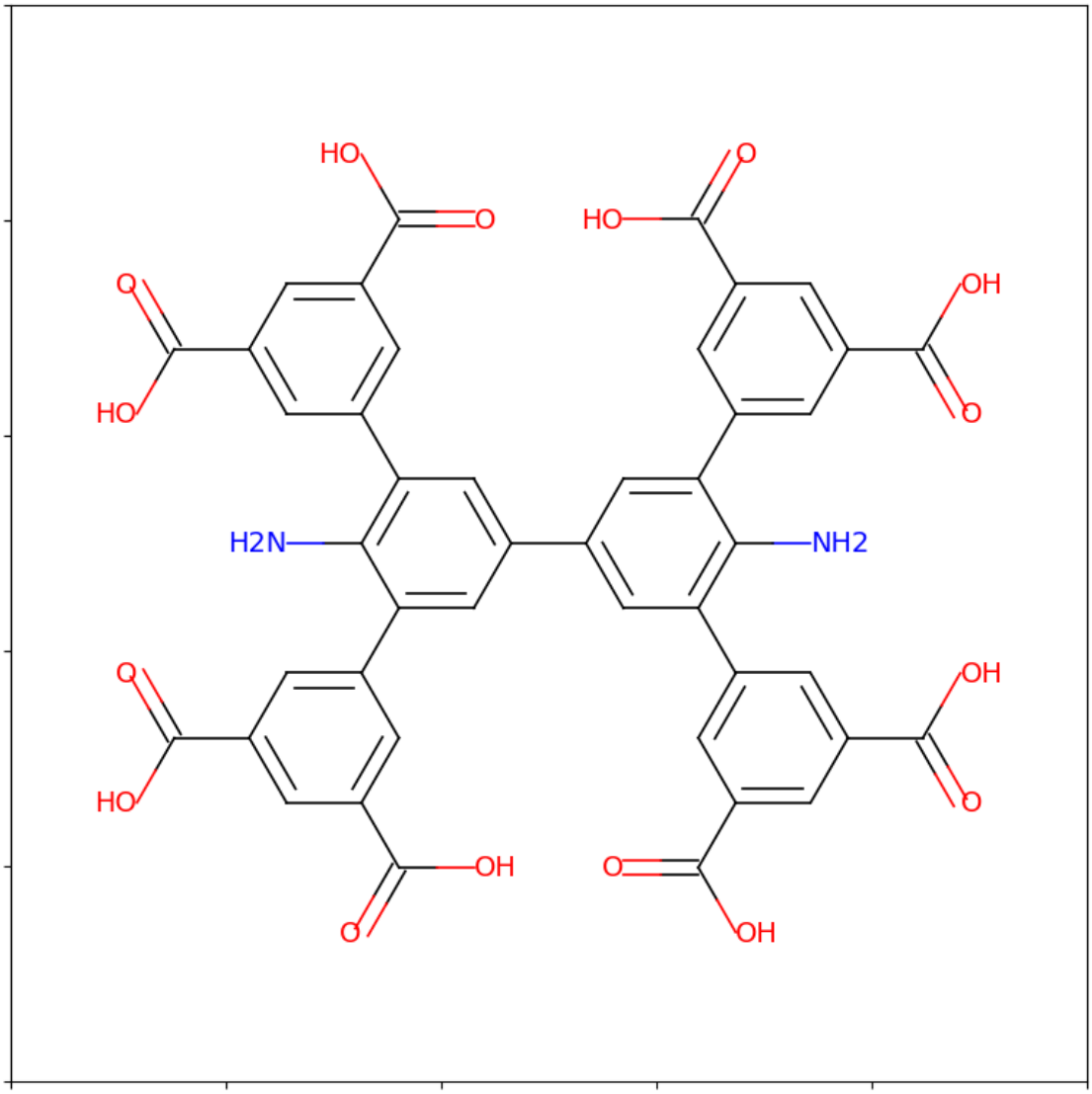
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: tetrahydrofuran (THF)
Solvent2: N,N-diethylformamide (DEF)
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.075
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Pretty sure about the crystallization, but not
about the quality of the crystals
```

```
# MOF 14
```

Here is the linker:

[61]:
```
Image('./AVEQID_cleansingle_linker0.png')
```

[61]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[62]:
```
nutils.viewer('./AVEQID_clean.cif')
```

[63]:
```
temperature_mof_14_Celsius  = 120.0 #@param {type:'number'}
time_mof_14_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_14 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
 ↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
 ↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
 ↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
 ↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
 ↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
 ↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_14 = 'ethanol' #@param ["None", "1-butanol",␣
 ↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
 ↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
 ↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
 ↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
 ↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
 ↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_14 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
additive_mof_14 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_14 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
 ↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
 ↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
 ↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
 ↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
 ↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_14_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_14_mol_per_liter  = 0.045 #@param {type:'number'}
concentration_second_linker_mof_14_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_14 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_14 =  'Not used to work with such a big␣
 ↪linkers, but if the crystallization works similarly than in cu-carboxylate␣
 ↪based MOFs the synthesis conditions could work for its crystallization'␣
 ↪#@param {type:'string'}
results['mof_14'] = {}
results['mof_14']['temperature']=temperature_mof_14_Celsius
```

```
results['mof_14']['time']=time_mof_14_hours
results['mof_14']['solvent1']=first_solvent_mof_14
results['mof_14']['solvent2']=second_solvent_mof_14
results['mof_14']['solvent3']=third_solvent_mof_14
results['mof_14']['additive']=additive_mof_14
results['mof_14']['counter']=counter_ion_mof_14
results['mof_14']['metal']=concentration_metal_mof_14_mol_per_liter
results['mof_14']['linker1']=concentration_first_linker_mof_14_mol_per_liter
results['mof_14']['linker2']=concentration_second_linker_mof_14_mol_per_liter
results['mof_14']['surely']=are_you_sure_about_your_selction_mof_14
results['mof_14']['additional']=what_makes_you_so_sure_or_unsure_mof_14
```

[64]:
```
nutils.print_choice(temperature_mof_14_Celsius, time_mof_14_hours,␣
↪first_solvent_mof_14,second_solvent_mof_14,third_solvent_mof_14 ,␣
↪counter_ion_mof_14, concentration_metal_mof_14_mol_per_liter,␣
↪concentration_first_linker_mof_14_mol_per_liter,concentration_second_linker_mof_14_mol_per_
↪, additive_mof_14,are_you_sure_about_your_selction_mof_14,␣
↪what_makes_you_so_sure_or_unsure_mof_14 )
```

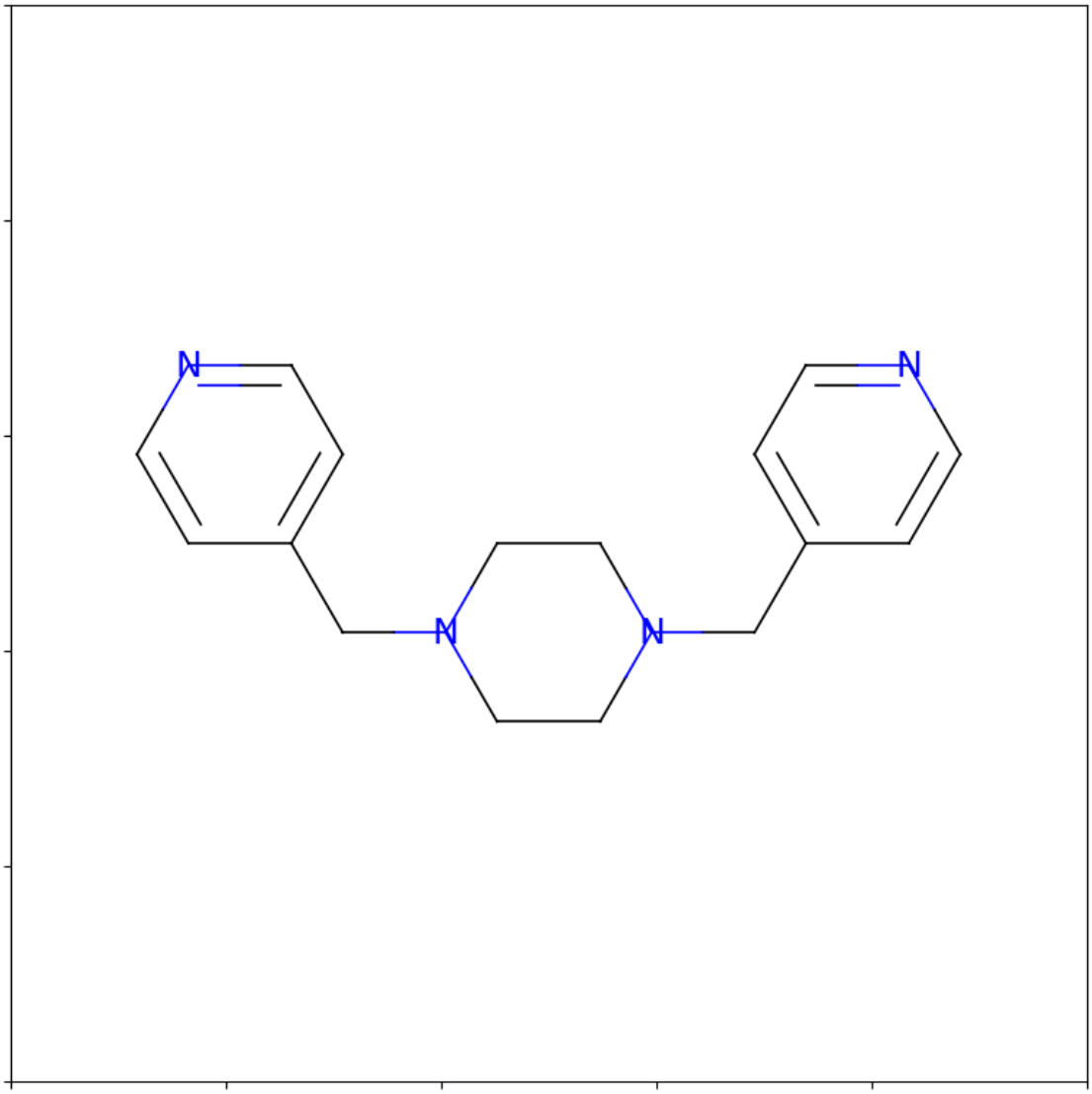
```
Thanks for your input
Your selection was:
Temperature: 120.0
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.075
First_Linker_Concentration: 0.045
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with such a big linkers, but if
the crystallization works similarly than in cu-carboxylate based MOFs the
synthesis conditions could work for its crystallization
```

```
# MOF 15
```

Here is the linker:

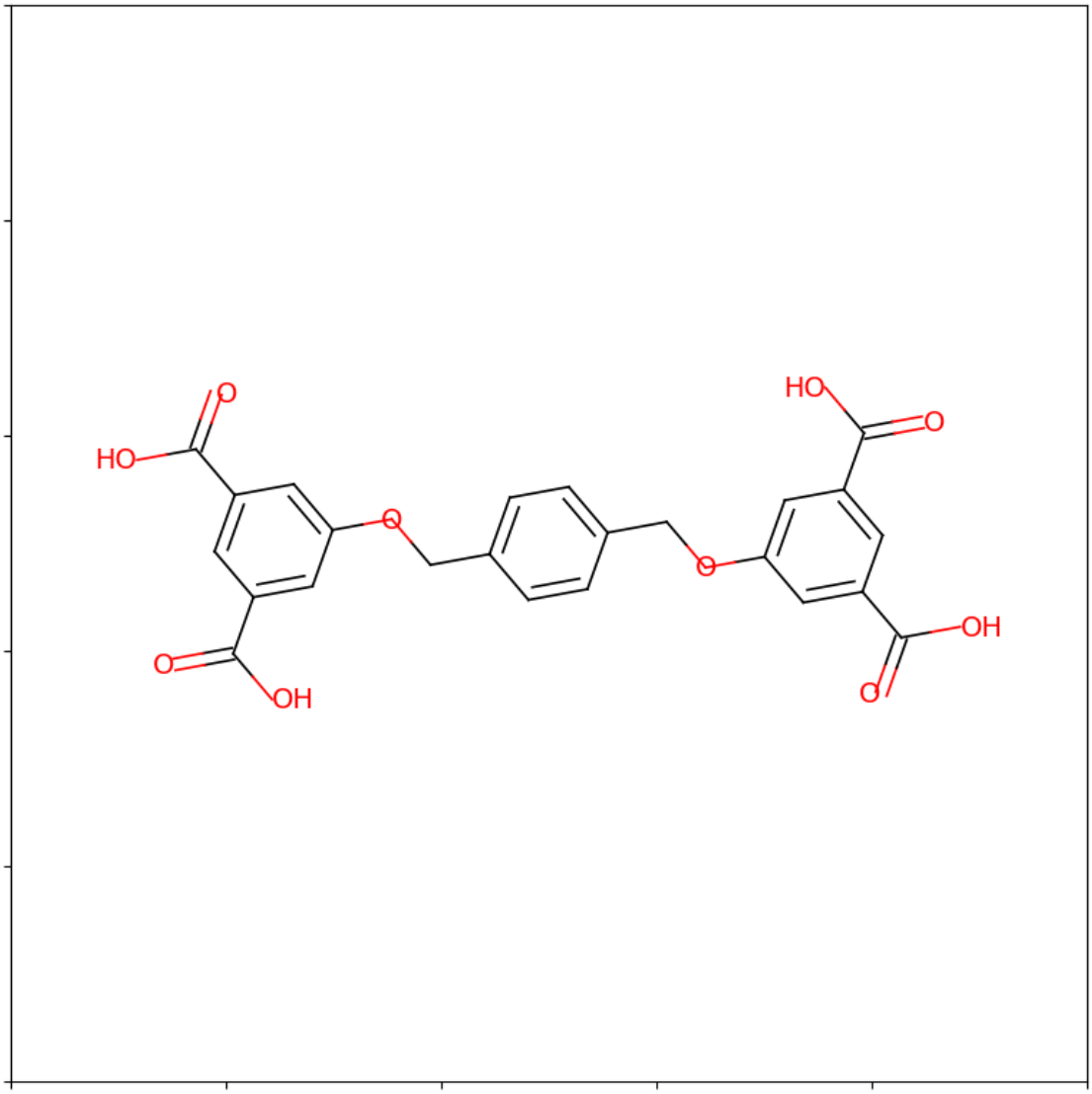
[65]:
```
Image('./REYCOP_cleansingle_linker0.png')
```

[65]:



[66]:
```
Image('./REYCOP_cleansingle_linker2.png')
```

[66]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[67]:
```
nutils.viewer('./REYCOP_clean.cif')
```

[68]:
```
temperature_mof_15_Celsius  = 135 #@param {type:'number'}
time_mof_15_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_15 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_15 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_15 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_15 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_15 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_15_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_15_mol_per_liter  = 0.2 #@param {type:'number'}
concentration_second_linker_mof_15_mol_per_liter  =  0.05#@param {type:'number'}
are_you_sure_about_your_selction_mof_15 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_15 =  'Not used to work with mixed linkers␣
↪of different types, but I think that the conditions can work for its␣
↪crystallization' #@param {type:'string'}
results['mof_15'] = {}
results['mof_15']['temperature']=temperature_mof_15_Celsius
results['mof_15']['time']=time_mof_15_hours
```

```
results['mof_15']['solvent1']=first_solvent_mof_15
results['mof_15']['solvent2']=second_solvent_mof_15
results['mof_15']['solvent3']=third_solvent_mof_15
results['mof_15']['additive']=additive_mof_15
results['mof_15']['counter']=counter_ion_mof_15
results['mof_15']['metal']=concentration_metal_mof_15_mol_per_liter
results['mof_15']['linker1']=concentration_first_linker_mof_15_mol_per_liter
results['mof_15']['linker2']=concentration_second_linker_mof_15_mol_per_liter
results['mof_15']['surely']=are_you_sure_about_your_selction_mof_15
results['mof_15']['additional']=what_makes_you_so_sure_or_unsure_mof_15
```

[69]:
```
nutils.print_choice(temperature_mof_15_Celsius, time_mof_15_hours,␣
↪first_solvent_mof_15,second_solvent_mof_15,third_solvent_mof_15 ,␣
↪counter_ion_mof_15, concentration_metal_mof_15_mol_per_liter,␣
↪concentration_first_linker_mof_15_mol_per_liter,concentration_second_linker_mof_15_mol_per_
↪, additive_mof_15,are_you_sure_about_your_selction_mof_15,␣
↪what_makes_you_so_sure_or_unsure_mof_15 )
```

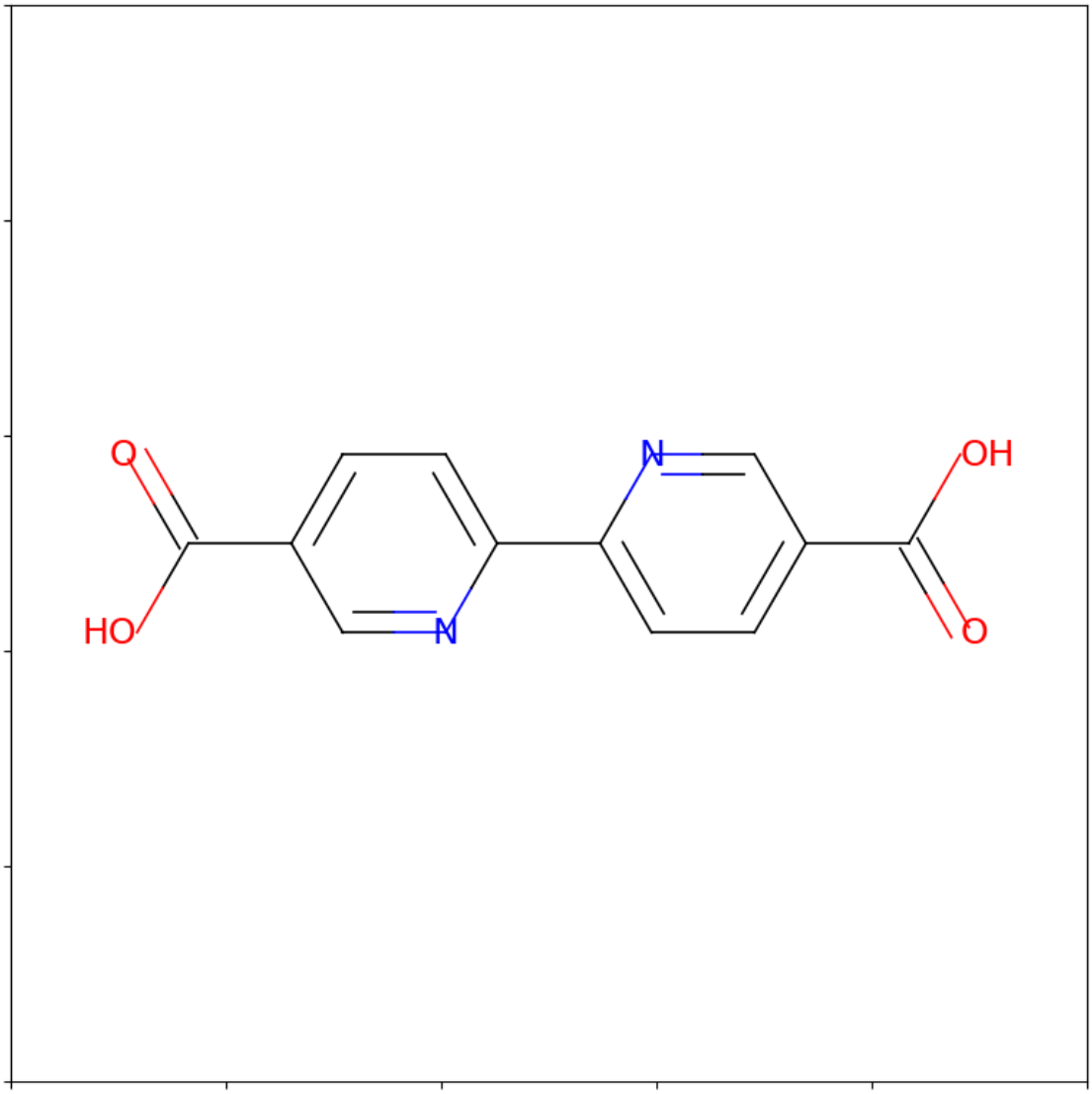
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.2
Second_Linker_Concentration: 0.05
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with mixed linkers of different
types, but I think that the conditions can work for its crystallization
```

```
# MOF 16
```

Here is the linker:

[70]:
```
Image('./EVADIQ_cleansingle_linker0.png')
```

[70]:



The metal center of this MOF is ``Dy''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[ ]:

[71]:
```
nutils.viewer('./EVADIQ_clean.cif')
```

[72]:
```
temperature_mof_16_Celsius  =  150#@param {type:'number'}
time_mof_16_hours  = 72 #@param {type:'number'}
first_solvent_mof_16 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
 ↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
 ↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
 ↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
 ↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
 ↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
 ↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_16 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
third_solvent_mof_16 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
additive_mof_16 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_16 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
 ↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
 ↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
 ↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
 ↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
 ↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_16_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_16_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_16_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_16 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_16 =  'I have no knowledge about Dy MOF␣
 ↪chemistry' #@param {type:'string'}
results['mof_16'] = {}
results['mof_16']['temperature']=temperature_mof_16_Celsius
```

```
results['mof_16']['time']=time_mof_16_hours
results['mof_16']['solvent1']=first_solvent_mof_16
results['mof_16']['solvent2']=second_solvent_mof_16
results['mof_16']['solvent3']=third_solvent_mof_16
results['mof_16']['additive']=additive_mof_16
results['mof_16']['counter']=counter_ion_mof_16
results['mof_16']['metal']=concentration_metal_mof_16_mol_per_liter
results['mof_16']['linker1']=concentration_first_linker_mof_16_mol_per_liter
results['mof_16']['linker2']=concentration_second_linker_mof_16_mol_per_liter
results['mof_16']['surely']=are_you_sure_about_your_selction_mof_16
results['mof_16']['additional']=what_makes_you_so_sure_or_unsure_mof_16
```

[73]:
```
nutils.print_choice(temperature_mof_16_Celsius, time_mof_16_hours,␣
↪first_solvent_mof_16,second_solvent_mof_16,third_solvent_mof_16 ,␣
↪counter_ion_mof_16, concentration_metal_mof_16_mol_per_liter,␣
↪concentration_first_linker_mof_16_mol_per_liter,concentration_second_linker_mof_16_mol_per_
↪, additive_mof_16,are_you_sure_about_your_selction_mof_16,␣
↪what_makes_you_so_sure_or_unsure_mof_16 )
```

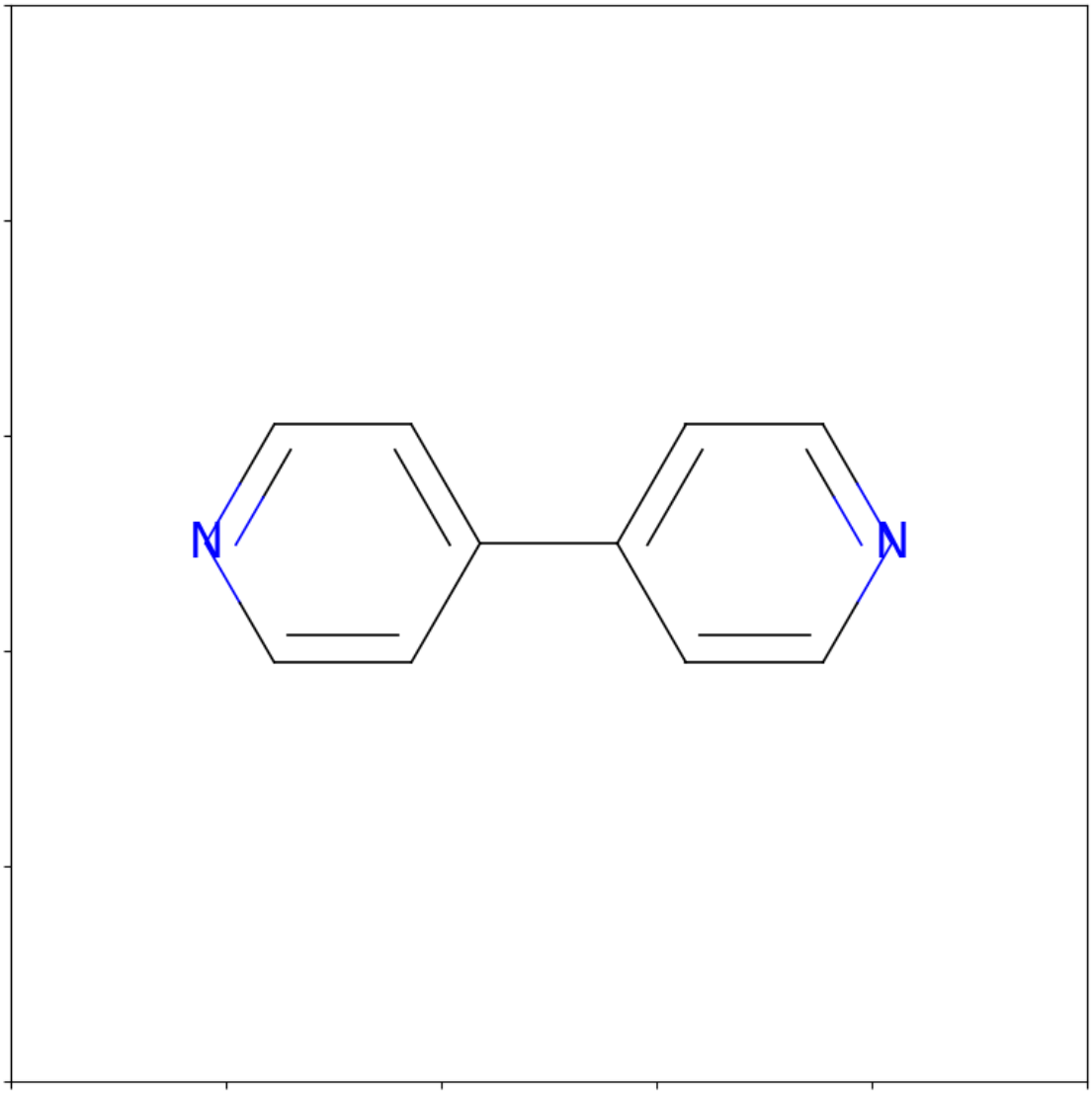
```
Thanks for your input
Your selection was:
Temperature: 150
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.05
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: I have no knowledge about Dy MOF chemistry
```

```
# MOF 17
```

Here is the linker:

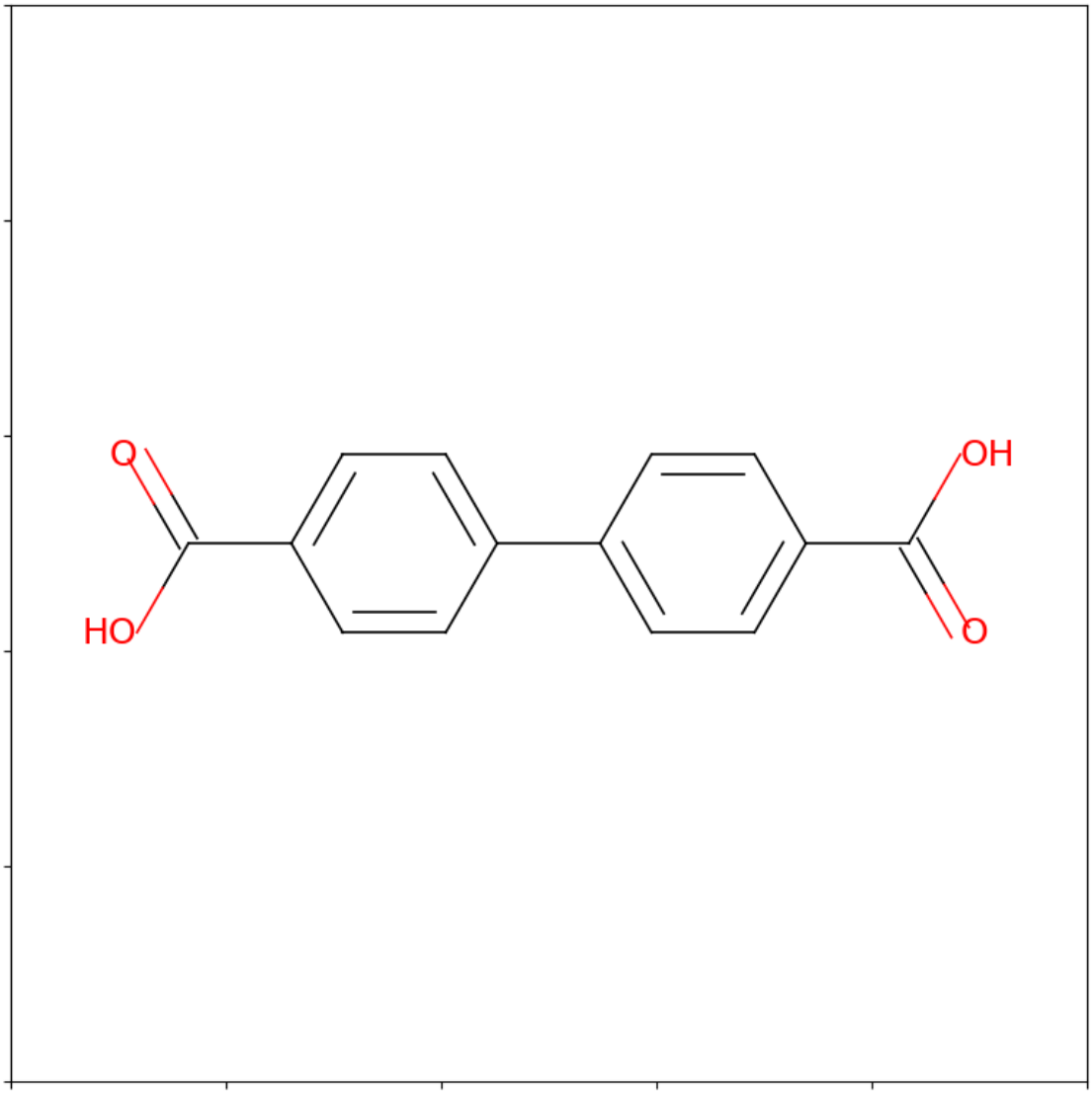
[74]:
```
Image('./AXOHIE_cleansingle_linker0.png')
```

[74]:



[75]:
```
Image('./AXOHIE_cleansingle_linker3.png')
```

[75]:



The metal center of this MOF is ``Cd''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[76]:
```
nutils.viewer('./AXOHIE_clean.cif')
```

[77]:
```
temperature_mof_17_Celsius  = 120.0 #@param {type:'number'}
time_mof_17_hours  = 36 #@param {type:'number'}
```

```
first_solvent_mof_17 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_17 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_17 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_17 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_17 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_17_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_first_linker_mof_17_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_17_mol_per_liter  = 0.025 #@param {type:
↪'number'}
are_you_sure_about_your_selction_mof_17 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_17 =  'Not used to work with cadmium MOFs'␣
↪#@param {type:'string'}
results['mof_17'] = {}
results['mof_17']['temperature']=temperature_mof_17_Celsius
```

```
results['mof_17']['time']=time_mof_17_hours
results['mof_17']['solvent1']=first_solvent_mof_17
results['mof_17']['solvent2']=second_solvent_mof_17
results['mof_17']['solvent3']=third_solvent_mof_17
results['mof_17']['additive']=additive_mof_17
results['mof_17']['counter']=counter_ion_mof_17
results['mof_17']['metal']=concentration_metal_mof_17_mol_per_liter
results['mof_17']['linker1']=concentration_first_linker_mof_17_mol_per_liter
results['mof_17']['linker2']=concentration_second_linker_mof_17_mol_per_liter
results['mof_17']['surely']=are_you_sure_about_your_selction_mof_17
results['mof_17']['additional']=what_makes_you_so_sure_or_unsure_mof_17
```

[78]:
```
nutils.print_choice(temperature_mof_17_Celsius, time_mof_17_hours,␣
↪first_solvent_mof_17,second_solvent_mof_17,third_solvent_mof_17 ,␣
↪counter_ion_mof_17, concentration_metal_mof_17_mol_per_liter,␣
↪concentration_first_linker_mof_17_mol_per_liter,concentration_second_linker_mof_17_mol_per_
↪, additive_mof_17,are_you_sure_about_your_selction_mof_17,␣
↪what_makes_you_so_sure_or_unsure_mof_17 )
```

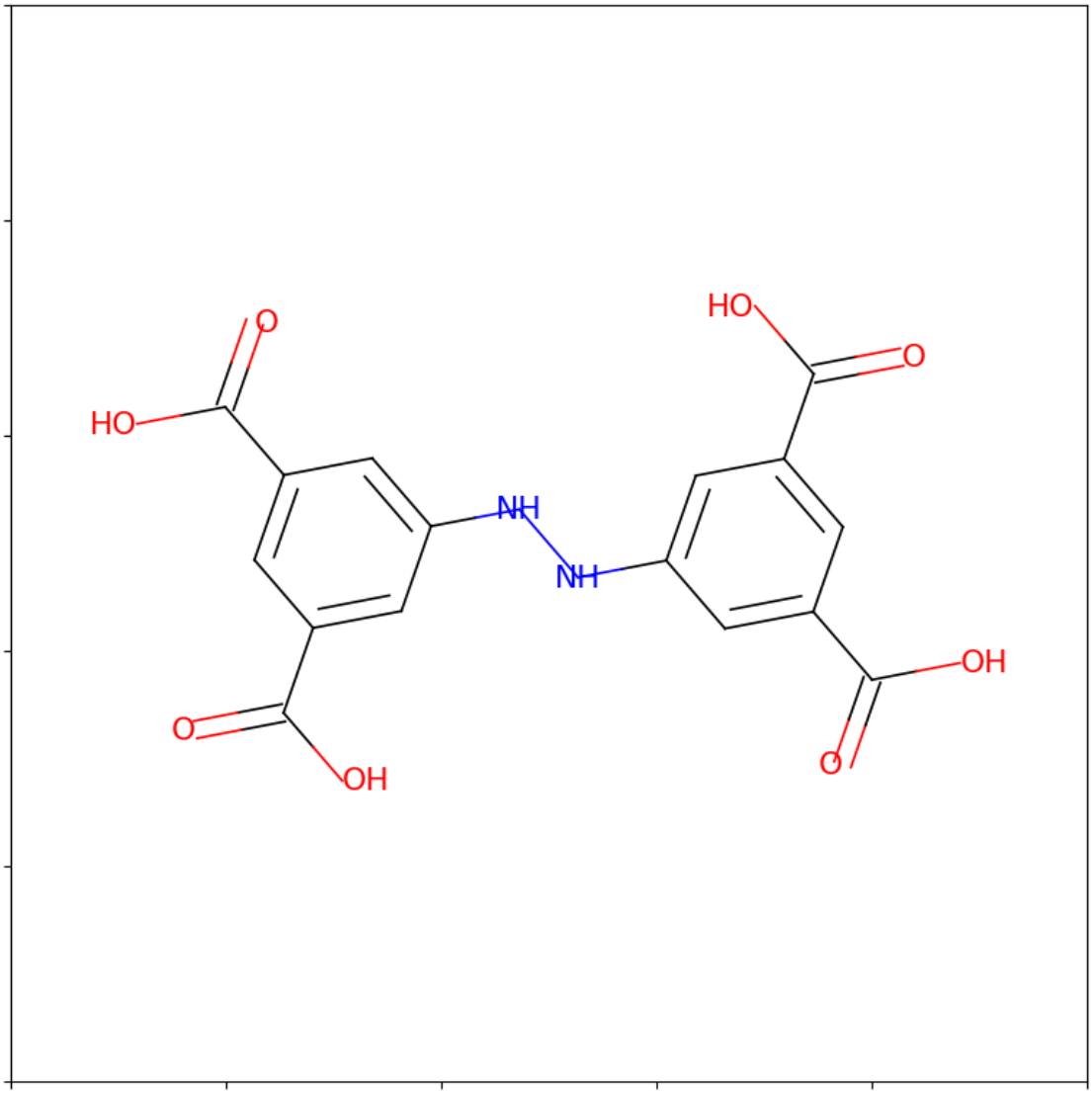
```
Thanks for your input
Your selection was:
Temperature: 120.0
Time: 36
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.025
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.025
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with cadmium MOFs
```

```
# MOF 18
```

Here is the linker:

[79]:
```
Image('./OFODET_cleansingle_linker0.png')
```

[79]:



The metal center of this MOF is ``Mn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[80]:
```
nutils.viewer('./OFODET_clean.cif')
```

[ ]:
```
```

[81]:
```
temperature_mof_18_Celsius  = 120.0 #@param {type:'number'}
time_mof_18_hours  = 72 #@param {type:'number'}
first_solvent_mof_18 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_18 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_18 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_18 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_18 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_18_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_18_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_second_linker_mof_18_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_18 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_18 =  'Quite sure that the crystallization␣
↪conditions can work, but not so sure if single crystals can be obtained'␣
↪#@param {type:'string'}
results['mof_18'] = {}
```

```
results['mof_18']['temperature']=temperature_mof_18_Celsius
results['mof_18']['time']=time_mof_18_hours
results['mof_18']['solvent1']=first_solvent_mof_18
results['mof_18']['solvent2']=second_solvent_mof_18
results['mof_18']['solvent3']=third_solvent_mof_18
results['mof_18']['additive']=additive_mof_18
results['mof_18']['counter']=counter_ion_mof_18
results['mof_18']['metal']=concentration_metal_mof_18_mol_per_liter
results['mof_18']['linker1']=concentration_first_linker_mof_18_mol_per_liter
results['mof_18']['linker2']=concentration_second_linker_mof_18_mol_per_liter
results['mof_18']['surely']=are_you_sure_about_your_selction_mof_18
results['mof_18']['additional']=what_makes_you_so_sure_or_unsure_mof_18
```

[82]:
```
nutils.print_choice(temperature_mof_18_Celsius, time_mof_18_hours,␣
↪first_solvent_mof_18,second_solvent_mof_18,third_solvent_mof_18 ,␣
↪counter_ion_mof_18, concentration_metal_mof_18_mol_per_liter,␣
↪concentration_first_linker_mof_18_mol_per_liter,concentration_second_linker_mof_18_mol_per_
↪, additive_mof_18,are_you_sure_about_your_selction_mof_18,␣
↪what_makes_you_so_sure_or_unsure_mof_18 )
```

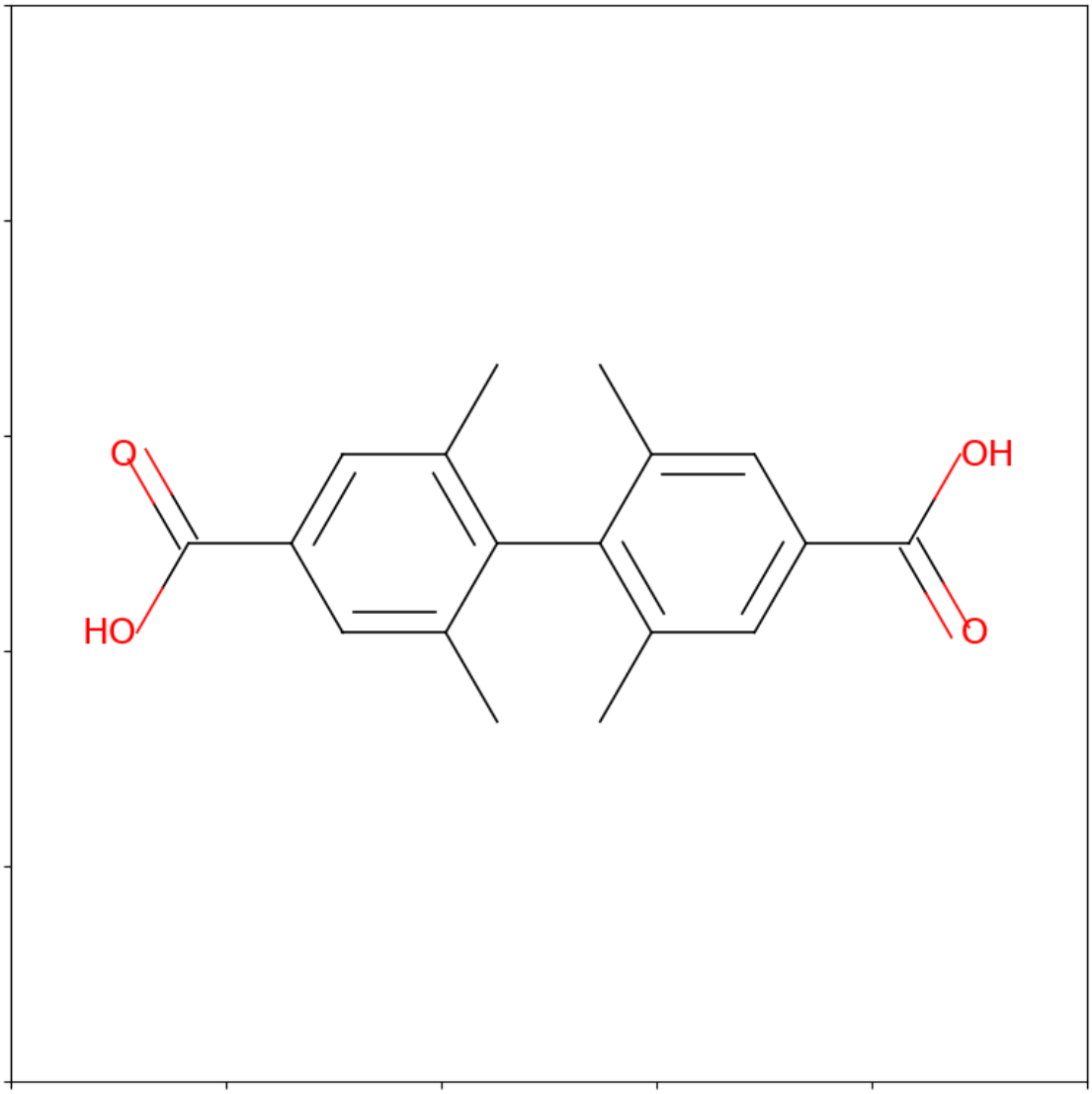
```
Thanks for your input
Your selection was:
Temperature: 120.0
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.025
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Quite sure that the crystallization conditions
can work, but not so sure if single crystals can be obtained
```

```
# MOF 19
```

Here is the linker:

[83]:
```
Image('./TEMPAE_cleansingle_linker0.png')
```

[83]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[84]:
```
nutils.viewer('./TEMPAE_clean.cif')
```

[85]:
```
temperature_mof_19_Celsius  = 135 #@param {type:'number'}
time_mof_19_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_19 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_19 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_19 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_19 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_19 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_19_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_19_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_19_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_19 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_19 =  'Relatively sure that the condition␣
↪can work to obtain the MOF, but not confident about the quality of the␣
↪crystals obatined' #@param {type:'string'}
results['mof_19'] = {}
results['mof_19']['temperature']=temperature_mof_19_Celsius
results['mof_19']['time']=time_mof_19_hours
```

```
results['mof_19']['solvent1']=first_solvent_mof_19
results['mof_19']['solvent2']=second_solvent_mof_19
results['mof_19']['solvent3']=third_solvent_mof_19
results['mof_19']['additive']=additive_mof_19
results['mof_19']['counter']=counter_ion_mof_19
results['mof_19']['metal']=concentration_metal_mof_19_mol_per_liter
results['mof_19']['linker1']=concentration_first_linker_mof_19_mol_per_liter
results['mof_19']['linker2']=concentration_second_linker_mof_19_mol_per_liter
results['mof_19']['surely']=are_you_sure_about_your_selction_mof_19
results['mof_19']['additional']=what_makes_you_so_sure_or_unsure_mof_19
```

[86]:
```
nutils.print_choice(temperature_mof_19_Celsius, time_mof_19_hours,␣
↪first_solvent_mof_19,second_solvent_mof_19,third_solvent_mof_19 ,␣
↪counter_ion_mof_19, concentration_metal_mof_19_mol_per_liter,␣
↪concentration_first_linker_mof_19_mol_per_liter,concentration_second_linker_mof_19_mol_per_
↪, additive_mof_19,are_you_sure_about_your_selction_mof_19,␣
↪what_makes_you_so_sure_or_unsure_mof_19 )
```

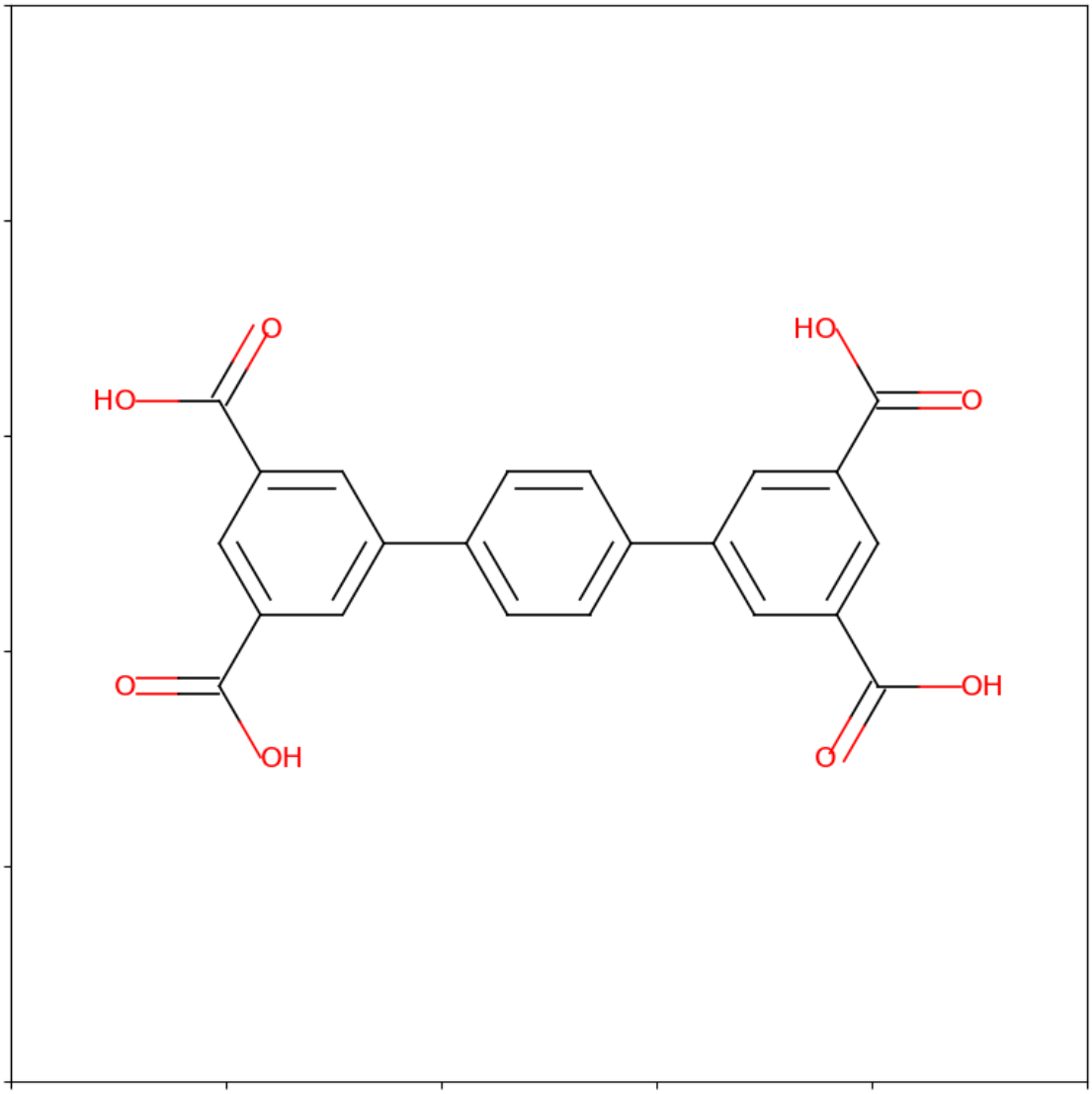
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.075
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Relatively sure that the condition can work to
obtain the MOF, but not confident about the quality of the crystals obatined
```

```
# MOF 20
```

Here is the linker:

[87]:
```
Image('./WIPLOY_cleansingle_linker0.png')
```

[87]:



The metal center of this MOF is ``Eu''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[88]:
```
nutils.viewer('./WIPLOY_clean.cif')
```

[89]:
```
temperature_mof_20_Celsius  = 150 #@param {type:'number'}
time_mof_20_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_20 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_20 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_20 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_20 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_20 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_20_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_first_linker_mof_20_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_20_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_20 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_20 =  '' #@param {type:'string'}
results['mof_20'] = {}
results['mof_20']['temperature']=temperature_mof_20_Celsius
results['mof_20']['time']=time_mof_20_hours
results['mof_20']['solvent1']=first_solvent_mof_20
results['mof_20']['solvent2']=second_solvent_mof_20
```

```
results['mof_20']['solvent3']=third_solvent_mof_20
results['mof_20']['additive']=additive_mof_20
results['mof_20']['counter']=counter_ion_mof_20
results['mof_20']['metal']=concentration_metal_mof_20_mol_per_liter
results['mof_20']['linker1']=concentration_first_linker_mof_20_mol_per_liter
results['mof_20']['linker2']=concentration_second_linker_mof_20_mol_per_liter
results['mof_20']['surely']=are_you_sure_about_your_selction_mof_20
results['mof_20']['additional']=what_makes_you_so_sure_or_unsure_mof_20
```

[90]:
```
nutils.print_choice(temperature_mof_20_Celsius, time_mof_20_hours,␣
↪first_solvent_mof_20,second_solvent_mof_20,third_solvent_mof_20 ,␣
↪counter_ion_mof_20, concentration_metal_mof_20_mol_per_liter,␣
↪concentration_first_linker_mof_20_mol_per_liter,concentration_second_linker_mof_20_mol_per_
↪, additive_mof_20,are_you_sure_about_your_selction_mof_20,␣
↪what_makes_you_so_sure_or_unsure_mof_20 )
```

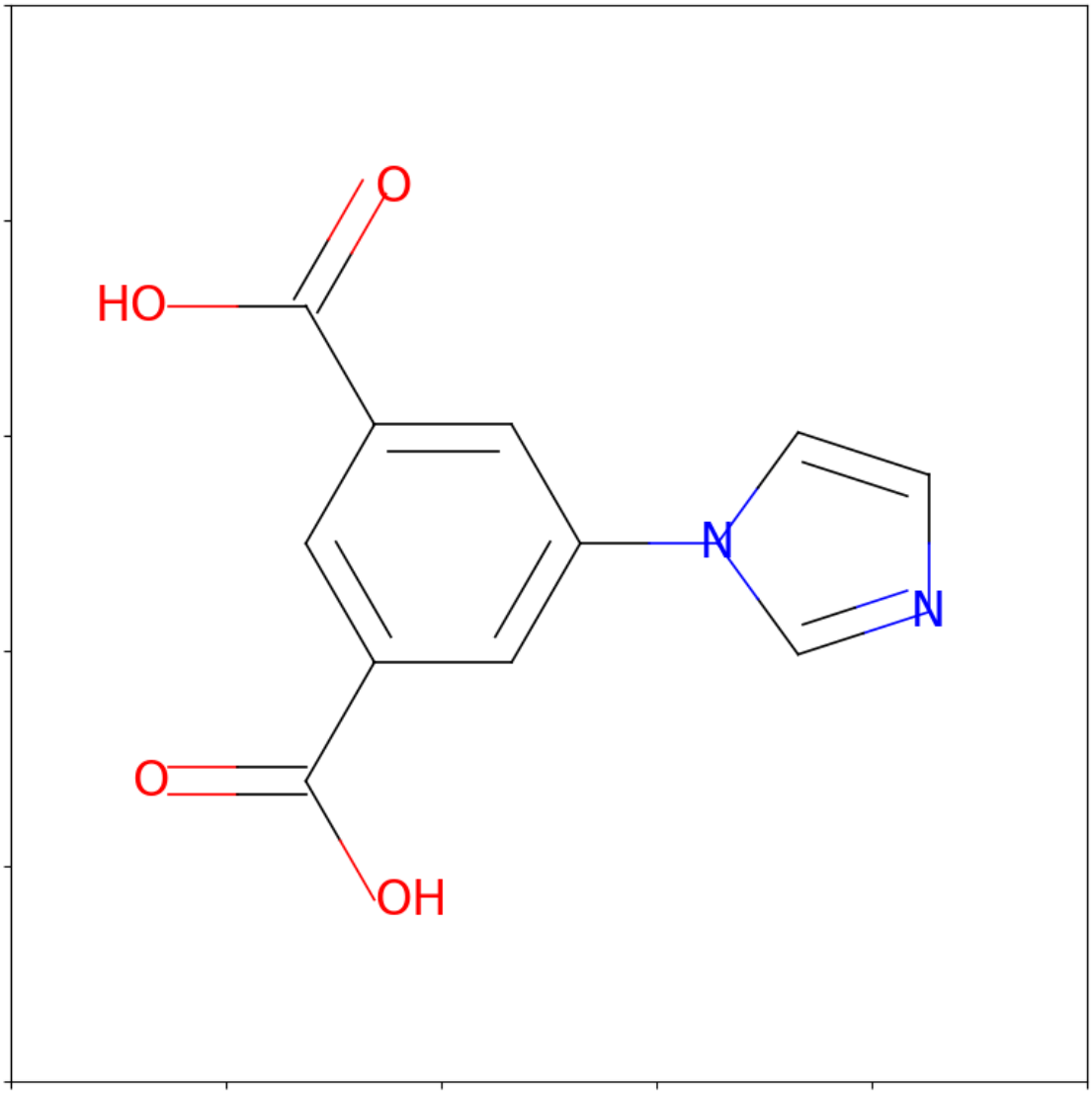
```
Thanks for your input
Your selection was:
Temperature: 150
Time: 72.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.025
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure:
```

```
# MOF 21
```

Here is the linker:

[91]:
```
Image('./NUBPIL_cleansingle_linker0.png')
```

[91]:



The metal center of this MOF is ``Cu''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[92]:
```
nutils.viewer('./NUBPIL_clean.cif')
```

[93]:
```
temperature_mof_21_Celsius  =  120#@param {type:'number'}
time_mof_21_hours  =  72#@param {type:'number'}
```

```
first_solvent_mof_21 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_21 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_21 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_21 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_21 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_21_mol_per_liter  =  0.035#@param {type:'number'}
concentration_first_linker_mof_21_mol_per_liter  =  0.05#@param {type:'number'}
concentration_second_linker_mof_21_mol_per_liter  =  0#@param {type:'number'}
are_you_sure_about_your_selction_mof_21 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_21 =  'Not used to work with linkers that␣
↪have different coordinating g' #@param {type:'string'}
results['mof_21'] = {}
results['mof_21']['temperature']=temperature_mof_21_Celsius
results['mof_21']['time']=time_mof_21_hours
results['mof_21']['solvent1']=first_solvent_mof_21
```

```
results['mof_21']['solvent2']=second_solvent_mof_21
results['mof_21']['solvent3']=third_solvent_mof_21
results['mof_21']['additive']=additive_mof_21
results['mof_21']['counter']=counter_ion_mof_21
results['mof_21']['metal']=concentration_metal_mof_21_mol_per_liter
results['mof_21']['linker1']=concentration_first_linker_mof_21_mol_per_liter
results['mof_21']['linker2']=concentration_second_linker_mof_21_mol_per_liter
results['mof_21']['surely']=are_you_sure_about_your_selction_mof_21
results['mof_21']['additional']=what_makes_you_so_sure_or_unsure_mof_21
```

[94]:
```
nutils.print_choice(temperature_mof_21_Celsius, time_mof_21_hours,␣
↪first_solvent_mof_21,second_solvent_mof_21,third_solvent_mof_21 ,␣
↪counter_ion_mof_21, concentration_metal_mof_21_mol_per_liter,␣
↪concentration_first_linker_mof_21_mol_per_liter,concentration_second_linker_mof_21_mol_per_
↪, additive_mof_21,are_you_sure_about_your_selction_mof_21,␣
↪what_makes_you_so_sure_or_unsure_mof_21 )
```

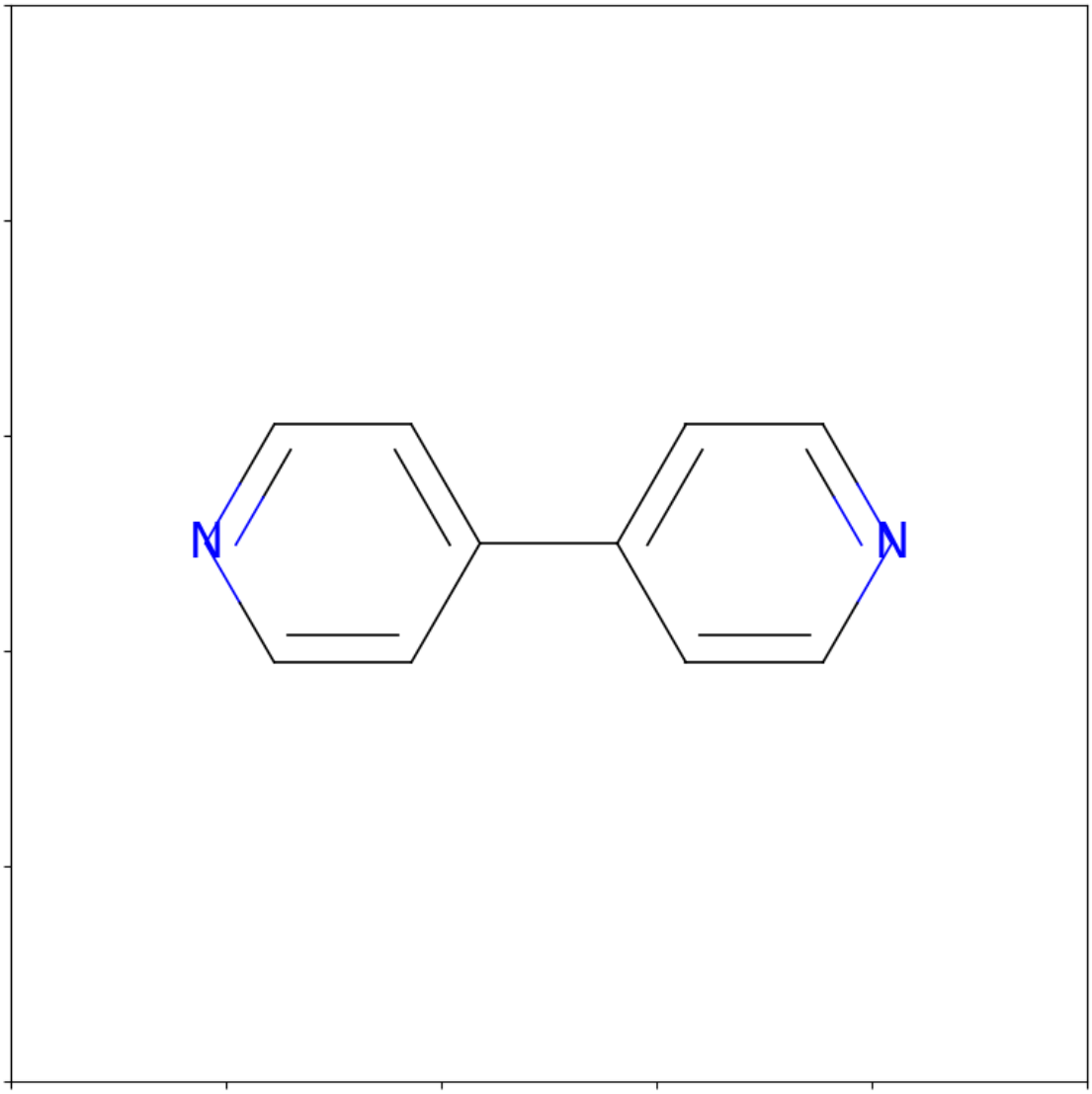
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.035
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with linkers that have different
coordinating g
```

```
# MOF 22
```

Here is the linker:

[95]:
```
Image('./PEKZIP_cleansingle_linker0.png')
```

[95]:



The metal center of this MOF is ``Cu''. The oxidation state of the metal is ``1''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[96]:
```
nutils.viewer('./PEKZIP_clean.cif')
```

[97]:
```
temperature_mof_22_Celsius  = 100.0 #@param {type:'number'}
time_mof_22_hours  = 48 #@param {type:'number'}
```

```
first_solvent_mof_22 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_22 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_22 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_22 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_22 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_22_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_first_linker_mof_22_mol_per_liter  = 0.25 #@param {type:'number'}
concentration_second_linker_mof_22_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_22 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_22 =  'crystallization may occur also at␣
↪room temperature after heating the system' #@param {type:'string'}
results['mof_22'] = {}
results['mof_22']['temperature']=temperature_mof_22_Celsius
results['mof_22']['time']=time_mof_22_hours
results['mof_22']['solvent1']=first_solvent_mof_22
```

```
results['mof_22']['solvent2']=second_solvent_mof_22
results['mof_22']['solvent3']=third_solvent_mof_22
results['mof_22']['additive']=additive_mof_22
results['mof_22']['counter']=counter_ion_mof_22
results['mof_22']['metal']=concentration_metal_mof_22_mol_per_liter
results['mof_22']['linker1']=concentration_first_linker_mof_22_mol_per_liter
results['mof_22']['linker2']=concentration_second_linker_mof_22_mol_per_liter
results['mof_22']['surely']=are_you_sure_about_your_selction_mof_22
results['mof_22']['additional']=what_makes_you_so_sure_or_unsure_mof_22
```

[98]:
```
nutils.print_choice(temperature_mof_22_Celsius, time_mof_22_hours,␣
↪first_solvent_mof_22,second_solvent_mof_22,third_solvent_mof_22 ,␣
↪counter_ion_mof_22, concentration_metal_mof_22_mol_per_liter,␣
↪concentration_first_linker_mof_22_mol_per_liter,concentration_second_linker_mof_22_mol_per_
↪, additive_mof_22,are_you_sure_about_your_selction_mof_22,␣
↪what_makes_you_so_sure_or_unsure_mof_22 )
```

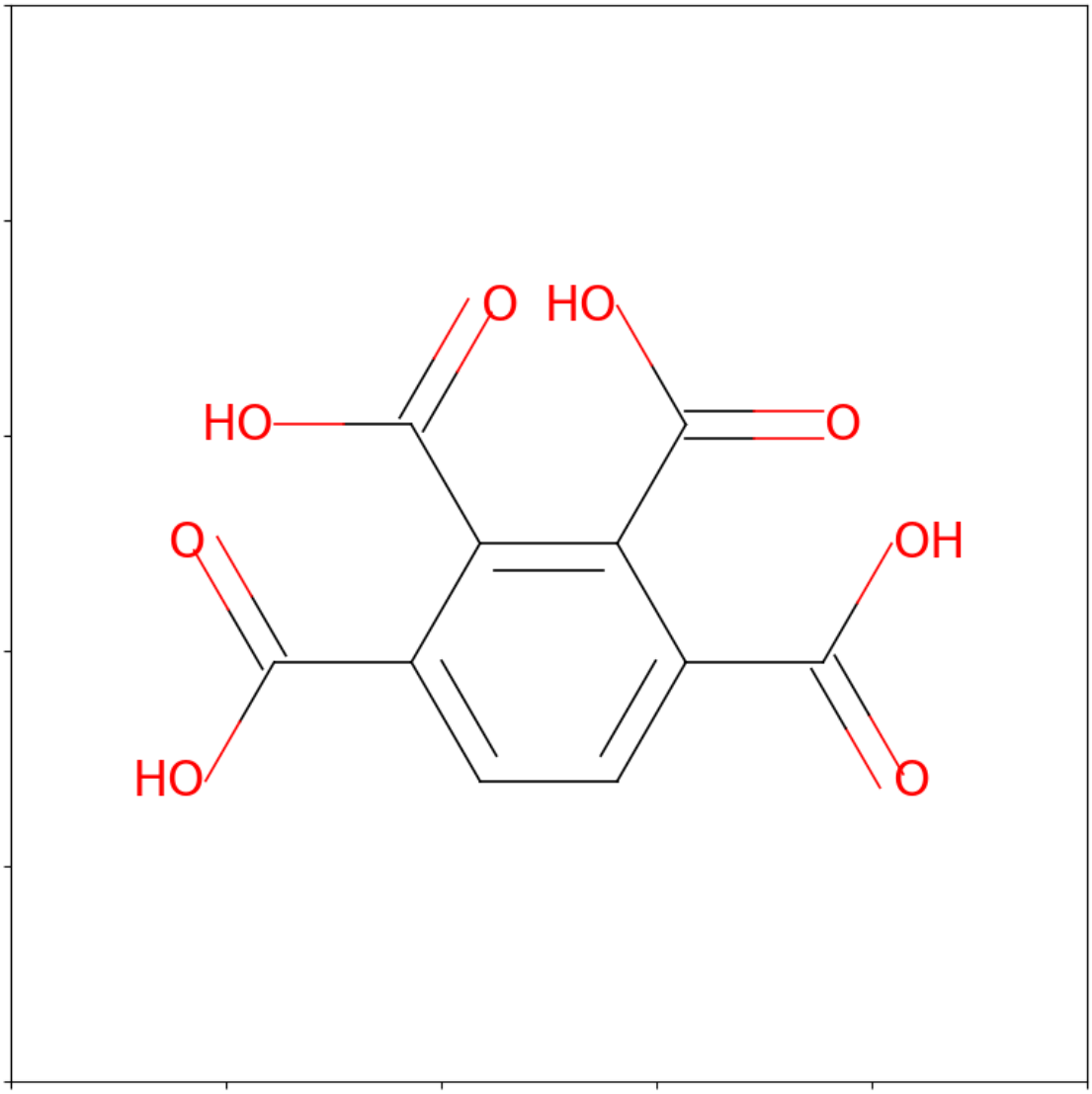
```
Thanks for your input
Your selection was:
Temperature: 100.0
Time: 48
Solvent1: ethanol
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.1
First_Linker_Concentration: 0.25
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: crystallization may occur also at room
temperature after heating the system
```

```
# MOF 23
```

Here is the linker:

[99]:
```
Image('./FIMXUW_cleansingle_linker2.png')
```

[99]:



The metal center of this MOF is ``La''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[100]:
```
nutils.viewer('./FIMXUW_clean.cif')
```

[101]:
```
temperature_mof_23_Celsius  = 150 #@param {type:'number'}
time_mof_23_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_23 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
 ↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
 ↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
 ↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
 ↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
 ↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
 ↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_23 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
third_solvent_mof_23 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
additive_mof_23 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_23 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
 ↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
 ↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
 ↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
 ↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
 ↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_23_mol_per_liter  = 0.055 #@param {type:'number'}
concentration_first_linker_mof_23_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_23_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_23 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_23 =  'Not sure about the overall␣
 ↪concentration of the reaction. I usually suggest diluted system to favour␣
 ↪the crystallization of the material as single crystals, but if the␣
 ↪concentration is lowered too much you take the risk to obtain only a␣
 ↪solution at the end of the reaction' #@param {type:'string'}
results['mof_23'] = {}
```

```
results['mof_23']['temperature']=temperature_mof_23_Celsius
results['mof_23']['time']=time_mof_23_hours
results['mof_23']['solvent1']=first_solvent_mof_23
results['mof_23']['solvent2']=second_solvent_mof_23
results['mof_23']['solvent3']=third_solvent_mof_23
results['mof_23']['additive']=additive_mof_23
results['mof_23']['counter']=counter_ion_mof_23
results['mof_23']['metal']=concentration_metal_mof_23_mol_per_liter
results['mof_23']['linker1']=concentration_first_linker_mof_23_mol_per_liter
results['mof_23']['linker2']=concentration_second_linker_mof_23_mol_per_liter
results['mof_23']['surely']=are_you_sure_about_your_selction_mof_23
results['mof_23']['additional']=what_makes_you_so_sure_or_unsure_mof_23
```

[102]:
```
nutils.print_choice(temperature_mof_23_Celsius, time_mof_23_hours,␣
↪first_solvent_mof_23,second_solvent_mof_23,third_solvent_mof_23 ,␣
↪counter_ion_mof_23, concentration_metal_mof_23_mol_per_liter,␣
↪concentration_first_linker_mof_23_mol_per_liter,concentration_second_linker_mof_23_mol_per_
↪, additive_mof_23,are_you_sure_about_your_selction_mof_23,␣
↪what_makes_you_so_sure_or_unsure_mof_23 )
```

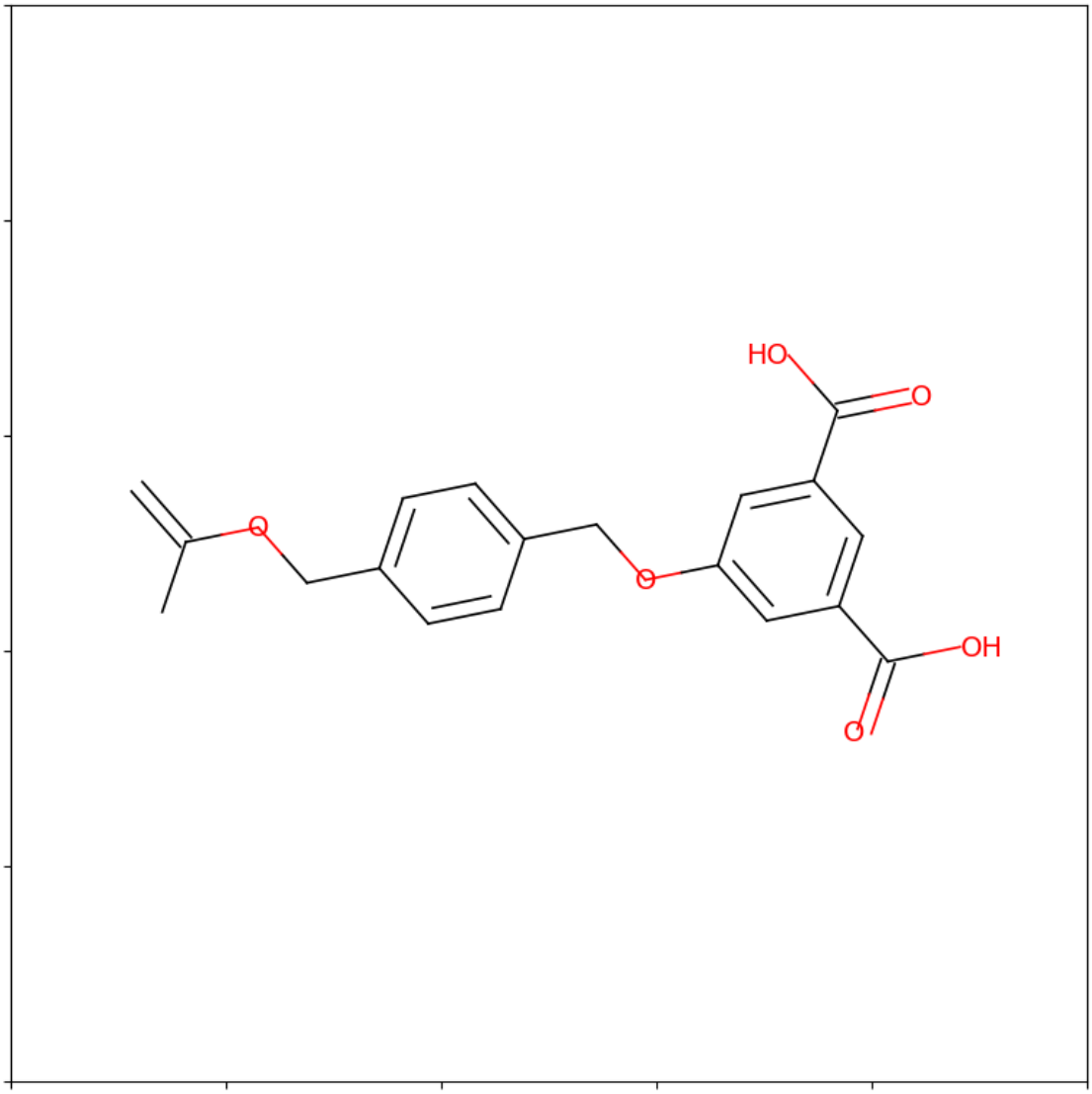
```
Thanks for your input
Your selection was:
Temperature: 150
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.055
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the overall concentration of the
reaction. I usually suggest diluted system to favour the crystallization of the
material as single crystals, but if the concentration is lowered too much you
take the risk to obtain only a solution at the end of the reaction
```

```
# MOF 24
```

Here is the linker:

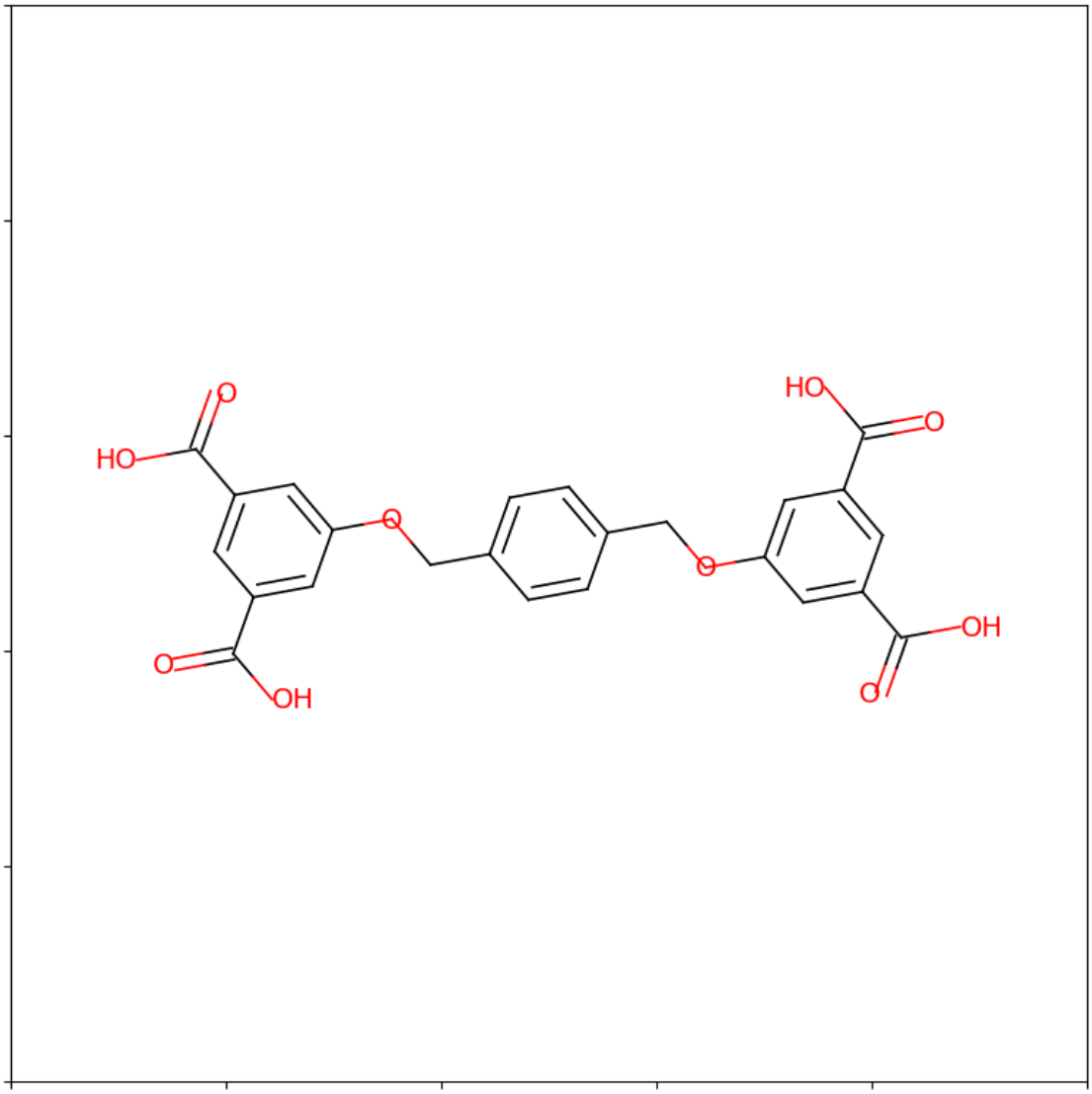
[103]:
```
Image('./REYCEF_cleansingle_linker0.png')
```

[103]:



[104]:
```
Image('./REYCEF_cleansingle_linker2.png')
```

[104]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[105]:
```
nutils.viewer('./REYCEF_clean.cif')
```

[106]:
```
temperature_mof_24_Celsius  = 135 #@param {type:'number'}
time_mof_24_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_24 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_24 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_24 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_24 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_24 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_24_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_24_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_24_mol_per_liter  = 0.075 #@param {type:
↪'number'}
are_you_sure_about_your_selction_mof_24 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_24 =  'I am not sure of the solubility of␣
↪the linkers without the addition of an acid/base' #@param {type:'string'}
results['mof_24'] = {}
results['mof_24']['temperature']=temperature_mof_24_Celsius
```

```
results['mof_24']['time']=time_mof_24_hours
results['mof_24']['solvent1']=first_solvent_mof_24
results['mof_24']['solvent2']=second_solvent_mof_24
results['mof_24']['solvent3']=third_solvent_mof_24
results['mof_24']['additive']=additive_mof_24
results['mof_24']['counter']=counter_ion_mof_24
results['mof_24']['metal']=concentration_metal_mof_24_mol_per_liter
results['mof_24']['linker1']=concentration_first_linker_mof_24_mol_per_liter
results['mof_24']['linker2']=concentration_second_linker_mof_24_mol_per_liter
results['mof_24']['surely']=are_you_sure_about_your_selction_mof_24
results['mof_24']['additional']=what_makes_you_so_sure_or_unsure_mof_24
```

[107]:
```
nutils.print_choice(temperature_mof_24_Celsius, time_mof_24_hours,␣
↪first_solvent_mof_24,second_solvent_mof_24,third_solvent_mof_24 ,␣
↪counter_ion_mof_24, concentration_metal_mof_24_mol_per_liter,␣
↪concentration_first_linker_mof_24_mol_per_liter,concentration_second_linker_mof_24_mol_per_
↪, additive_mof_24,are_you_sure_about_your_selction_mof_24,␣
↪what_makes_you_so_sure_or_unsure_mof_24 )
```

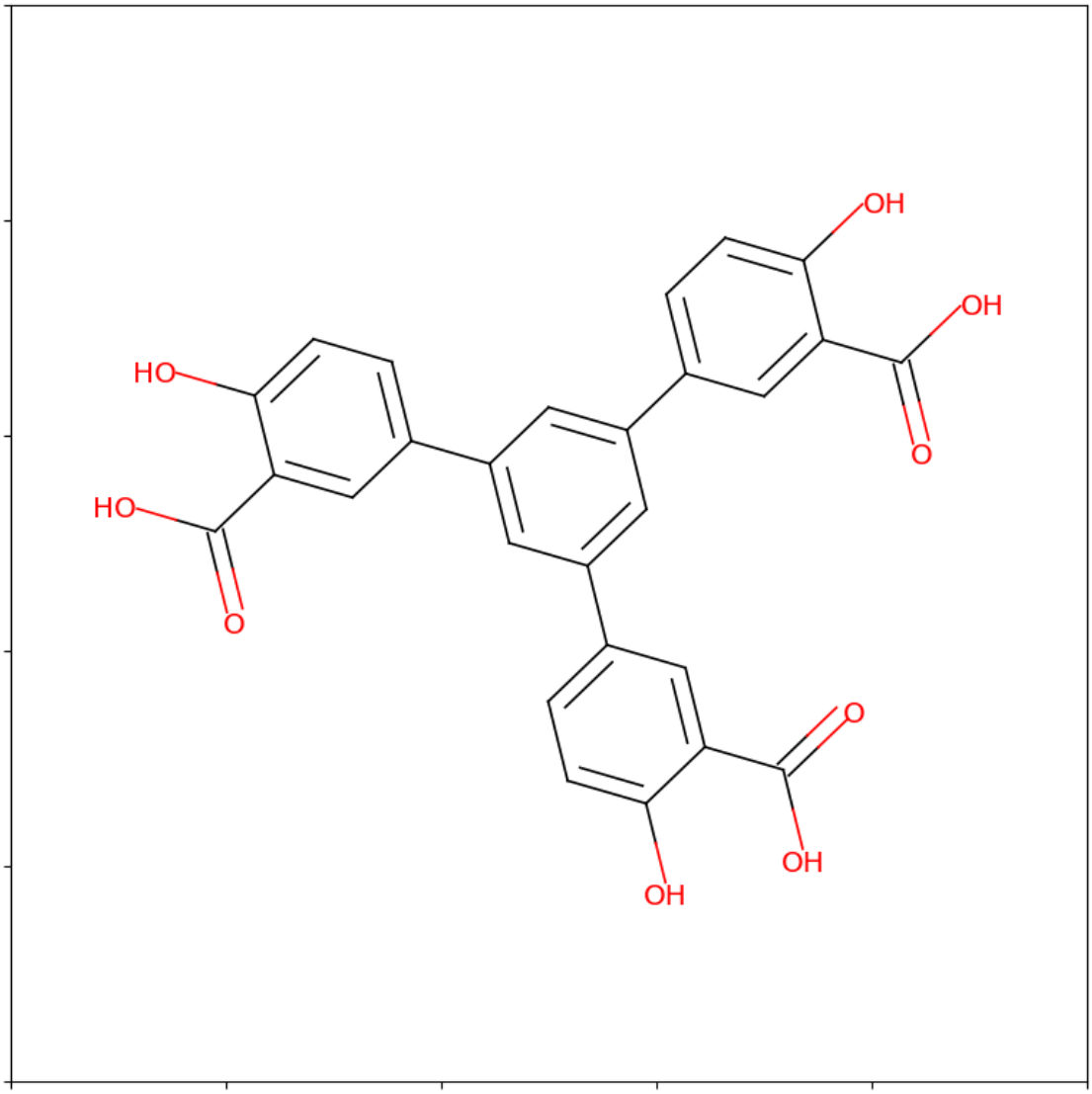
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.075
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: I am not sure of the solubility of the linkers
without the addition of an acid/base
```

```
# MOF 25
```

Here is the linker:

[108]:
```
Image('./IZEWAN_cleansingle_linker0.png')
```

[108]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[109]:
```
nutils.viewer('./IZEWAN_clean.cif')
```

[110]:
```
temperature_mof_25_Celsius  = 135 #@param {type:'number'}
time_mof_25_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_25 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_25 = 'tetrahydrofuran (THF)' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_25 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_25 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_25 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_25_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_25_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_second_linker_mof_25_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_25 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_25 =  'Not sure about the overall␣
↪concentration of the system. Temperature and solvent conditions could be␣
↪close to the good ones at least to crystallize the material' #@param {type:
↪'string'}
results['mof_25'] = {}
results['mof_25']['temperature']=temperature_mof_25_Celsius
```

```
results['mof_25']['time']=time_mof_25_hours
results['mof_25']['solvent1']=first_solvent_mof_25
results['mof_25']['solvent2']=second_solvent_mof_25
results['mof_25']['solvent3']=third_solvent_mof_25
results['mof_25']['additive']=additive_mof_25
results['mof_25']['counter']=counter_ion_mof_25
results['mof_25']['metal']=concentration_metal_mof_25_mol_per_liter
results['mof_25']['linker1']=concentration_first_linker_mof_25_mol_per_liter
results['mof_25']['linker2']=concentration_second_linker_mof_25_mol_per_liter
results['mof_25']['surely']=are_you_sure_about_your_selction_mof_25
results['mof_25']['additional']=what_makes_you_so_sure_or_unsure_mof_25
```

[111]:
```
nutils.print_choice(temperature_mof_25_Celsius, time_mof_25_hours,␣
↪first_solvent_mof_25,second_solvent_mof_25,third_solvent_mof_25 ,␣
↪counter_ion_mof_25, concentration_metal_mof_25_mol_per_liter,␣
↪concentration_first_linker_mof_25_mol_per_liter,concentration_second_linker_mof_25_mol_per_
↪, additive_mof_25,are_you_sure_about_your_selction_mof_25,␣
↪what_makes_you_so_sure_or_unsure_mof_25 )
```

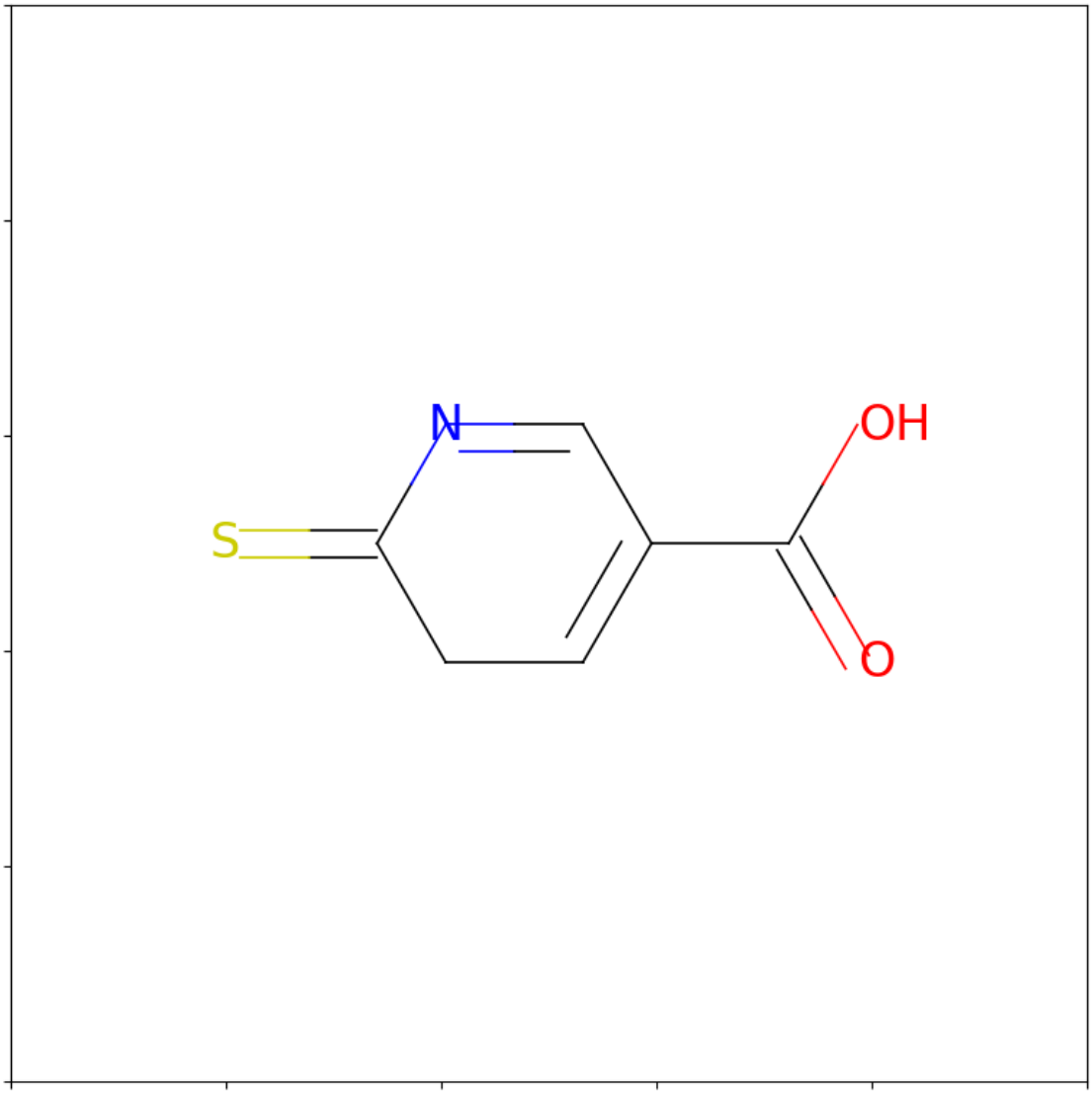
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: tetrahydrofuran (THF)
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.075
First_Linker_Concentration: 0.1
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the overall concentration of the
system. Temperature and solvent conditions could be close to the good ones at
least to crystallize the material
```

```
# MOF 26
```

Here is the linker:

[112]:
```
Image('./WEGDIX_chargedsingle_linker0.png')
```

[112]:



The metal center of this MOF is ``Cd''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[113]:
```
nutils.viewer('./WEGDIX_charged.cif')
```

[114]:
```
temperature_mof_26_Celsius  = 120 #@param {type:'number'}
time_mof_26_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_26 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_26 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_26 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_26 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_26 =  'SO4' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_26_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_26_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_second_linker_mof_26_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_26 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_26 =  'given the structure, the conditions␣
↪need to be oxidizing... but not sur how these are obtained during the␣
↪synthesis' #@param {type:'string'}
results['mof_26'] = {}
results['mof_26']['temperature']=temperature_mof_26_Celsius
results['mof_26']['time']=time_mof_26_hours
```

```
results['mof_26']['solvent1']=first_solvent_mof_26
results['mof_26']['solvent2']=second_solvent_mof_26
results['mof_26']['solvent3']=third_solvent_mof_26
results['mof_26']['additive']=additive_mof_26
results['mof_26']['counter']=counter_ion_mof_26
results['mof_26']['metal']=concentration_metal_mof_26_mol_per_liter
results['mof_26']['linker1']=concentration_first_linker_mof_26_mol_per_liter
results['mof_26']['linker2']=concentration_second_linker_mof_26_mol_per_liter
results['mof_26']['surely']=are_you_sure_about_your_selction_mof_26
results['mof_26']['additional']=what_makes_you_so_sure_or_unsure_mof_26
```

[115]:
```
nutils.print_choice(temperature_mof_26_Celsius, time_mof_26_hours,␣
↪first_solvent_mof_26,second_solvent_mof_26,third_solvent_mof_26 ,␣
↪counter_ion_mof_26, concentration_metal_mof_26_mol_per_liter,␣
↪concentration_first_linker_mof_26_mol_per_liter,concentration_second_linker_mof_26_mol_per_
↪, additive_mof_26,are_you_sure_about_your_selction_mof_26,␣
↪what_makes_you_so_sure_or_unsure_mof_26 )
```

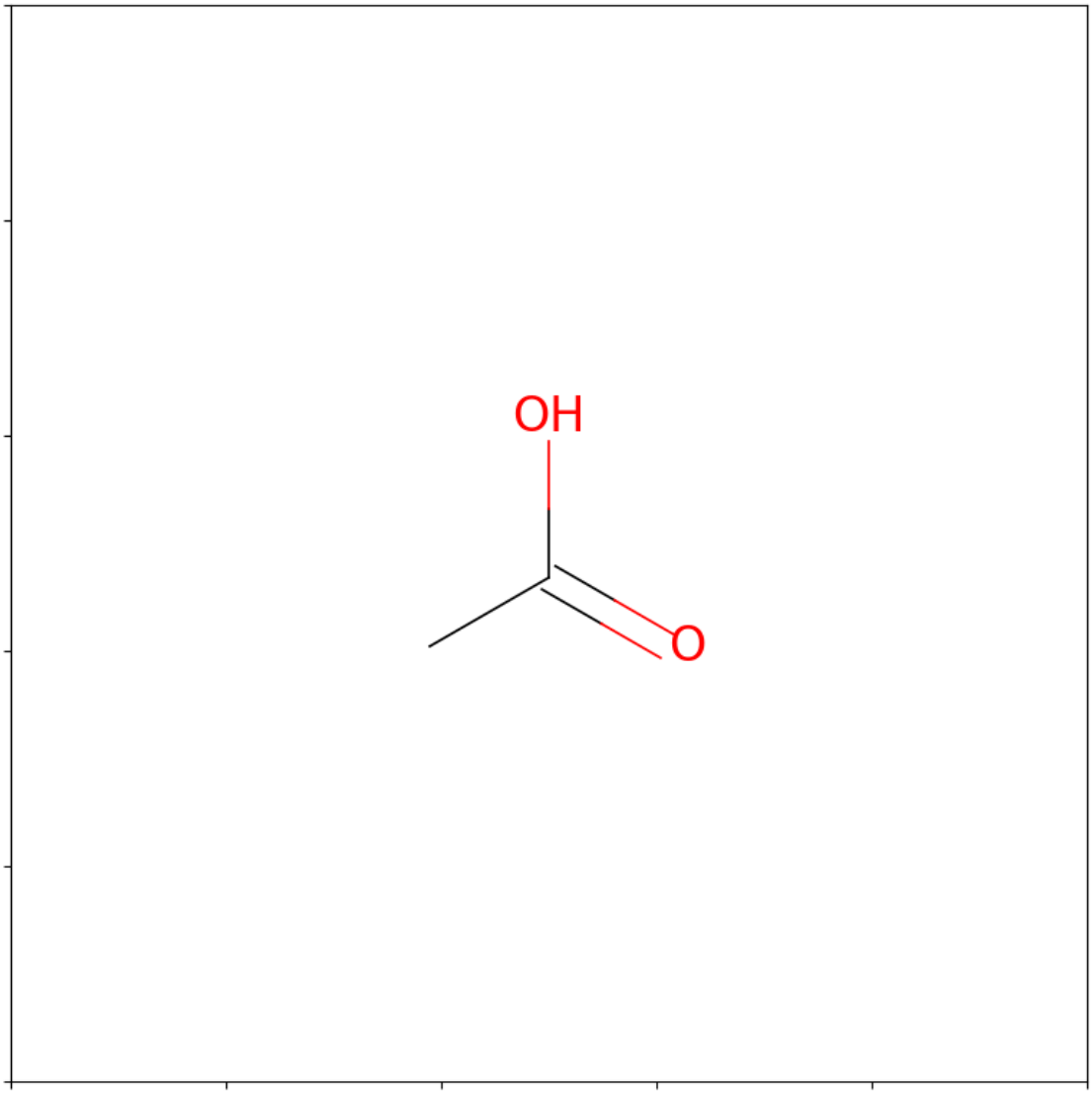
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 72
Solvent1: ethanol
Solvent2: None
Solvent3: None
Counter Ion: SO4
Metal_Concentration: 0.075
First_Linker_Concentration: 0.1
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: given the structure, the conditions need to be
oxidizing… but not sur how these are obtained during the synthesis
```

```
# MOF 27
```

Here is the linker:

[116]:
```
Image('./CABQEB_cleansingle_linker0.png')
```

[116]:



The metal center of this MOF is ``Co''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[117]:
```
nutils.viewer('./CABQEB_clean.cif')
```

[118]:
```
temperature_mof_27_Celsius  = 135 #@param {type:'number'}
time_mof_27_hours  = 48 #@param {type:'number'}
```

```
first_solvent_mof_27 = 'H2O' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
second_solvent_mof_27 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_27 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_27 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_27 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_27_mol_per_liter  = 0.25 #@param {type:'number'}
concentration_first_linker_mof_27_mol_per_liter  = 0.75 #@param {type:'number'}
concentration_second_linker_mof_27_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_27 = 'yes' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_27 =  "Quite sure, but not completely, we␣
↪use to synthesise Zr-clusters in similar conditions. Overall concentration␣
↪of the reagents could need to be tuned to obtain syngle crystals" #@param␣
↪{type:'string'}
results['mof_27'] = {}
results['mof_27']['temperature']=temperature_mof_27_Celsius
```

```
results['mof_27']['time']=time_mof_27_hours
results['mof_27']['solvent1']=first_solvent_mof_27
results['mof_27']['solvent2']=second_solvent_mof_27
results['mof_27']['solvent3']=third_solvent_mof_27
results['mof_27']['additive']=additive_mof_27
results['mof_27']['counter']=counter_ion_mof_27
results['mof_27']['metal']=concentration_metal_mof_27_mol_per_liter
results['mof_27']['linker1']=concentration_first_linker_mof_27_mol_per_liter
results['mof_27']['linker2']=concentration_second_linker_mof_27_mol_per_liter
results['mof_27']['surely']=are_you_sure_about_your_selction_mof_27
results['mof_27']['additional']=what_makes_you_so_sure_or_unsure_mof_27
```

[119]:
```
nutils.print_choice(temperature_mof_27_Celsius, time_mof_27_hours,␣
↪first_solvent_mof_27,second_solvent_mof_27,third_solvent_mof_27 ,␣
↪counter_ion_mof_27, concentration_metal_mof_27_mol_per_liter,␣
↪concentration_first_linker_mof_27_mol_per_liter,concentration_second_linker_mof_27_mol_per_
↪, additive_mof_27,are_you_sure_about_your_selction_mof_27,␣
↪what_makes_you_so_sure_or_unsure_mof_27 )
```

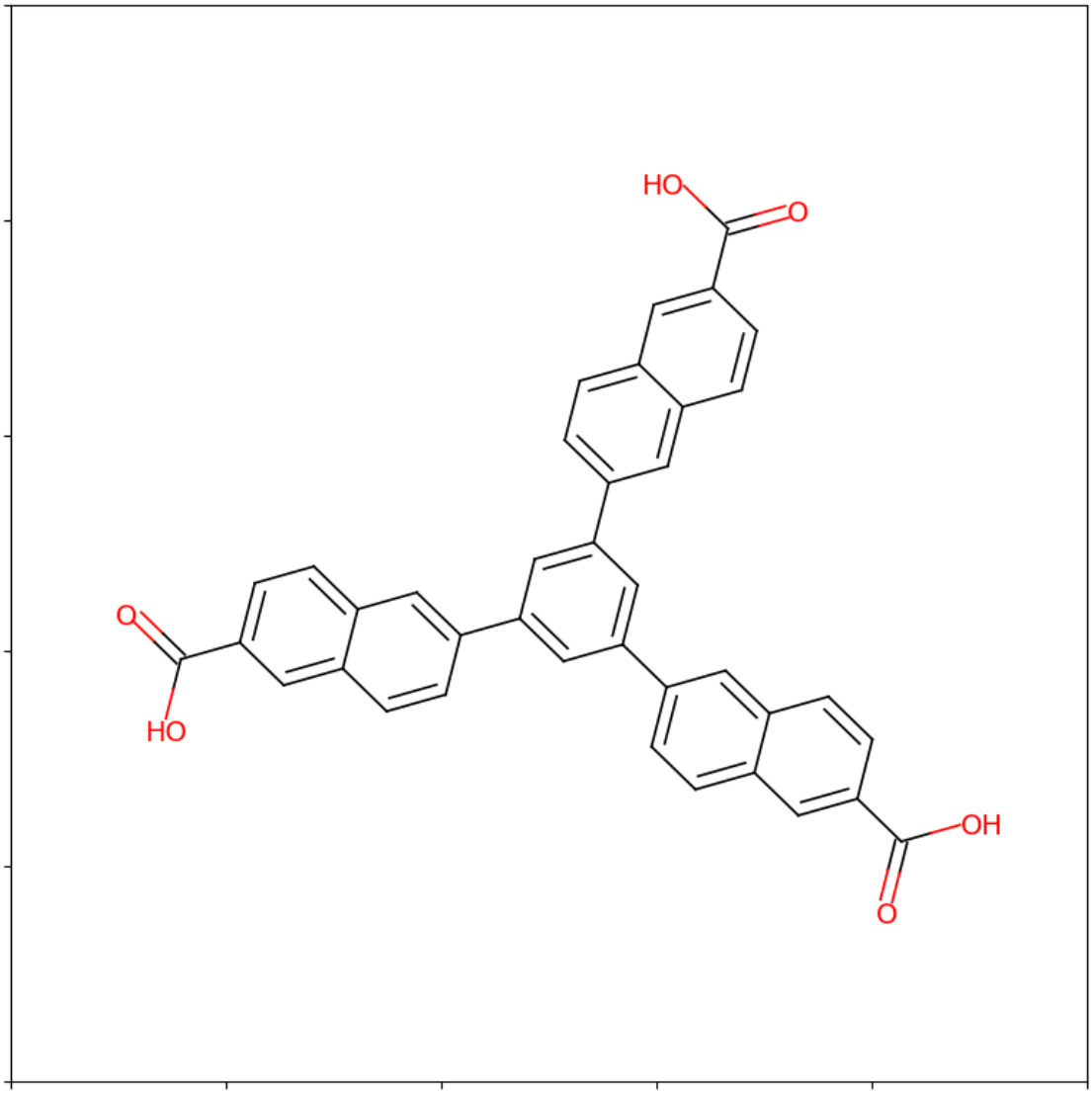
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 48
Solvent1: H2O
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.25
First_Linker_Concentration: 0.75
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: yes
What_Makes_You_So_Sure/Unsure: Quite sure, but not completely, we use to
synthesise Zr-clusters in similar conditions. Overall concentration of the
reagents could need to be tuned to obtain syngle crystals
```

```
# MOF 28
```

Here is the linker:

[120]:
```
Image('./BINSAU_cleansingle_linker0.png')
```

[120]:



The metal center of this MOF is ``Mn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[121]:
```
nutils.viewer('./BINSAU_clean.cif')
```

[122]:
```
temperature_mof_28_Celsius  =  135#@param {type:'number'}
time_mof_28_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_28 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_28 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_28 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_28 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_28 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_28_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_28_mol_per_liter  = 0.150 #@param {type:'number'}
concentration_second_linker_mof_28_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_28 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_28 =  'Not sure about the crystallization␣
↪of  the material as single crystals' #@param {type:'string'}
results['mof_28'] = {}
results['mof_28']['temperature']=temperature_mof_28_Celsius
results['mof_28']['time']=time_mof_28_hours
results['mof_28']['solvent1']=first_solvent_mof_28
```

```
results['mof_28']['solvent2']=second_solvent_mof_28
results['mof_28']['solvent3']=third_solvent_mof_28
results['mof_28']['additive']=additive_mof_28
results['mof_28']['counter']=counter_ion_mof_28
results['mof_28']['metal']=concentration_metal_mof_28_mol_per_liter
results['mof_28']['linker1']=concentration_first_linker_mof_28_mol_per_liter
results['mof_28']['linker2']=concentration_second_linker_mof_28_mol_per_liter
results['mof_28']['surely']=are_you_sure_about_your_selction_mof_28
results['mof_28']['additional']=what_makes_you_so_sure_or_unsure_mof_28
```

[123]:
```
nutils.print_choice(temperature_mof_28_Celsius, time_mof_28_hours,␣
↪first_solvent_mof_28,second_solvent_mof_28,third_solvent_mof_28 ,␣
↪counter_ion_mof_28, concentration_metal_mof_28_mol_per_liter,␣
↪concentration_first_linker_mof_28_mol_per_liter,concentration_second_linker_mof_28_mol_per_
↪, additive_mof_28,are_you_sure_about_your_selction_mof_28,␣
↪what_makes_you_so_sure_or_unsure_mof_28 )
```

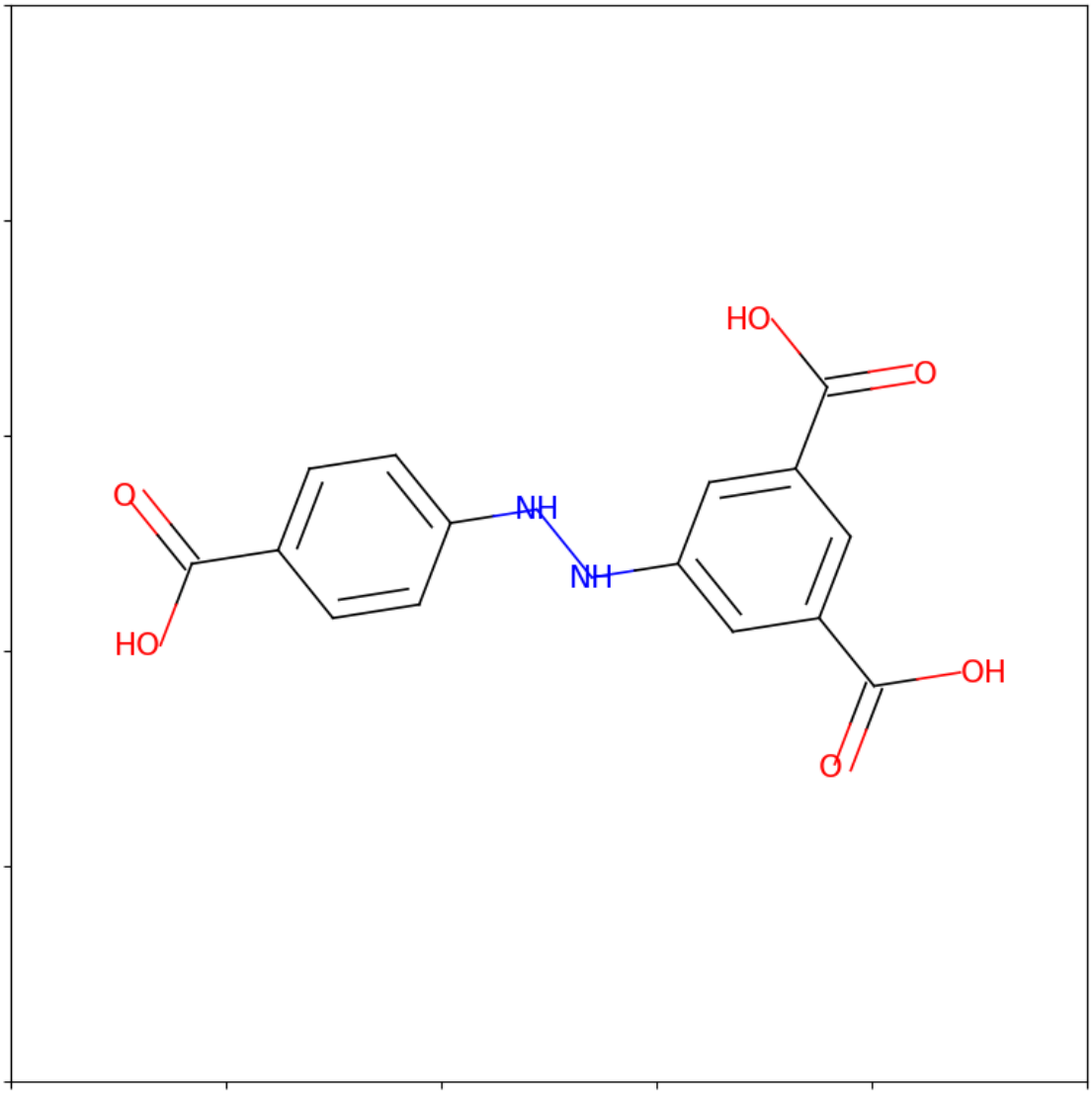
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.075
First_Linker_Concentration: 0.15
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the crystallization of  the
material as single crystals
```

```
# MOF 29
```

Here is the linker:

[124]:
```
Image('./EBUREA_cleansingle_linker0.png')
```

[124]:



The metal center of this MOF is ``Mn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[125]:
```
nutils.viewer('./EBUREA_clean.cif')
```

[126]:
```
temperature_mof_29_Celsius  = 135 #@param {type:'number'}
time_mof_29_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_29 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_29 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_29 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_29 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_29 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_29_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_29_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_second_linker_mof_29_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_29 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_29 =  'Not sure about the crystallization␣
↪of the material as single crystals of enough quality' #@param {type:'string'}
results['mof_29'] = {}
results['mof_29']['temperature']=temperature_mof_29_Celsius
results['mof_29']['time']=time_mof_29_hours
results['mof_29']['solvent1']=first_solvent_mof_29
```

```
results['mof_29']['solvent2']=second_solvent_mof_29
results['mof_29']['solvent3']=third_solvent_mof_29
results['mof_29']['additive']=additive_mof_29
results['mof_29']['counter']=counter_ion_mof_29
results['mof_29']['metal']=concentration_metal_mof_29_mol_per_liter
results['mof_29']['linker1']=concentration_first_linker_mof_29_mol_per_liter
results['mof_29']['linker2']=concentration_second_linker_mof_29_mol_per_liter
results['mof_29']['surely']=are_you_sure_about_your_selction_mof_29
results['mof_29']['additional']=what_makes_you_so_sure_or_unsure_mof_29
```

[127]:
```
nutils.print_choice(temperature_mof_29_Celsius, time_mof_29_hours,␣
↪first_solvent_mof_29,second_solvent_mof_29,third_solvent_mof_29 ,␣
↪counter_ion_mof_29, concentration_metal_mof_29_mol_per_liter,␣
↪concentration_first_linker_mof_29_mol_per_liter,concentration_second_linker_mof_29_mol_per_
↪, additive_mof_29,are_you_sure_about_your_selction_mof_29,␣
↪what_makes_you_so_sure_or_unsure_mof_29 )
```

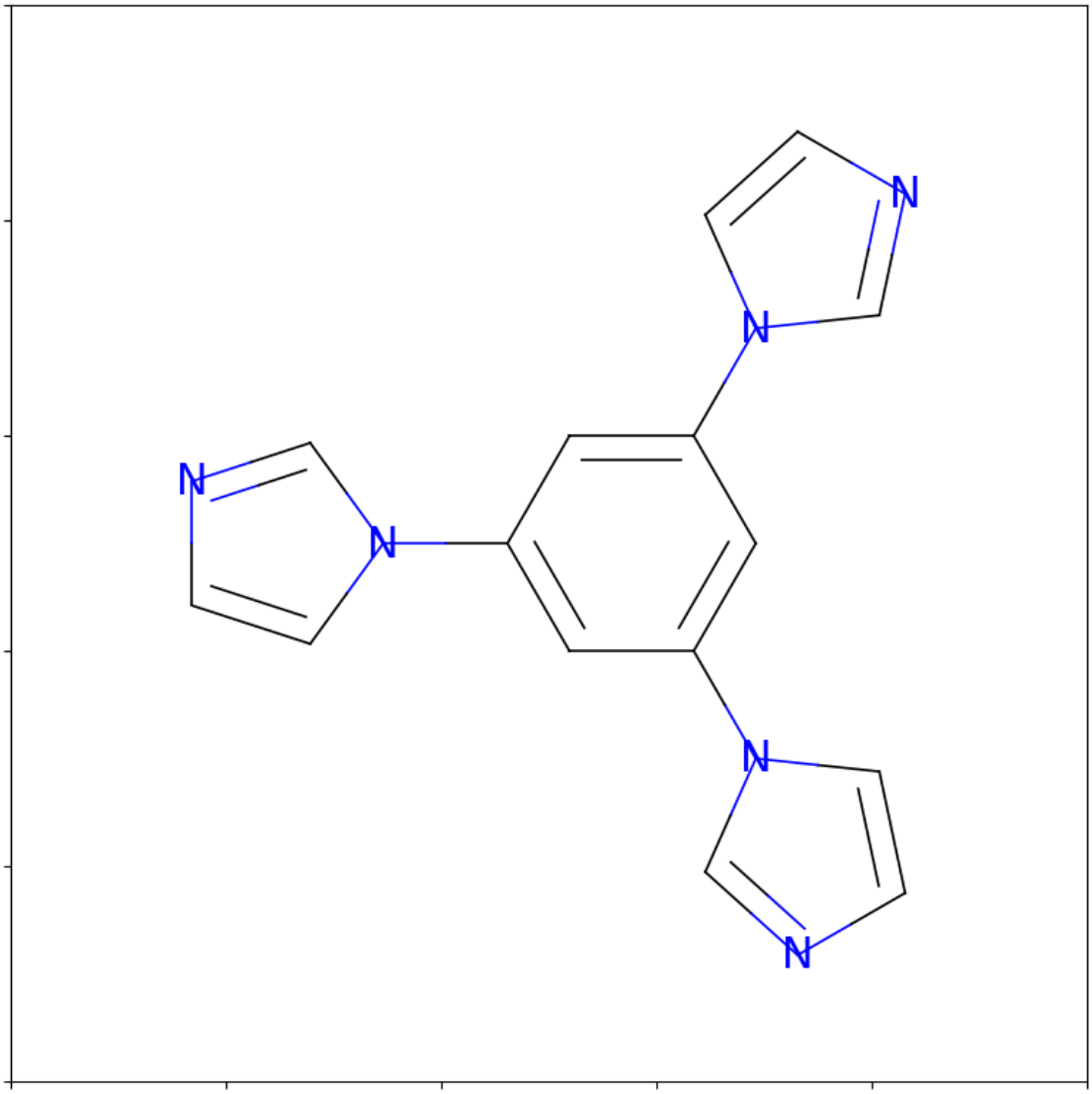
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.075
First_Linker_Concentration: 0.1
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the crystallization of the
material as single crystals of enough quality
```

```
# MOF 30
```

Here is the linker:

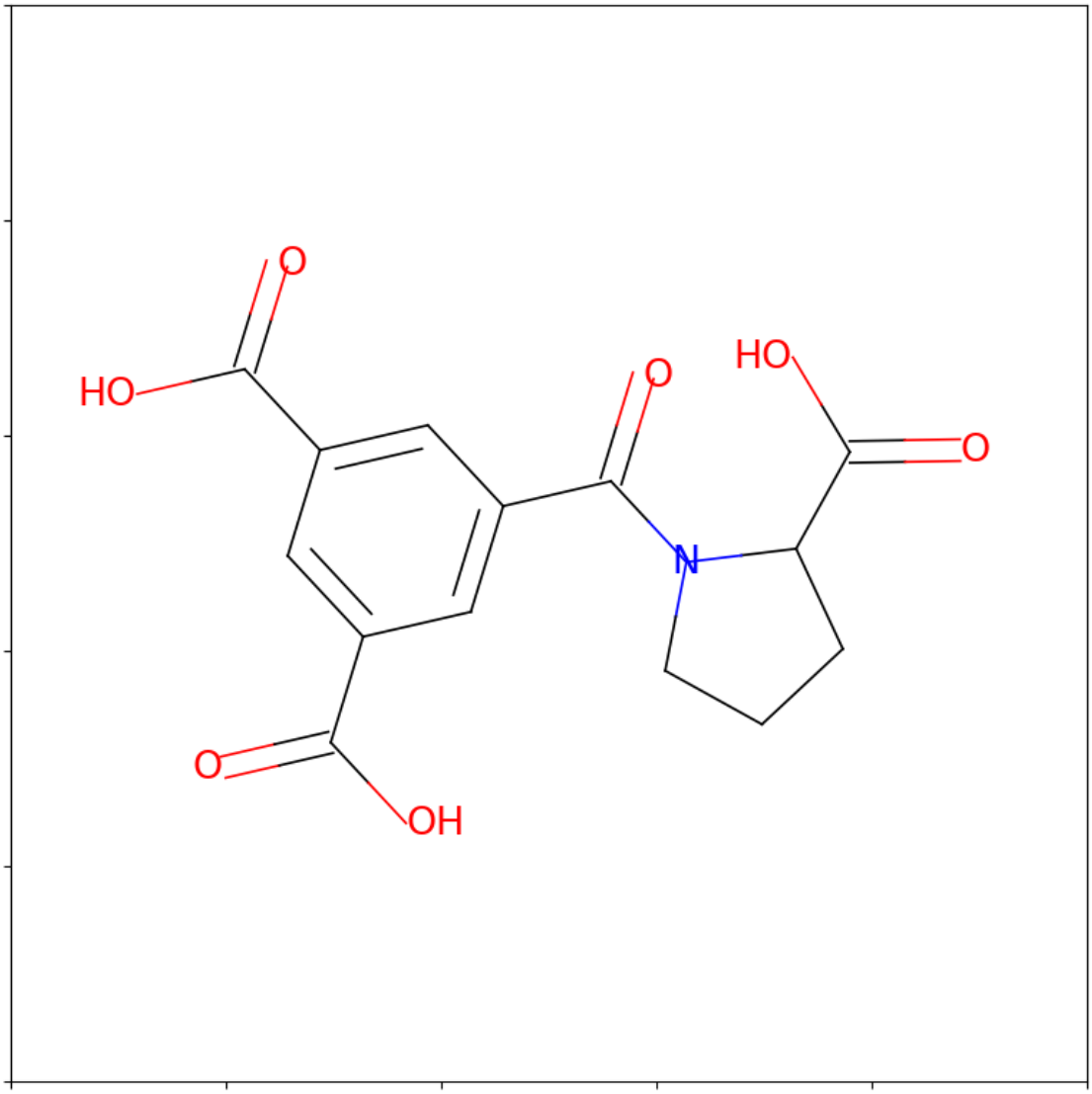
[128]:
```
Image('./LOXBEH_cleansingle_linker0.png')
```

[128]:



[129]:
```
Image('./LOXBEH_cleansingle_linker2.png')
```

[129]:



The metal center of this MOF is ``Cd''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[130]:
```
nutils.viewer('./LOXBEH_clean.cif')
```

[131]:
```
temperature_mof_30_Celsius  = 135 #@param {type:'number'}
time_mof_30_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_30 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_30 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_30 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_30 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_30 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_30_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_30_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_30_mol_per_liter  = 0.1 #@param {type:'number'}
are_you_sure_about_your_selction_mof_30 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_30 =  'Nos used to crystallize MOFs with␣
↪linkers containing different coordinating groups ' #@param {type:'string'}
results['mof_30'] = {}
results['mof_30']['temperature']=temperature_mof_30_Celsius
results['mof_30']['time']=time_mof_30_hours
results['mof_30']['solvent1']=first_solvent_mof_30
```

```
results['mof_30']['solvent2']=second_solvent_mof_30
results['mof_30']['solvent3']=third_solvent_mof_30
results['mof_30']['additive']=additive_mof_30
results['mof_30']['counter']=counter_ion_mof_30
results['mof_30']['metal']=concentration_metal_mof_30_mol_per_liter
results['mof_30']['linker1']=concentration_first_linker_mof_30_mol_per_liter
results['mof_30']['linker2']=concentration_second_linker_mof_30_mol_per_liter
results['mof_30']['surely']=are_you_sure_about_your_selction_mof_30
results['mof_30']['additional']=what_makes_you_so_sure_or_unsure_mof_30
```

[132]:
```
nutils.print_choice(temperature_mof_30_Celsius, time_mof_30_hours,␣
↪first_solvent_mof_30,second_solvent_mof_30,third_solvent_mof_30 ,␣
↪counter_ion_mof_30, concentration_metal_mof_30_mol_per_liter,␣
↪concentration_first_linker_mof_30_mol_per_liter,concentration_second_linker_mof_30_mol_per_
↪, additive_mof_30,are_you_sure_about_your_selction_mof_30,␣
↪what_makes_you_so_sure_or_unsure_mof_30 )
```

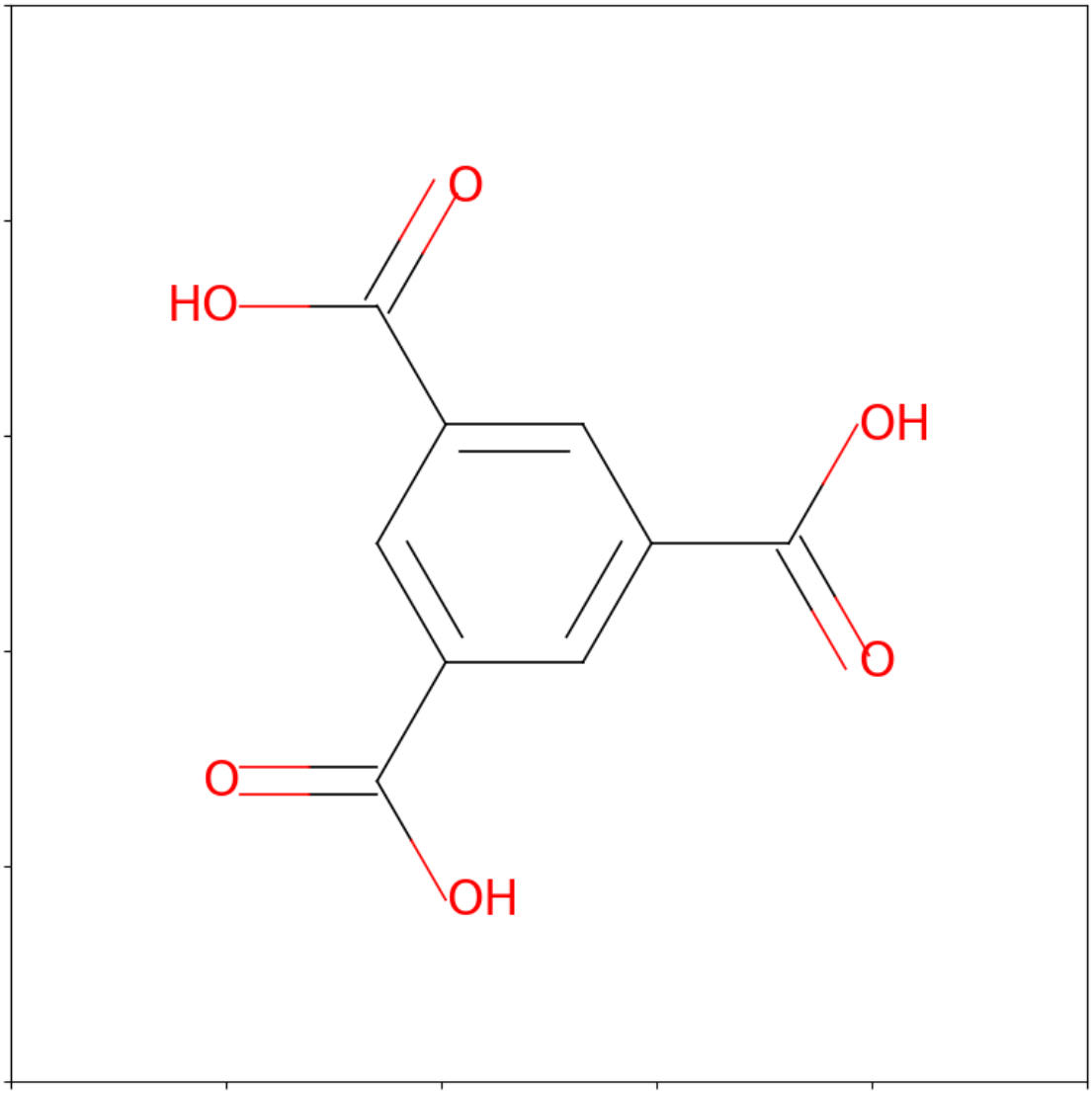
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.075
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.1
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Nos used to crystallize MOFs with linkers
containing different coordinating groups
```

```
# MOF 31
```

Here is the linker:

[133]:
```
Image('./ZUDQEW_cleansingle_linker0.png')
```

[133]:



The metal center of this MOF is ``Cd''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[134]:
```
nutils.viewer('./ZUDQEW_clean.cif')
```

[135]:
```
temperature_mof_31_Celsius  = 135 #@param {type:'number'}
time_mof_31_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_31 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_31 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_31 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_31 = 'base' #@param ['no additive', 'acid', 'base']
counter_ion_mof_31 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_31_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_first_linker_mof_31_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_31_mol_per_liter  = 0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_31 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_31 =  'I am not sure if the DBCO fragment␣
↪of the structure is considered as a ligand or as a base including during the␣
↪reaction' #@param {type:'string'}
results['mof_31'] = {}
results['mof_31']['temperature']=temperature_mof_31_Celsius
results['mof_31']['time']=time_mof_31_hours
```

```
results['mof_31']['solvent1']=first_solvent_mof_31
results['mof_31']['solvent2']=second_solvent_mof_31
results['mof_31']['solvent3']=third_solvent_mof_31
results['mof_31']['additive']=additive_mof_31
results['mof_31']['counter']=counter_ion_mof_31
results['mof_31']['metal']=concentration_metal_mof_31_mol_per_liter
results['mof_31']['linker1']=concentration_first_linker_mof_31_mol_per_liter
results['mof_31']['linker2']=concentration_second_linker_mof_31_mol_per_liter
results['mof_31']['surely']=are_you_sure_about_your_selction_mof_31
results['mof_31']['additional']=what_makes_you_so_sure_or_unsure_mof_31
```

[136]:
```
nutils.print_choice(temperature_mof_31_Celsius, time_mof_31_hours,␣
↪first_solvent_mof_31,second_solvent_mof_31,third_solvent_mof_31 ,␣
↪counter_ion_mof_31, concentration_metal_mof_31_mol_per_liter,␣
↪concentration_first_linker_mof_31_mol_per_liter,concentration_second_linker_mof_31_mol_per_
↪, additive_mof_31,are_you_sure_about_your_selction_mof_31,␣
↪what_makes_you_so_sure_or_unsure_mof_31 )
```

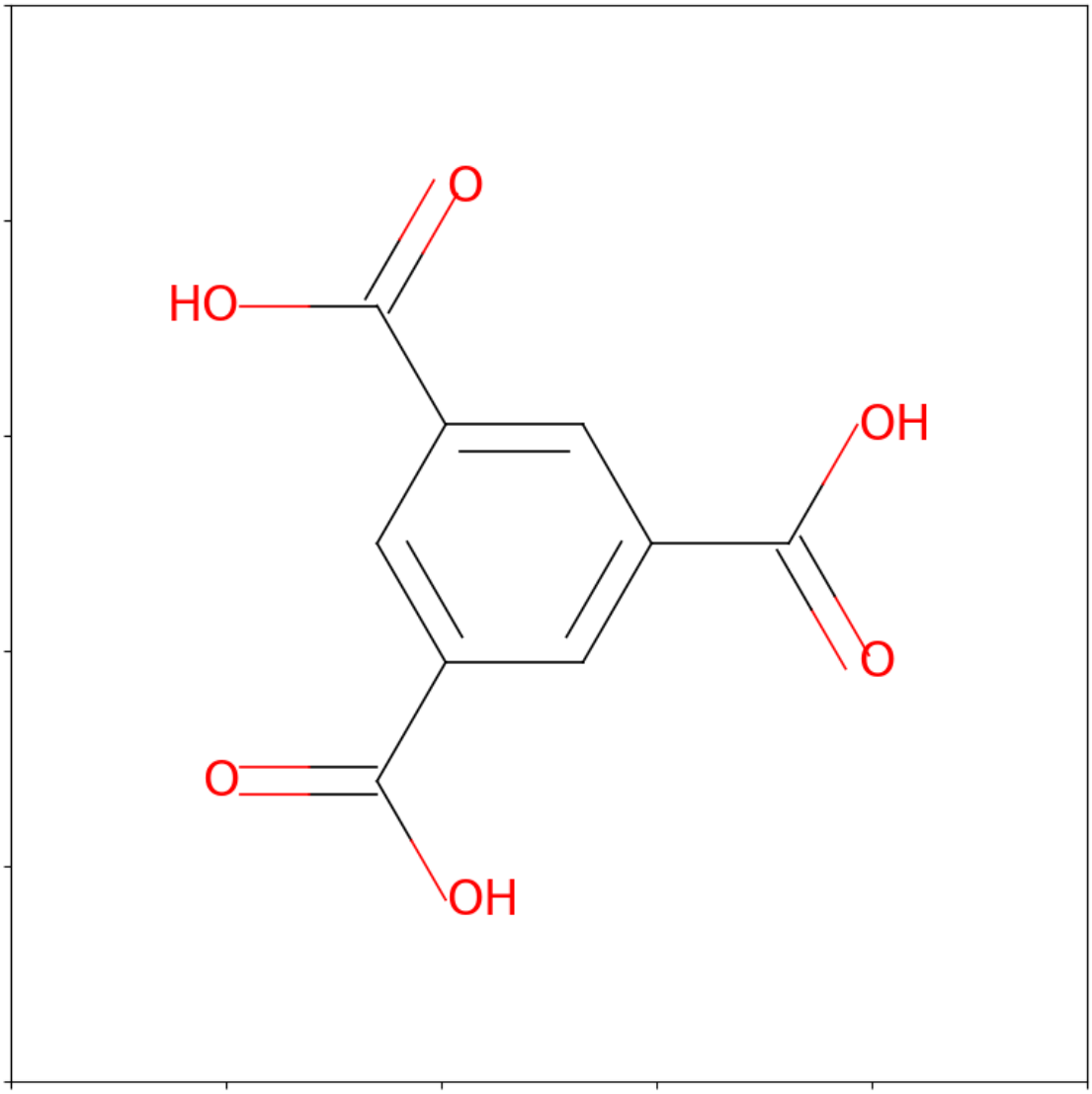
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.1
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0
Additive: base
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: I am not sure if the DBCO fragment of the
structure is considered as a ligand or as a base including during the reaction
```

```
# MOF 32
```

Here is the linker:

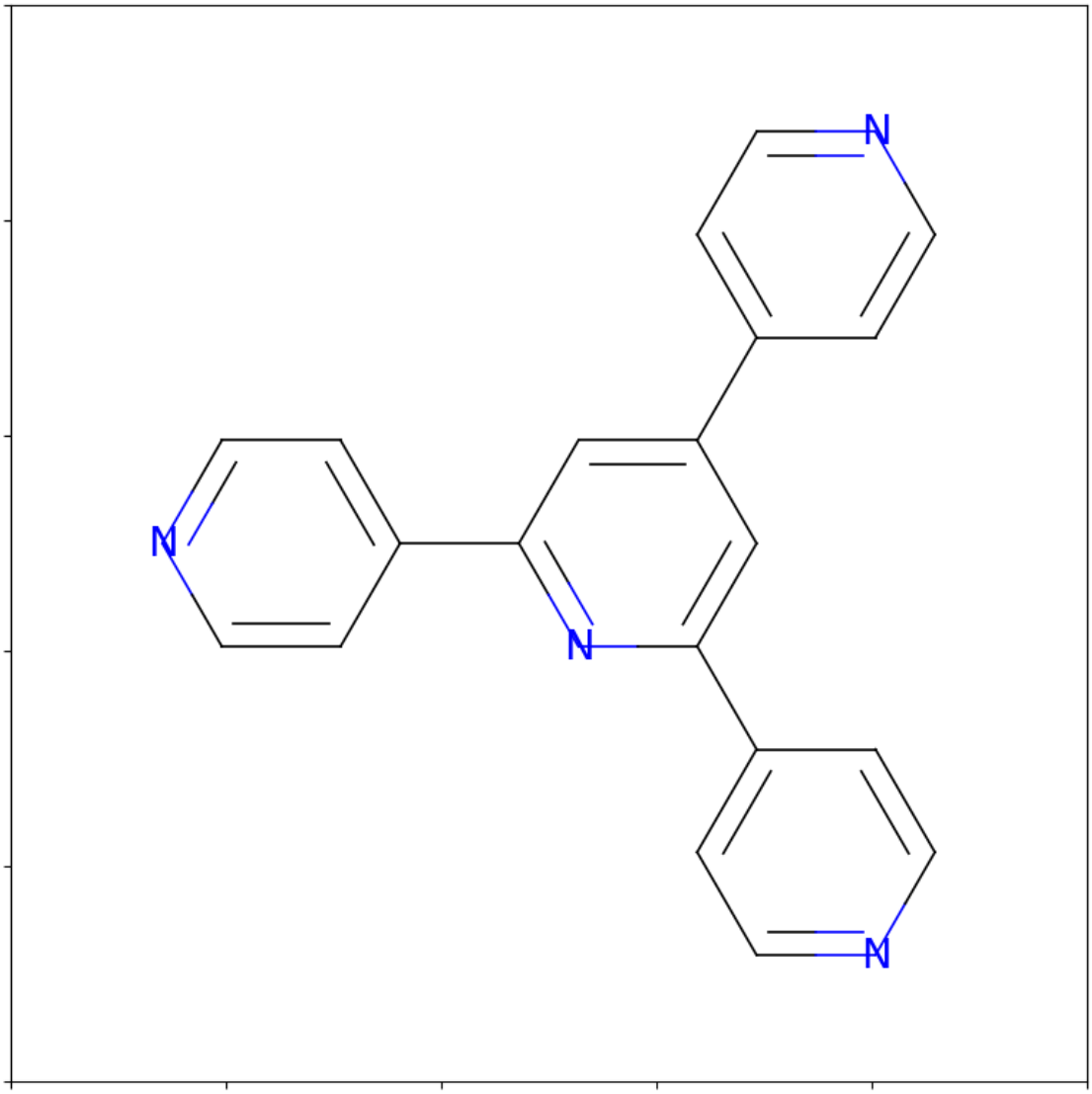
[137]:
```
Image('./TOFLAD_cleansingle_linker0.png')
```

[137]:



[138]:
```
Image('./TOFLAD_cleansingle_linker1.png')
```

[138]:



The metal center of this MOF is ``Cd''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[139]:
```
nutils.viewer('./TOFLAD_clean.cif')
```

[140]:
```
temperature_mof_32_Celsius  = 135 #@param {type:'number'}
time_mof_32_hours  = 48.0 #@param {type:'number'}
```

```
first_solvent_mof_32 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_32 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_32 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_32 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_32 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_32_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_32_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_32_mol_per_liter  = 0.075 #@param {type:
↪'number'}
are_you_sure_about_your_selction_mof_32 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_32 =  'Not used to work with MOFs␣
↪containing different type of linkers ' #@param {type:'string'}
results['mof_32'] = {}
results['mof_32']['temperature']=temperature_mof_32_Celsius
```

```
results['mof_32']['time']=time_mof_32_hours
results['mof_32']['solvent1']=first_solvent_mof_32
results['mof_32']['solvent2']=second_solvent_mof_32
results['mof_32']['solvent3']=third_solvent_mof_32
results['mof_32']['additive']=additive_mof_32
results['mof_32']['counter']=counter_ion_mof_32
results['mof_32']['metal']=concentration_metal_mof_32_mol_per_liter
results['mof_32']['linker1']=concentration_first_linker_mof_32_mol_per_liter
results['mof_32']['linker2']=concentration_second_linker_mof_32_mol_per_liter
results['mof_32']['surely']=are_you_sure_about_your_selction_mof_32
results['mof_32']['additional']=what_makes_you_so_sure_or_unsure_mof_32
```

[141]:
```
nutils.print_choice(temperature_mof_32_Celsius, time_mof_32_hours,␣
↪first_solvent_mof_32,second_solvent_mof_32,third_solvent_mof_32 ,␣
↪counter_ion_mof_32, concentration_metal_mof_32_mol_per_liter,␣
↪concentration_first_linker_mof_32_mol_per_liter,concentration_second_linker_mof_32_mol_per_
↪, additive_mof_32,are_you_sure_about_your_selction_mof_32,␣
↪what_makes_you_so_sure_or_unsure_mof_32 )
```

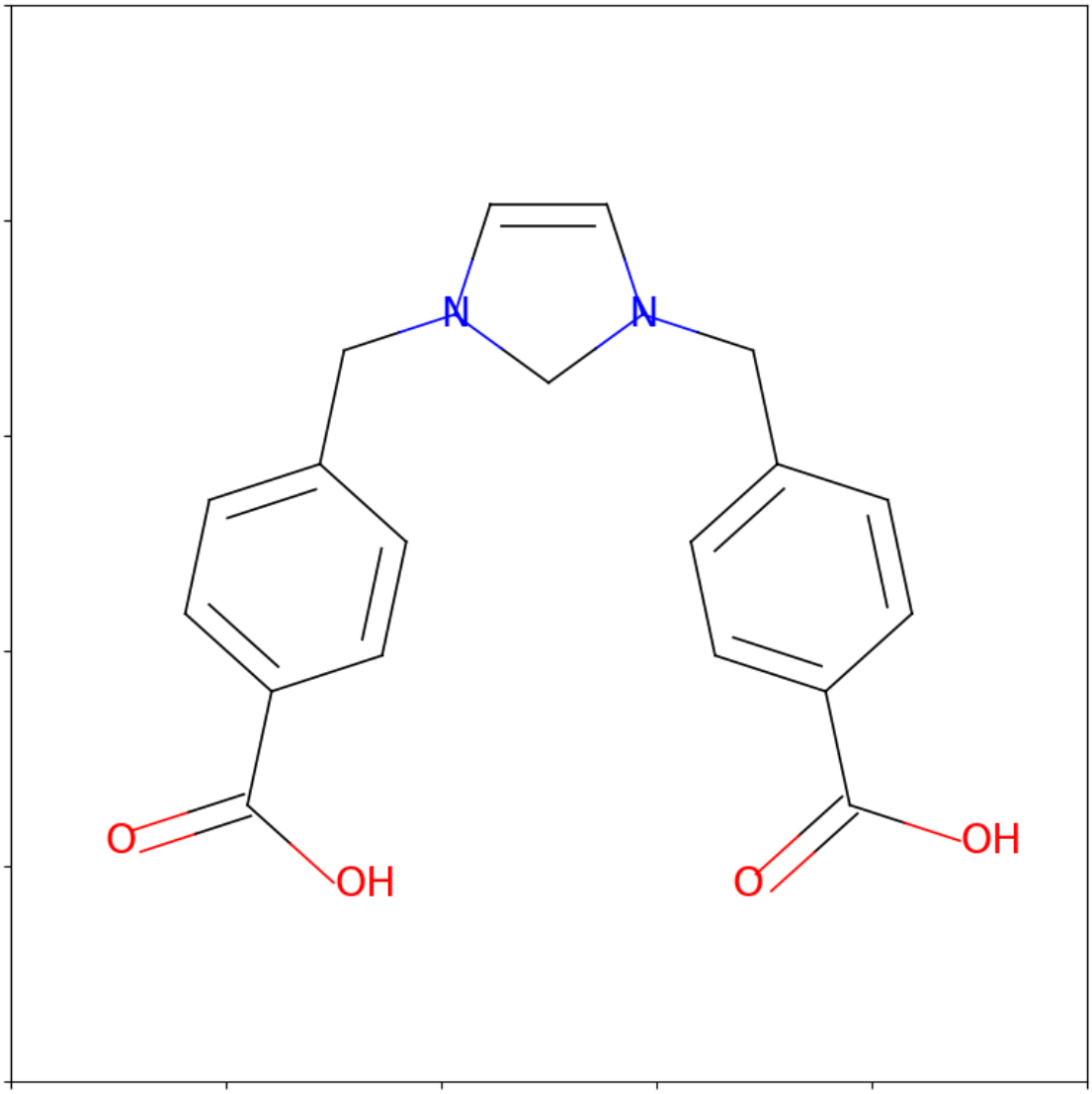
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 48.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.075
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.075
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with MOFs containing different
type of linkers
```

```
# MOF 33
```

Here is the linker:

[142]:
```
Image('./TEJBAN_cleansingle_linker0.png')
```

[142]:



The metal center of this MOF is ``Eu''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[143]:
```
nutils.viewer('./TEJBAN_clean.cif')
```

[144]:
```
temperature_mof_33_Celsius  = 135 #@param {type:'number'}
time_mof_33_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_33 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_33 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_33 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_33 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_33 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_33_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_33_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_33_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_33 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_33 =  'Not sure about the overall␣
↪concentration of the reagents. Maybe a little bit more concentrate system␣
↪could be needed for the MOF crystallization as single crystals ' #@param␣
↪{type:'string'}
results['mof_33'] = {}
results['mof_33']['temperature']=temperature_mof_33_Celsius
```

```
results['mof_33']['time']=time_mof_33_hours
results['mof_33']['solvent1']=first_solvent_mof_33
results['mof_33']['solvent2']=second_solvent_mof_33
results['mof_33']['solvent3']=third_solvent_mof_33
results['mof_33']['additive']=additive_mof_33
results['mof_33']['counter']=counter_ion_mof_33
results['mof_33']['metal']=concentration_metal_mof_33_mol_per_liter
results['mof_33']['linker1']=concentration_first_linker_mof_33_mol_per_liter
results['mof_33']['linker2']=concentration_second_linker_mof_33_mol_per_liter
results['mof_33']['surely']=are_you_sure_about_your_selction_mof_33
results['mof_33']['additional']=what_makes_you_so_sure_or_unsure_mof_33
```

[145]:
```
nutils.print_choice(temperature_mof_33_Celsius, time_mof_33_hours,␣
↪first_solvent_mof_33,second_solvent_mof_33,third_solvent_mof_33 ,␣
↪counter_ion_mof_33, concentration_metal_mof_33_mol_per_liter,␣
↪concentration_first_linker_mof_33_mol_per_liter,concentration_second_linker_mof_33_mol_per_
↪, additive_mof_33,are_you_sure_about_your_selction_mof_33,␣
↪what_makes_you_so_sure_or_unsure_mof_33 )
```

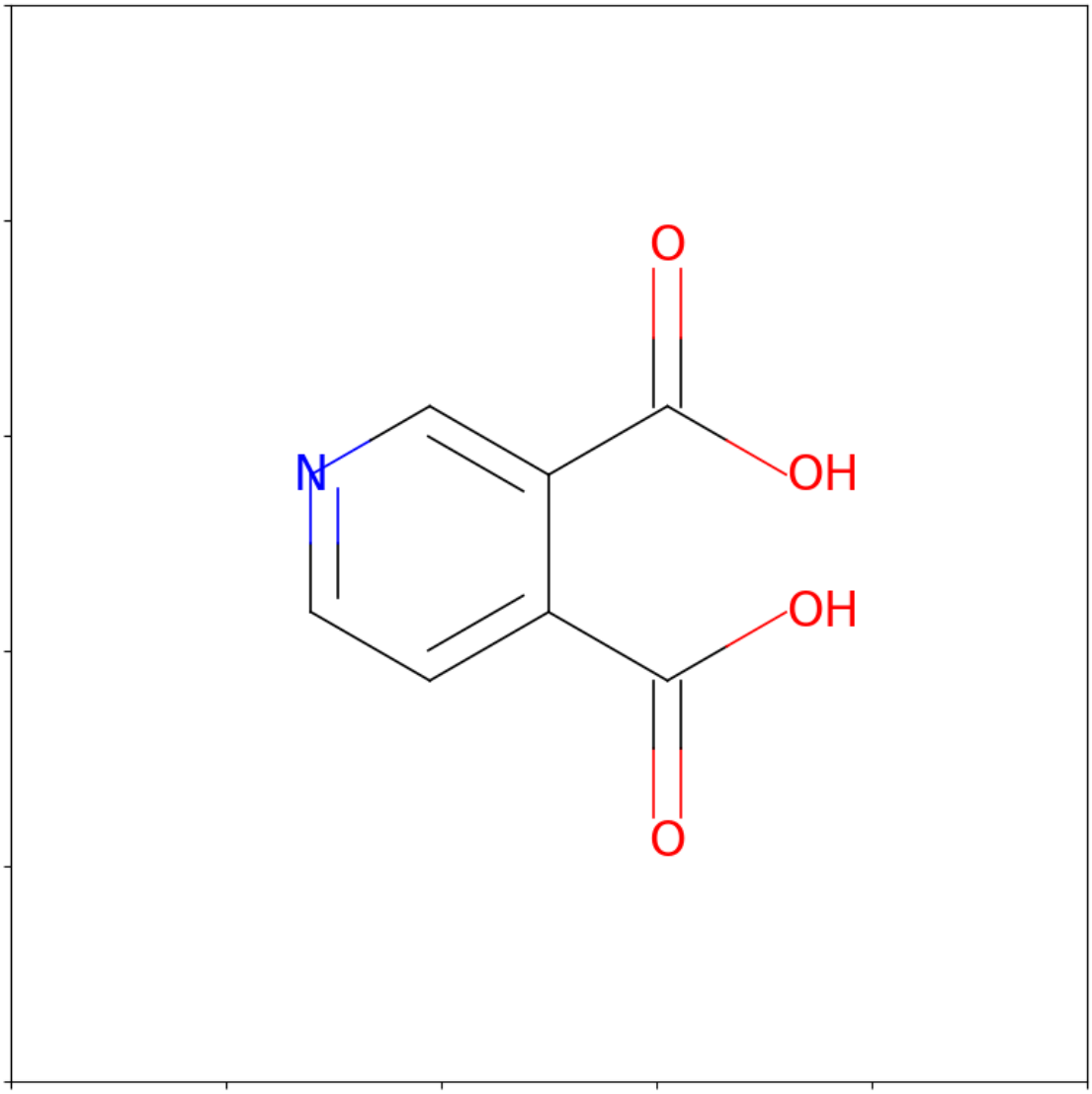
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.075
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the overall concentration of the
reagents. Maybe a little bit more concentrate system could be needed for the MOF
crystallization as single crystals
```

```
# MOF 34
```

Here is the linker:

[146]:
```
Image('./DEPXAY_cleansingle_linker0.png')
```

[146]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[147]:
```
nutils.viewer('./DEPXAY_clean.cif')
```

[148]:
```
temperature_mof_34_Celsius  = 120.0 #@param {type:'number'}
time_mof_34_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_34 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_34 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_34 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_34 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_34 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_34_mol_per_liter  = 0.15 #@param {type:'number'}
concentration_first_linker_mof_34_mol_per_liter  = 0.15 #@param {type:'number'}
concentration_second_linker_mof_34_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_34 = 'yes' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_34 =  'quite sure about the␣
↪crystallization of the MOF. Nos so sure of the quallity of the syngle␣
↪crystals' #@param {type:'string'}
results['mof_34'] = {}
results['mof_34']['temperature']=temperature_mof_34_Celsius
results['mof_34']['time']=time_mof_34_hours
```

```
results['mof_34']['solvent1']=first_solvent_mof_34
results['mof_34']['solvent2']=second_solvent_mof_34
results['mof_34']['solvent3']=third_solvent_mof_34
results['mof_34']['additive']=additive_mof_34
results['mof_34']['counter']=counter_ion_mof_34
results['mof_34']['metal']=concentration_metal_mof_34_mol_per_liter
results['mof_34']['linker1']=concentration_first_linker_mof_34_mol_per_liter
results['mof_34']['linker2']=concentration_second_linker_mof_34_mol_per_liter
results['mof_34']['surely']=are_you_sure_about_your_selction_mof_34
results['mof_34']['additional']=what_makes_you_so_sure_or_unsure_mof_34
```

[149]:
```
nutils.print_choice(temperature_mof_34_Celsius, time_mof_34_hours,␣
↪first_solvent_mof_34,second_solvent_mof_34,third_solvent_mof_34 ,␣
↪counter_ion_mof_34, concentration_metal_mof_34_mol_per_liter,␣
↪concentration_first_linker_mof_34_mol_per_liter,concentration_second_linker_mof_34_mol_per_
↪, additive_mof_34,are_you_sure_about_your_selction_mof_34,␣
↪what_makes_you_so_sure_or_unsure_mof_34 )
```

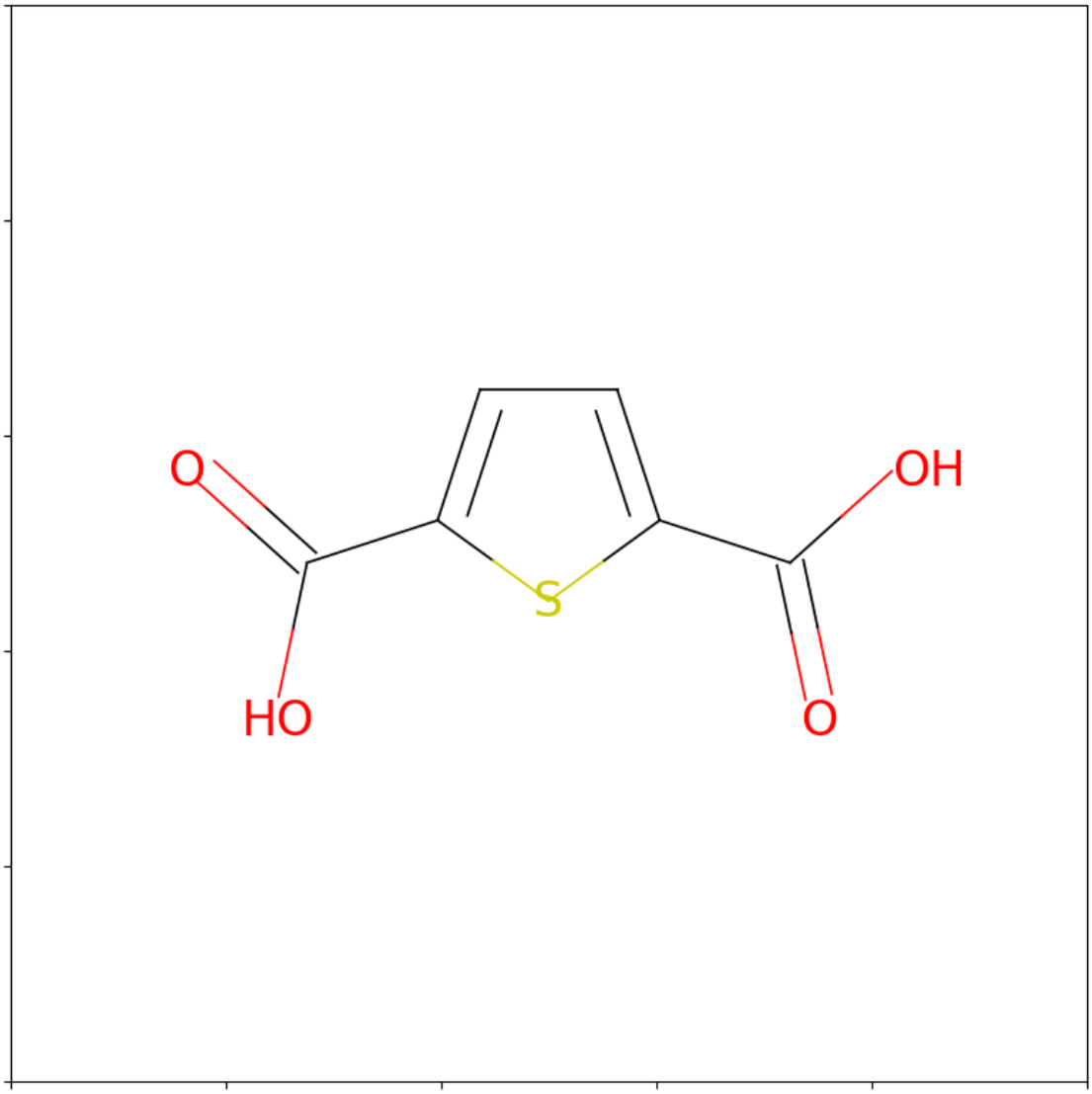
```
Thanks for your input
Your selection was:
Temperature: 120.0
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.15
First_Linker_Concentration: 0.15
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: yes
What_Makes_You_So_Sure/Unsure: quite sure about the crystallization of the MOF.
Nos so sure of the quallity of the syngle crystals
```

```
# MOF 35
```

Here is the linker:

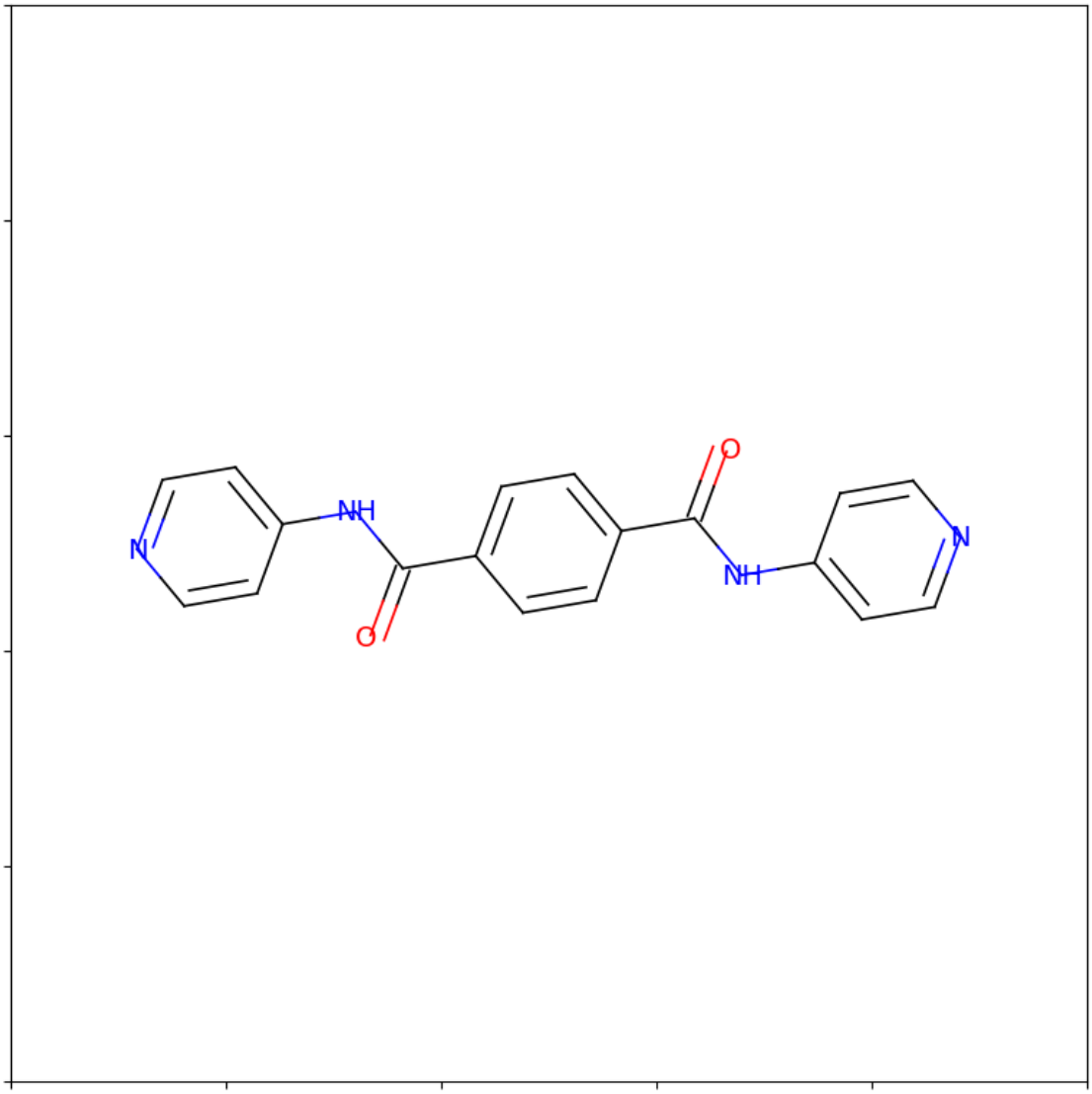
[150]:
```
Image('./TETZID_cleansingle_linker0.png')
```

[150]:



[151]:
```
Image('./TETZID_cleansingle_linker2.png')
```

[151]:



The metal center of this MOF is ``Cd''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[152]:
```
nutils.viewer('./TETZID_clean.cif')
```

[153]:
```
temperature_mof_35_Celsius  = 120.0 #@param {type:'number'}
time_mof_35_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_35 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_35 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_35 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_35 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_35 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_35_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_35_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_35_mol_per_liter  = 0.1 #@param {type:'number'}
are_you_sure_about_your_selction_mof_35 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_35 =  'Not used to work with MOFs build up␣
↪from different linkers' #@param {type:'string'}
results['mof_35'] = {}
results['mof_35']['temperature']=temperature_mof_35_Celsius
results['mof_35']['time']=time_mof_35_hours
results['mof_35']['solvent1']=first_solvent_mof_35
```

```
results['mof_35']['solvent2']=second_solvent_mof_35
results['mof_35']['solvent3']=third_solvent_mof_35
results['mof_35']['additive']=additive_mof_35
results['mof_35']['counter']=counter_ion_mof_35
results['mof_35']['metal']=concentration_metal_mof_35_mol_per_liter
results['mof_35']['linker1']=concentration_first_linker_mof_35_mol_per_liter
results['mof_35']['linker2']=concentration_second_linker_mof_35_mol_per_liter
results['mof_35']['surely']=are_you_sure_about_your_selction_mof_35
results['mof_35']['additional']=what_makes_you_so_sure_or_unsure_mof_35
```

[154]:
```
nutils.print_choice(temperature_mof_35_Celsius, time_mof_35_hours,␣
↪first_solvent_mof_35,second_solvent_mof_35,third_solvent_mof_35 ,␣
↪counter_ion_mof_35, concentration_metal_mof_35_mol_per_liter,␣
↪concentration_first_linker_mof_35_mol_per_liter,concentration_second_linker_mof_35_mol_per_
↪, additive_mof_35,are_you_sure_about_your_selction_mof_35,␣
↪what_makes_you_so_sure_or_unsure_mof_35 )
```

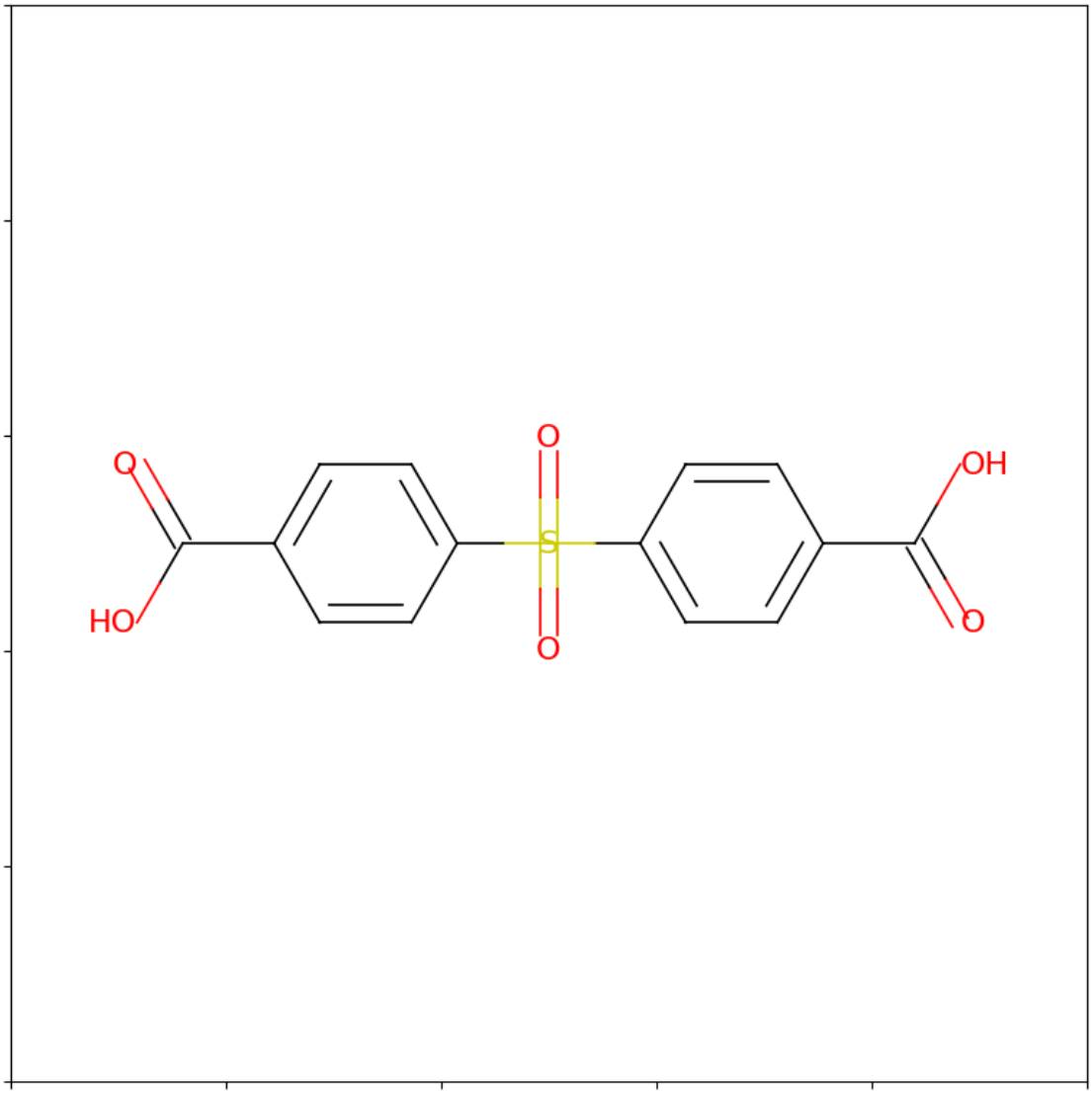
```
Thanks for your input
Your selection was:
Temperature: 120.0
Time: 72.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.05
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.1
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with MOFs build up from
different linkers
```

```
# MOF 36
```

Here is the linker:

[155]:
```
Image('./VIZQEC_cleansingle_linker0.png')
```

[155]:



The metal center of this MOF is ``Co''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[156]:
```
nutils.viewer('./VIZQEC_clean.cif')
```

[157]:
```
temperature_mof_36_Celsius  = 135 #@param {type:'number'}
time_mof_36_hours  =  72#@param {type:'number'}
```

```
first_solvent_mof_36 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_36 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_36 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_36 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_36 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_36_mol_per_liter  =  0.1#@param {type:'number'}
concentration_first_linker_mof_36_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_36_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_36 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_36 =  'Not sure about the crystallization␣
↪of the MOF as syngle crystals' #@param {type:'string'}
results['mof_36'] = {}
results['mof_36']['temperature']=temperature_mof_36_Celsius
results['mof_36']['time']=time_mof_36_hours
results['mof_36']['solvent1']=first_solvent_mof_36
```

```
results['mof_36']['solvent2']=second_solvent_mof_36
results['mof_36']['solvent3']=third_solvent_mof_36
results['mof_36']['additive']=additive_mof_36
results['mof_36']['counter']=counter_ion_mof_36
results['mof_36']['metal']=concentration_metal_mof_36_mol_per_liter
results['mof_36']['linker1']=concentration_first_linker_mof_36_mol_per_liter
results['mof_36']['linker2']=concentration_second_linker_mof_36_mol_per_liter
results['mof_36']['surely']=are_you_sure_about_your_selction_mof_36
results['mof_36']['additional']=what_makes_you_so_sure_or_unsure_mof_36
```

[158]:
```
nutils.print_choice(temperature_mof_36_Celsius, time_mof_36_hours,␣
↪first_solvent_mof_36,second_solvent_mof_36,third_solvent_mof_36 ,␣
↪counter_ion_mof_36, concentration_metal_mof_36_mol_per_liter,␣
↪concentration_first_linker_mof_36_mol_per_liter,concentration_second_linker_mof_36_mol_per_
↪, additive_mof_36,are_you_sure_about_your_selction_mof_36,␣
↪what_makes_you_so_sure_or_unsure_mof_36 )
```

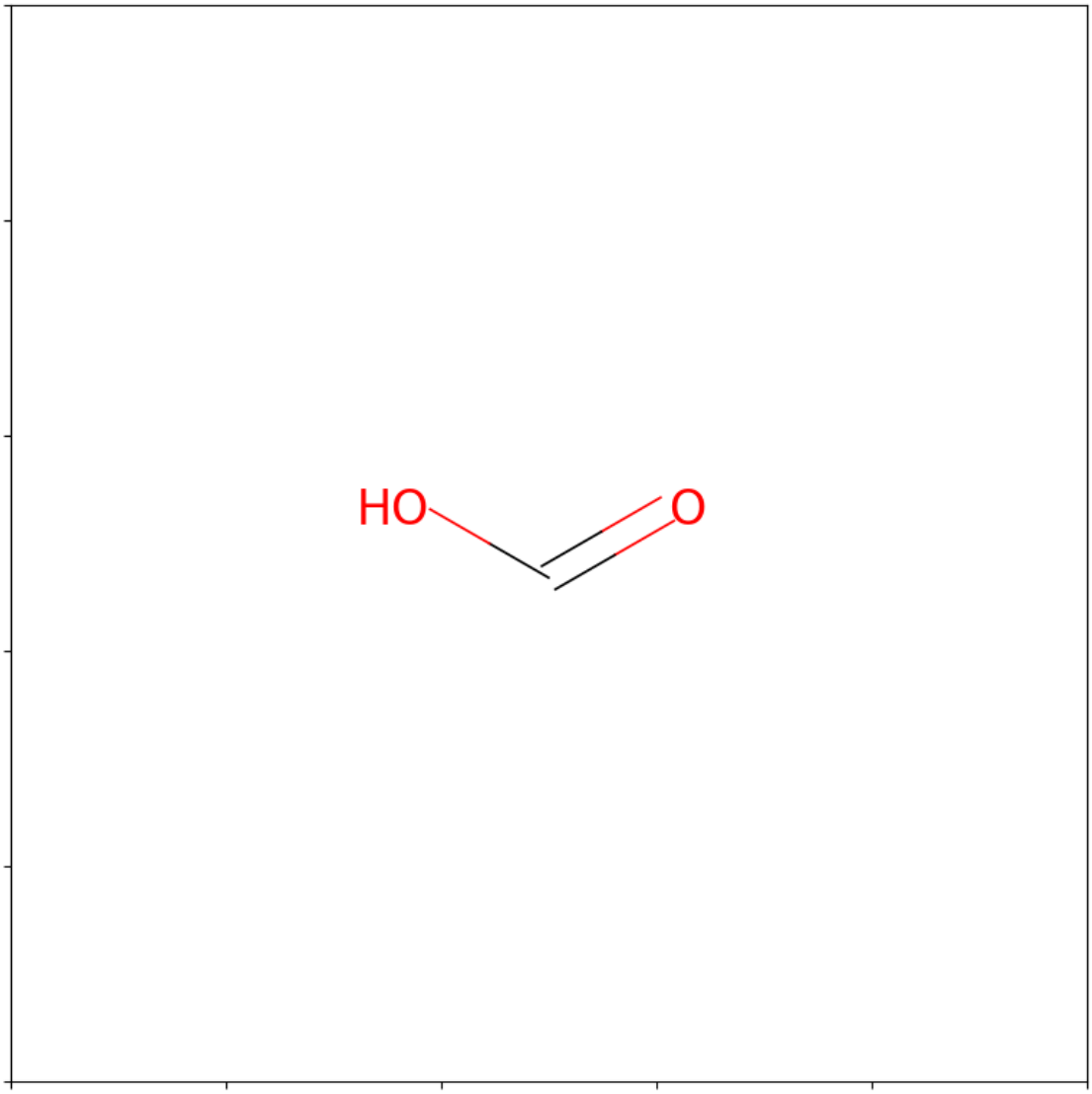
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-diethylformamide (DEF)
Solvent2: ethanol
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.1
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the crystallization of the MOF as
syngle crystals
```

```
# MOF 37
```

Here is the linker:

[159]:
```
Image('./ATIBOU02_cleansingle_linker0.png')
```

[159]:



The metal center of this MOF is ``Mn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[160]:
```
nutils.viewer('./ATIBOU02_clean.cif')
```

[161]:
```
temperature_mof_37_Celsius  = 135 #@param {type:'number'}
time_mof_37_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_37 = 'H2O' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
second_solvent_mof_37 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_37 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_37 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_37 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_37_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_first_linker_mof_37_mol_per_liter  =  0.05#@param {type:'number'}
concentration_second_linker_mof_37_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_37 = 'yes' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_37 =  'Quite sure about the␣
↪crystallization of the material, but not if it will crystallize as single␣
↪crystals' #@param {type:'string'}
results['mof_37'] = {}
results['mof_37']['temperature']=temperature_mof_37_Celsius
results['mof_37']['time']=time_mof_37_hours
```

```
results['mof_37']['solvent1']=first_solvent_mof_37
results['mof_37']['solvent2']=second_solvent_mof_37
results['mof_37']['solvent3']=third_solvent_mof_37
results['mof_37']['additive']=additive_mof_37
results['mof_37']['counter']=counter_ion_mof_37
results['mof_37']['metal']=concentration_metal_mof_37_mol_per_liter
results['mof_37']['linker1']=concentration_first_linker_mof_37_mol_per_liter
results['mof_37']['linker2']=concentration_second_linker_mof_37_mol_per_liter
results['mof_37']['surely']=are_you_sure_about_your_selction_mof_37
results['mof_37']['additional']=what_makes_you_so_sure_or_unsure_mof_37
```

[162]:
```
nutils.print_choice(temperature_mof_37_Celsius, time_mof_37_hours,␣
↪first_solvent_mof_37,second_solvent_mof_37,third_solvent_mof_37 ,␣
↪counter_ion_mof_37, concentration_metal_mof_37_mol_per_liter,␣
↪concentration_first_linker_mof_37_mol_per_liter,concentration_second_linker_mof_37_mol_per_
↪, additive_mof_37,are_you_sure_about_your_selction_mof_37,␣
↪what_makes_you_so_sure_or_unsure_mof_37 )
```

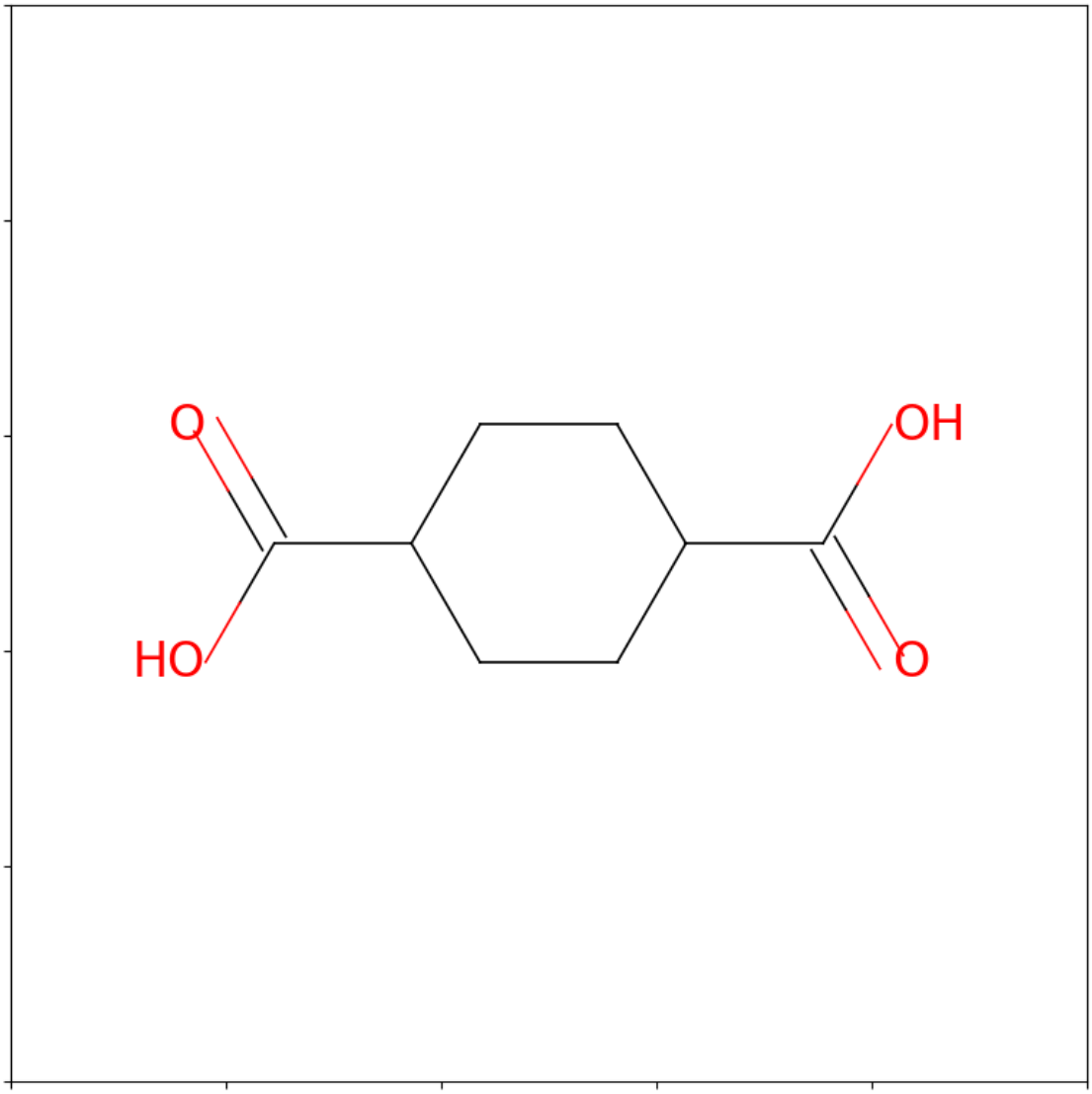
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: H2O
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.1
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: yes
What_Makes_You_So_Sure/Unsure: Quite sure about the crystallization of the
material, but not if it will crystallize as single crystals
```

```
# MOF 38
```

Here is the linker:

[163]:
```
Image('./XAXQEU_SLsingle_linker1.png')
```

[163]:



The metal center of this MOF is ``In''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[164]:
```
nutils.viewer('./XAXQEU_SL.cif')
```

[165]:
```
temperature_mof_38_Celsius  = 135 #@param {type:'number'}
time_mof_38_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_38 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_38 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_38 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_38 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_38 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_38_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_38_mol_per_liter  = 0.025 #@param {type:'number'}
concentration_second_linker_mof_38_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_38 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_38 =  'Not sure about the concentration of␣
↪the system. Maybe the suggested metal and linker mol/L is under the thresold␣
↪of the crystallization of the material' #@param {type:'string'}
results['mof_38'] = {}
results['mof_38']['temperature']=temperature_mof_38_Celsius
results['mof_38']['time']=time_mof_38_hours
```

```
results['mof_38']['solvent1']=first_solvent_mof_38
results['mof_38']['solvent2']=second_solvent_mof_38
results['mof_38']['solvent3']=third_solvent_mof_38
results['mof_38']['additive']=additive_mof_38
results['mof_38']['counter']=counter_ion_mof_38
results['mof_38']['metal']=concentration_metal_mof_38_mol_per_liter
results['mof_38']['linker1']=concentration_first_linker_mof_38_mol_per_liter
results['mof_38']['linker2']=concentration_second_linker_mof_38_mol_per_liter
results['mof_38']['surely']=are_you_sure_about_your_selction_mof_38
results['mof_38']['additional']=what_makes_you_so_sure_or_unsure_mof_38
```

[166]:
```
nutils.print_choice(temperature_mof_38_Celsius, time_mof_38_hours,␣
↪first_solvent_mof_38,second_solvent_mof_38,third_solvent_mof_38 ,␣
↪counter_ion_mof_38, concentration_metal_mof_38_mol_per_liter,␣
↪concentration_first_linker_mof_38_mol_per_liter,concentration_second_linker_mof_38_mol_per_
↪, additive_mof_38,are_you_sure_about_your_selction_mof_38,␣
↪what_makes_you_so_sure_or_unsure_mof_38 )
```

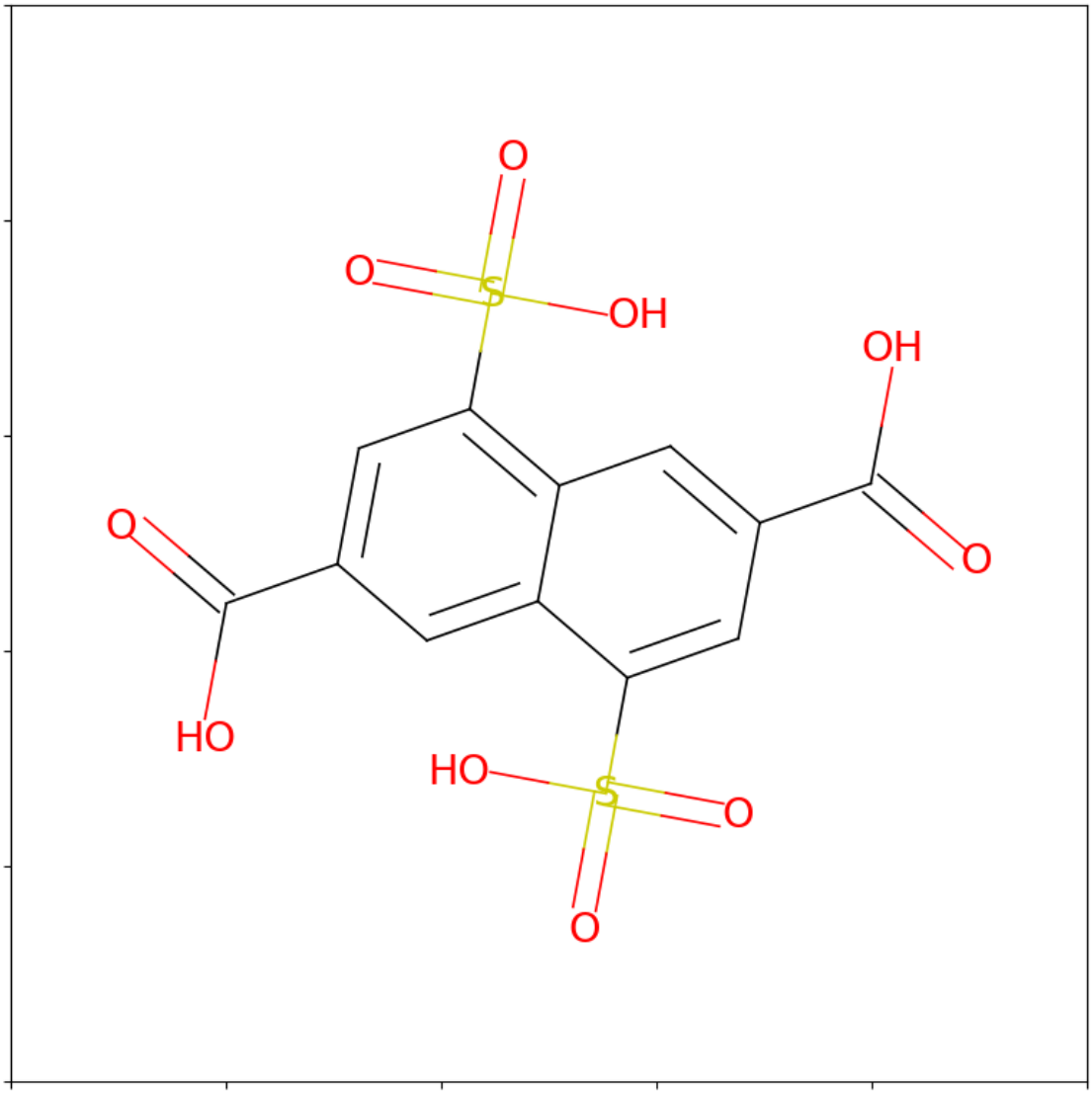
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.025
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the concentration of the system.
Maybe the suggested metal and linker mol/L is under the thresold of the
crystallization of the material
```

```
# MOF 39
```

Here is the linker:

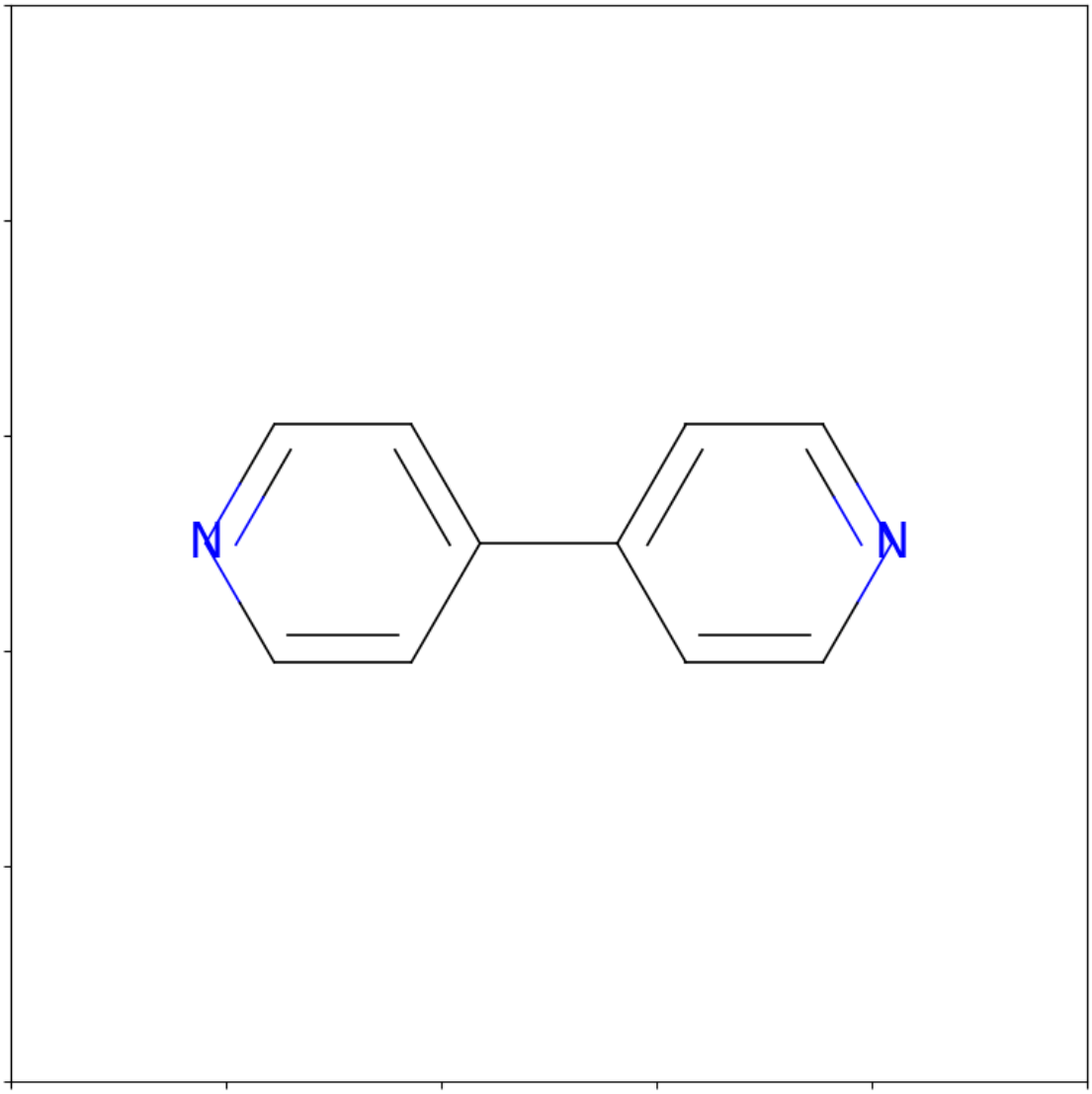
[167]:
```
Image('./MUVLUM_cleansingle_linker0.png')
```

[167]:



[168]:
```
Image('./MUVLUM_cleansingle_linker4.png')
```

[168]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[169]:
```
nutils.viewer('./MUVLUM_clean.cif')
```

[170]:
```
temperature_mof_39_Celsius  = 120 #@param {type:'number'}
time_mof_39_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_39 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_39 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_39 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_39 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_39 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_39_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_39_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_39_mol_per_liter  = 0.075 #@param {type:
↪'number'}
are_you_sure_about_your_selction_mof_39 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_39 =  'Not used to work with mixed ligand␣
↪MOFs' #@param {type:'string'}
results['mof_39'] = {}
results['mof_39']['temperature']=temperature_mof_39_Celsius
```

```
results['mof_39']['time']=time_mof_39_hours
results['mof_39']['solvent1']=first_solvent_mof_39
results['mof_39']['solvent2']=second_solvent_mof_39
results['mof_39']['solvent3']=third_solvent_mof_39
results['mof_39']['additive']=additive_mof_39
results['mof_39']['counter']=counter_ion_mof_39
results['mof_39']['metal']=concentration_metal_mof_39_mol_per_liter
results['mof_39']['linker1']=concentration_first_linker_mof_39_mol_per_liter
results['mof_39']['linker2']=concentration_second_linker_mof_39_mol_per_liter
results['mof_39']['surely']=are_you_sure_about_your_selction_mof_39
results['mof_39']['additional']=what_makes_you_so_sure_or_unsure_mof_39
```

[171]:
```
nutils.print_choice(temperature_mof_39_Celsius, time_mof_39_hours,␣
↪first_solvent_mof_39,second_solvent_mof_39,third_solvent_mof_39 ,␣
↪counter_ion_mof_39, concentration_metal_mof_39_mol_per_liter,␣
↪concentration_first_linker_mof_39_mol_per_liter,concentration_second_linker_mof_39_mol_per_
↪, additive_mof_39,are_you_sure_about_your_selction_mof_39,␣
↪what_makes_you_so_sure_or_unsure_mof_39 )
```

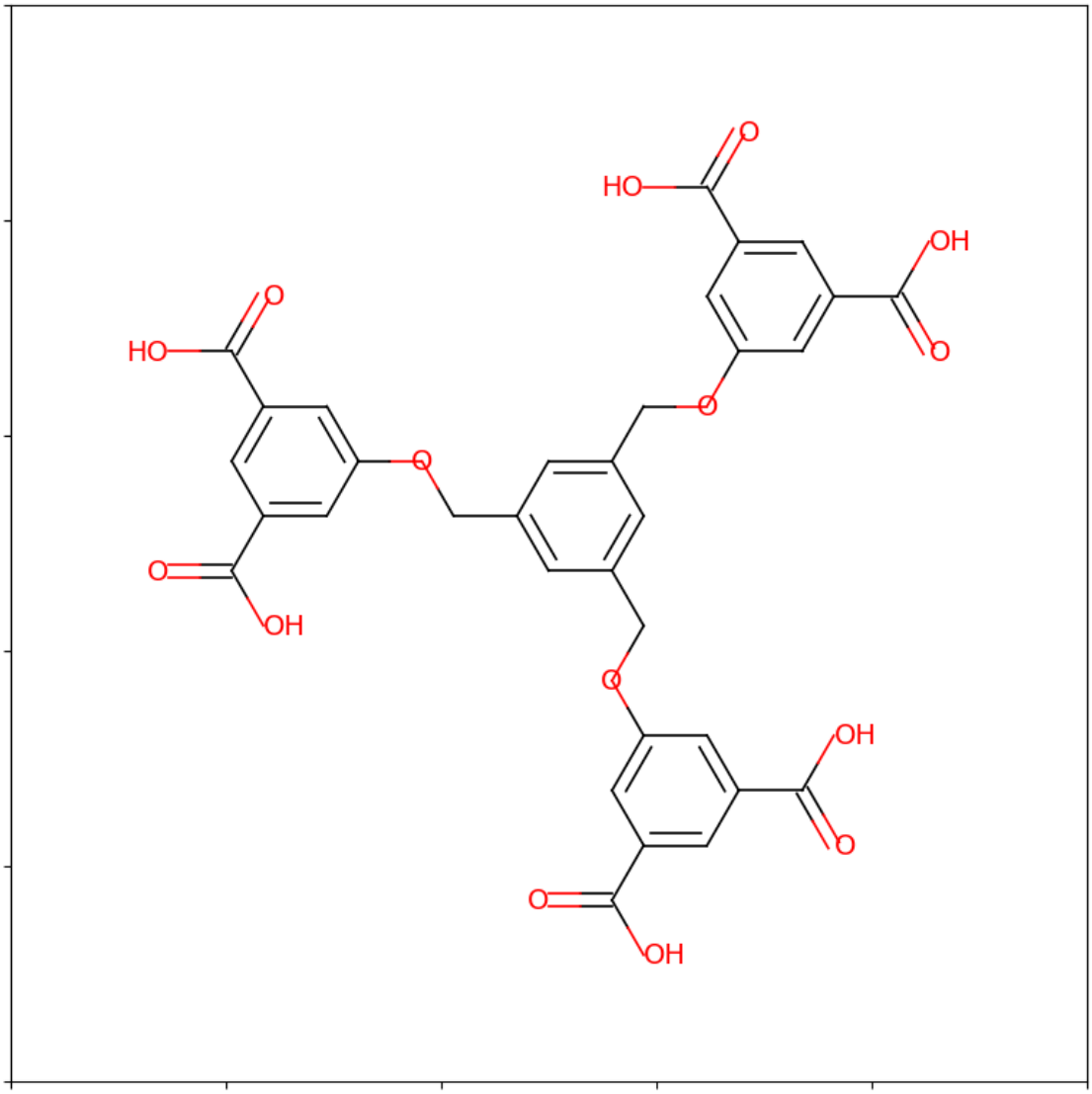
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.075
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.075
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with mixed ligand MOFs
```

```
# MOF 40
```

Here is the linker:

[172]:
```
Image('./ADASOP_cleansingle_linker0.png')
```

[172]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[173]:
```
nutils.viewer('./ADASOP_clean.cif')
```

[174]:
```
temperature_mof_40_Celsius  = 120.0 #@param {type:'number'}
time_mof_40_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_40 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_40 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_40 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_40 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_40 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_40_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_first_linker_mof_40_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_second_linker_mof_40_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_40 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_40 =  'Not sure about the crystallization␣
↪conditions with such a large linkers' #@param {type:'string'}
results['mof_40'] = {}
results['mof_40']['temperature']=temperature_mof_40_Celsius
results['mof_40']['time']=time_mof_40_hours
results['mof_40']['solvent1']=first_solvent_mof_40
```

```
results['mof_40']['solvent2']=second_solvent_mof_40
results['mof_40']['solvent3']=third_solvent_mof_40
results['mof_40']['additive']=additive_mof_40
results['mof_40']['counter']=counter_ion_mof_40
results['mof_40']['metal']=concentration_metal_mof_40_mol_per_liter
results['mof_40']['linker1']=concentration_first_linker_mof_40_mol_per_liter
results['mof_40']['linker2']=concentration_second_linker_mof_40_mol_per_liter
results['mof_40']['surely']=are_you_sure_about_your_selction_mof_40
results['mof_40']['additional']=what_makes_you_so_sure_or_unsure_mof_40
```

[175]:
```
nutils.print_choice(temperature_mof_40_Celsius, time_mof_40_hours,␣
↪first_solvent_mof_40,second_solvent_mof_40,third_solvent_mof_40 ,␣
↪counter_ion_mof_40, concentration_metal_mof_40_mol_per_liter,␣
↪concentration_first_linker_mof_40_mol_per_liter,concentration_second_linker_mof_40_mol_per_
↪, additive_mof_40,are_you_sure_about_your_selction_mof_40,␣
↪what_makes_you_so_sure_or_unsure_mof_40 )
```

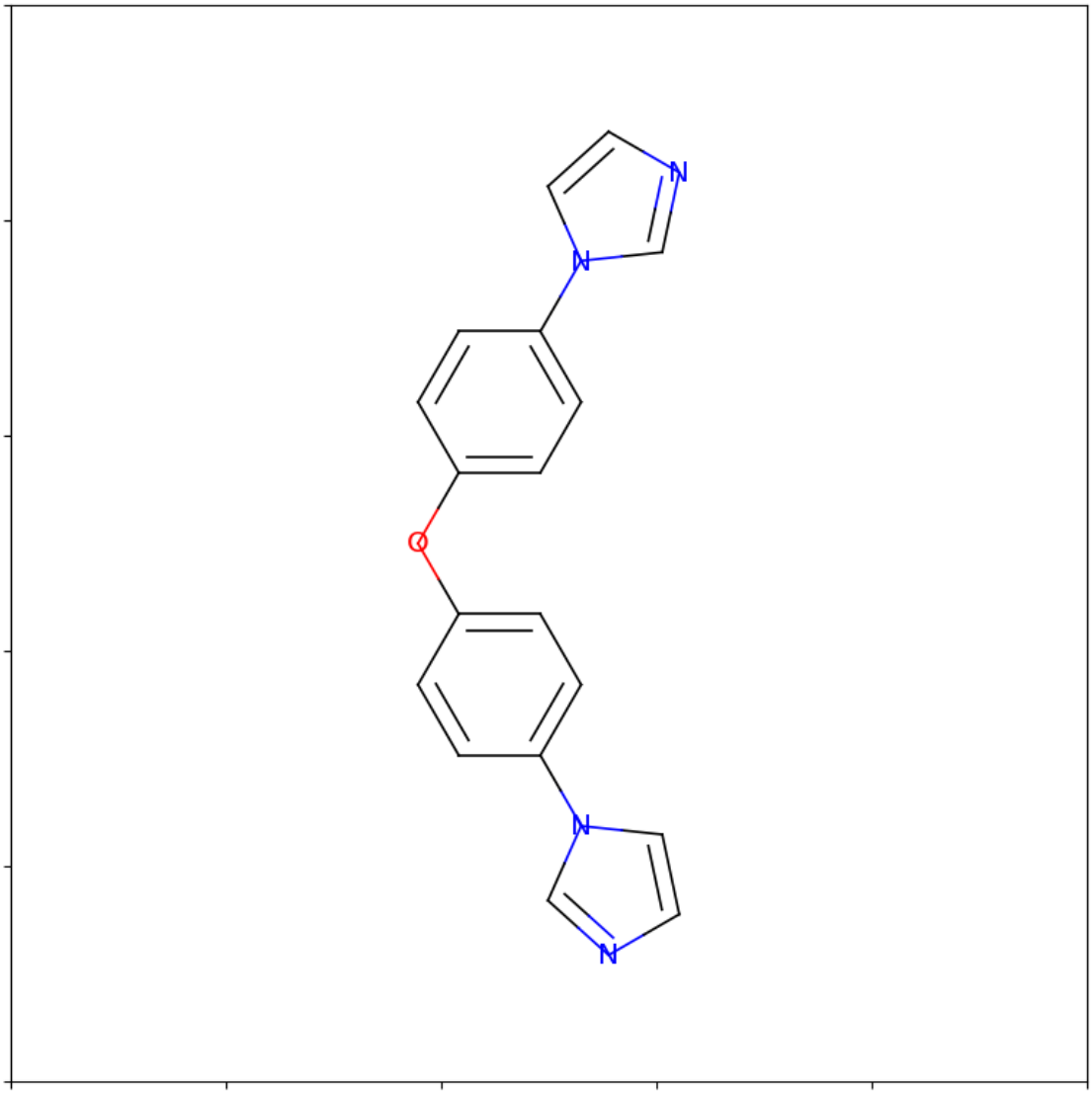
```
Thanks for your input
Your selection was:
Temperature: 120.0
Time: 72
Solvent1: N,N-diethylformamide (DEF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.1
First_Linker_Concentration: 0.1
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the crystallization conditions
with such a large linkers
```

```
# MOF 41
```

Here is the linker:

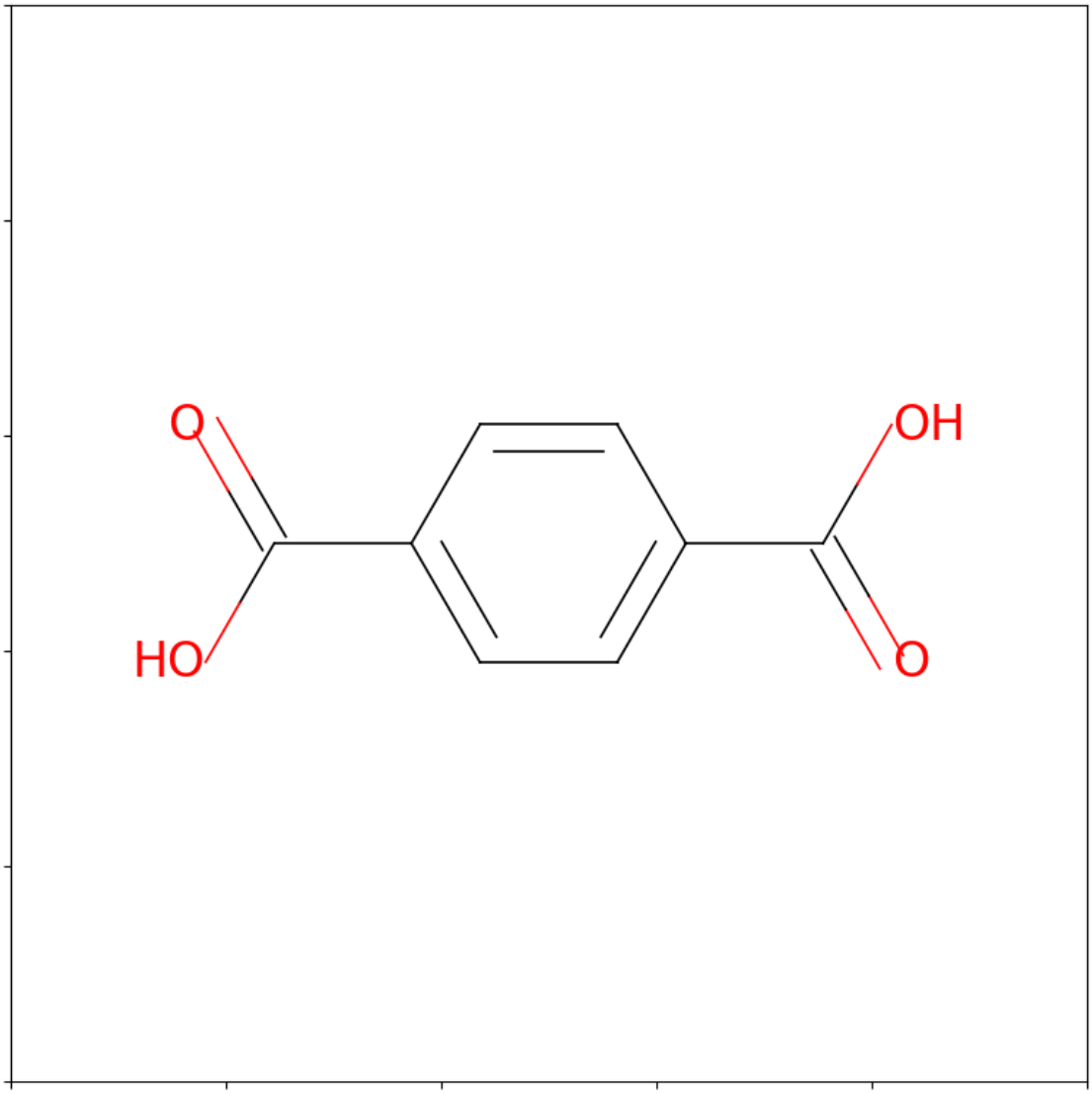
[176]:
```
Image('./OKIPUU_cleansingle_linker0.png')
```

[176]:



[177]:
```
Image('./OKIPUU_cleansingle_linker2.png')
```

[177]:



The metal center of this MOF is ``Cd''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[178]:
```
nutils.viewer('./OKIPUU_clean.cif')
```

[179]:
```
temperature_mof_41_Celsius  = 120 #@param {type:'number'}
time_mof_41_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_41 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_41 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
third_solvent_mof_41 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_41 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_41 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_41_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_41_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_second_linker_mof_41_mol_per_liter  = 0.05 #@param {type:'number'}
are_you_sure_about_your_selction_mof_41 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_41 =  'Not used to work with MOFs␣
↪containing different type of linkers' #@param {type:'string'}
results['mof_41'] = {}
results['mof_41']['temperature']=temperature_mof_41_Celsius
results['mof_41']['time']=time_mof_41_hours
results['mof_41']['solvent1']=first_solvent_mof_41
```

```
results['mof_41']['solvent2']=second_solvent_mof_41
results['mof_41']['solvent3']=third_solvent_mof_41
results['mof_41']['additive']=additive_mof_41
results['mof_41']['counter']=counter_ion_mof_41
results['mof_41']['metal']=concentration_metal_mof_41_mol_per_liter
results['mof_41']['linker1']=concentration_first_linker_mof_41_mol_per_liter
results['mof_41']['linker2']=concentration_second_linker_mof_41_mol_per_liter
results['mof_41']['surely']=are_you_sure_about_your_selction_mof_41
results['mof_41']['additional']=what_makes_you_so_sure_or_unsure_mof_41
```

[180]:
```
nutils.print_choice(temperature_mof_41_Celsius, time_mof_41_hours,␣
↪first_solvent_mof_41,second_solvent_mof_41,third_solvent_mof_41 ,␣
↪counter_ion_mof_41, concentration_metal_mof_41_mol_per_liter,␣
↪concentration_first_linker_mof_41_mol_per_liter,concentration_second_linker_mof_41_mol_per_
↪, additive_mof_41,are_you_sure_about_your_selction_mof_41,␣
↪what_makes_you_so_sure_or_unsure_mof_41 )
```

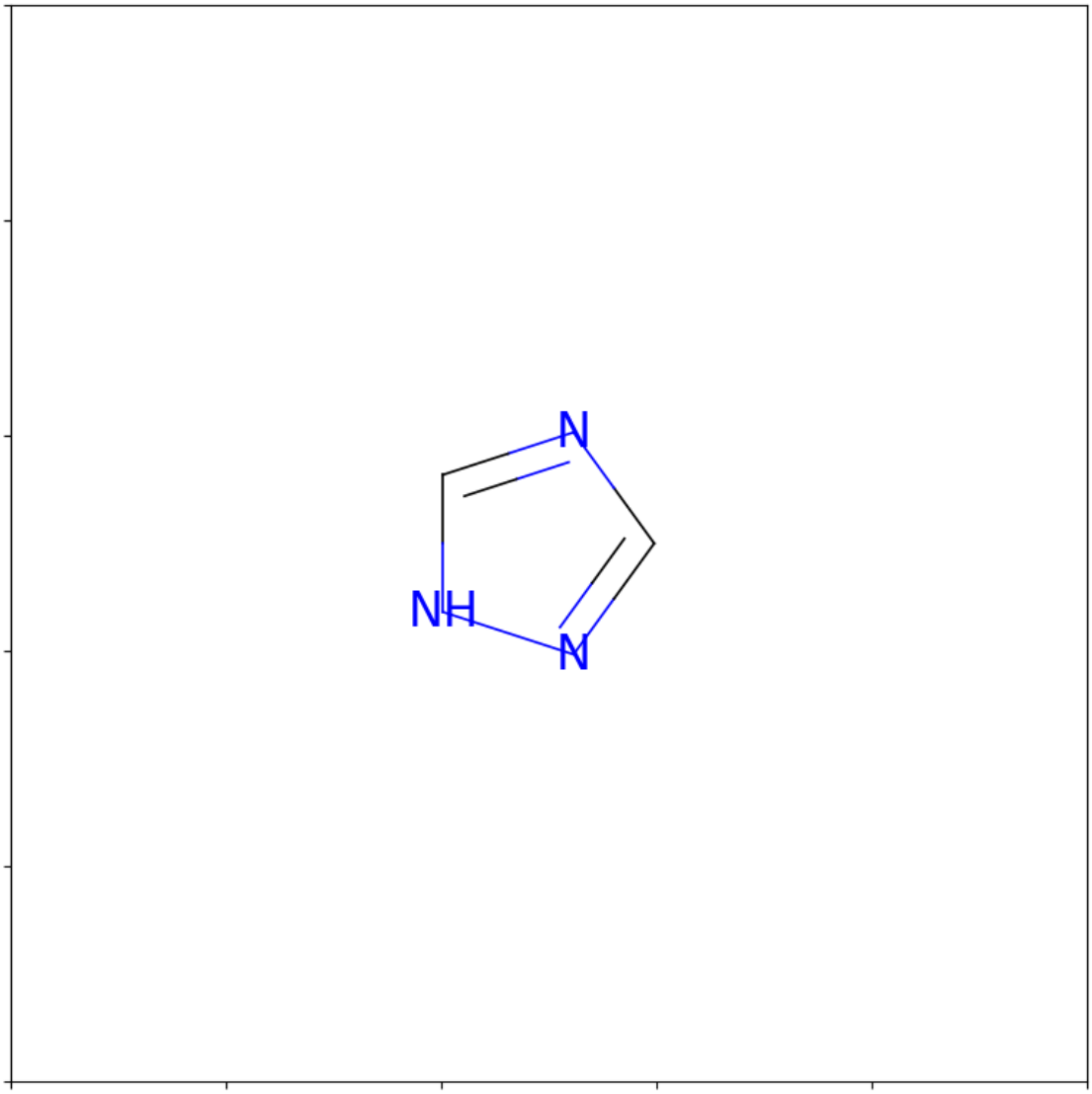
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 72.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: ethanol
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.05
First_Linker_Concentration: 0.1
Second_Linker_Concentration: 0.05
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not used to work with MOFs containing different
type of linkers
```

```
# MOF 42
```

Here is the linker:

[181]:
```
Image('./LATPIG_cleansingle_linker0.png')
```

[181]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[182]:
```
nutils.viewer('./LATPIG_clean.cif')
```

[183]:
```
temperature_mof_42_Celsius  = 120 #@param {type:'number'}
time_mof_42_hours  = 24 #@param {type:'number'}
```

```
first_solvent_mof_42 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_42 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_42 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_42 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_42 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_42_mol_per_liter  = 0.25 #@param {type:'number'}
concentration_first_linker_mof_42_mol_per_liter  =  0.75#@param {type:'number'}
concentration_second_linker_mof_42_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_42 = 'yes' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_42 =  'Quite sure since it can be similar␣
↪to the ZIF-8 crystallization conditions' #@param {type:'string'}
results['mof_42'] = {}
results['mof_42']['temperature']=temperature_mof_42_Celsius
results['mof_42']['time']=time_mof_42_hours
results['mof_42']['solvent1']=first_solvent_mof_42
```

```
results['mof_42']['solvent2']=second_solvent_mof_42
results['mof_42']['solvent3']=third_solvent_mof_42
results['mof_42']['additive']=additive_mof_42
results['mof_42']['counter']=counter_ion_mof_42
results['mof_42']['metal']=concentration_metal_mof_42_mol_per_liter
results['mof_42']['linker1']=concentration_first_linker_mof_42_mol_per_liter
results['mof_42']['linker2']=concentration_second_linker_mof_42_mol_per_liter
results['mof_42']['surely']=are_you_sure_about_your_selction_mof_42
results['mof_42']['additional']=what_makes_you_so_sure_or_unsure_mof_42
```

[184]:
```
nutils.print_choice(temperature_mof_42_Celsius, time_mof_42_hours,␣
↪first_solvent_mof_42,second_solvent_mof_42,third_solvent_mof_42 ,␣
↪counter_ion_mof_42, concentration_metal_mof_42_mol_per_liter,␣
↪concentration_first_linker_mof_42_mol_per_liter,concentration_second_linker_mof_42_mol_per_
↪, additive_mof_42,are_you_sure_about_your_selction_mof_42,␣
↪what_makes_you_so_sure_or_unsure_mof_42 )
```

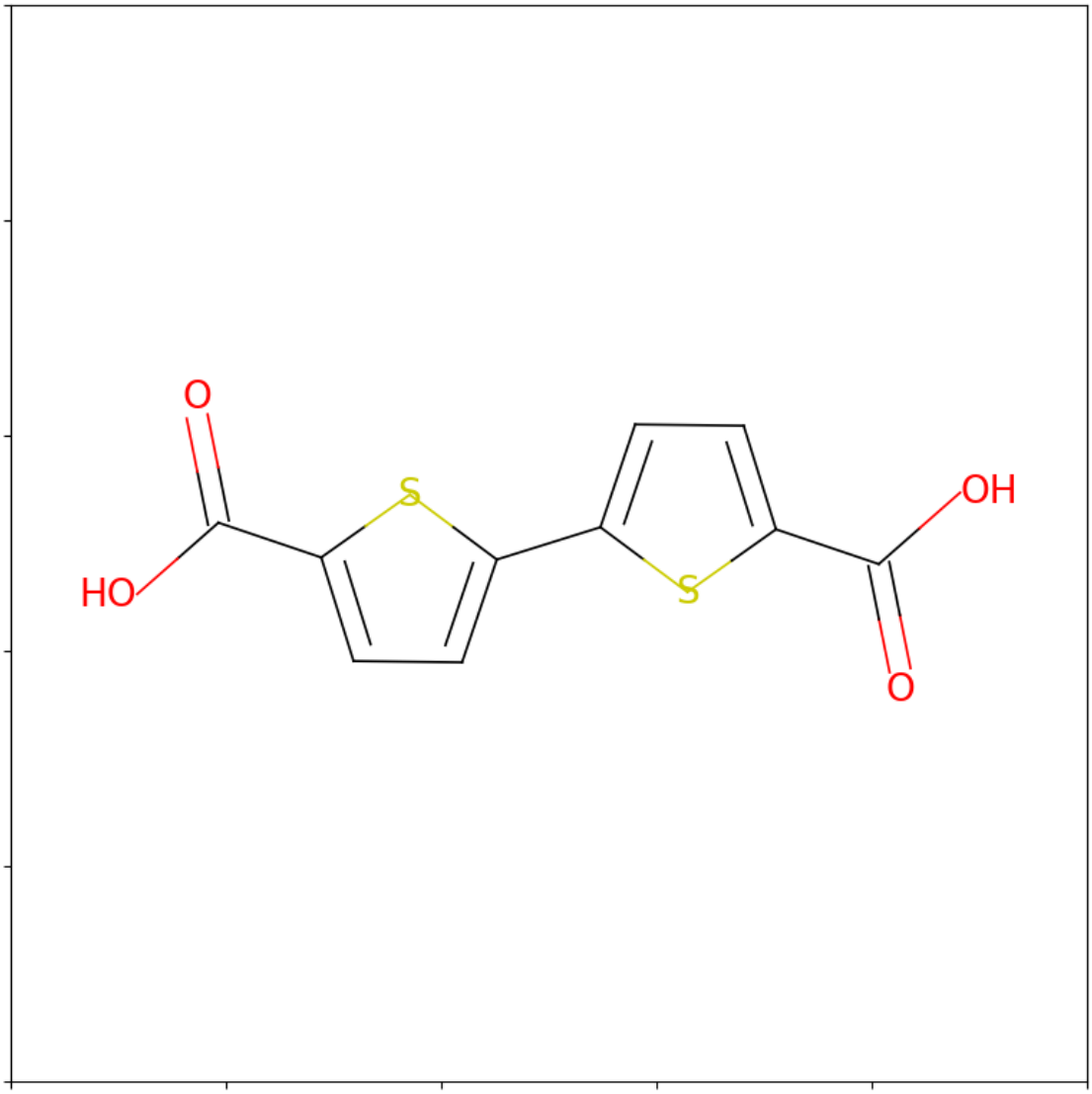
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 24
Solvent1: ethanol
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.25
First_Linker_Concentration: 0.75
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: yes
What_Makes_You_So_Sure/Unsure: Quite sure since it can be similar to the ZIF-8
crystallization conditions
```

```
# MOF 43
```

Here is the linker:

[185]:
```
Image('./UWOWAF_cleansingle_linker0.png')
```

[185]:



The metal center of this MOF is ``Mn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[186]:
```
nutils.viewer('./UWOWAF_clean.cif')
```

[187]:
```
temperature_mof_43_Celsius  = 135 #@param {type:'number'}
time_mof_43_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_43 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
 ↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
 ↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
 ↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
 ↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
 ↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
 ↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
 ↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
 ↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
 ↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_43 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
third_solvent_mof_43 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
 ↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
 ↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
 ↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
 ↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
 ↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
 ↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
 ↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
 ↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
 ↪"dimethylaniline"]
additive_mof_43 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_43 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
 ↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
 ↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
 ↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
 ↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
 ↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_43_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_43_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_43_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_43 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_43 =  'Not sure of the overall␣
 ↪concentration of metal and linker to be used in the synthesis, but␣
 ↪relatively sure that the proposed conditions can work for the MOF␣
 ↪crystallization' #@param {type:'string'}
results['mof_43'] = {}
results['mof_43']['temperature']=temperature_mof_43_Celsius
```

```
results['mof_43']['time']=time_mof_43_hours
results['mof_43']['solvent1']=first_solvent_mof_43
results['mof_43']['solvent2']=second_solvent_mof_43
results['mof_43']['solvent3']=third_solvent_mof_43
results['mof_43']['additive']=additive_mof_43
results['mof_43']['counter']=counter_ion_mof_43
results['mof_43']['metal']=concentration_metal_mof_43_mol_per_liter
results['mof_43']['linker1']=concentration_first_linker_mof_43_mol_per_liter
results['mof_43']['linker2']=concentration_second_linker_mof_43_mol_per_liter
results['mof_43']['surely']=are_you_sure_about_your_selction_mof_43
results['mof_43']['additional']=what_makes_you_so_sure_or_unsure_mof_43
```

[188]:
```
nutils.print_choice(temperature_mof_43_Celsius, time_mof_43_hours,␣
↪first_solvent_mof_43,second_solvent_mof_43,third_solvent_mof_43 ,␣
↪counter_ion_mof_43, concentration_metal_mof_43_mol_per_liter,␣
↪concentration_first_linker_mof_43_mol_per_liter,concentration_second_linker_mof_43_mol_per_
↪, additive_mof_43,are_you_sure_about_your_selction_mof_43,␣
↪what_makes_you_so_sure_or_unsure_mof_43 )
```

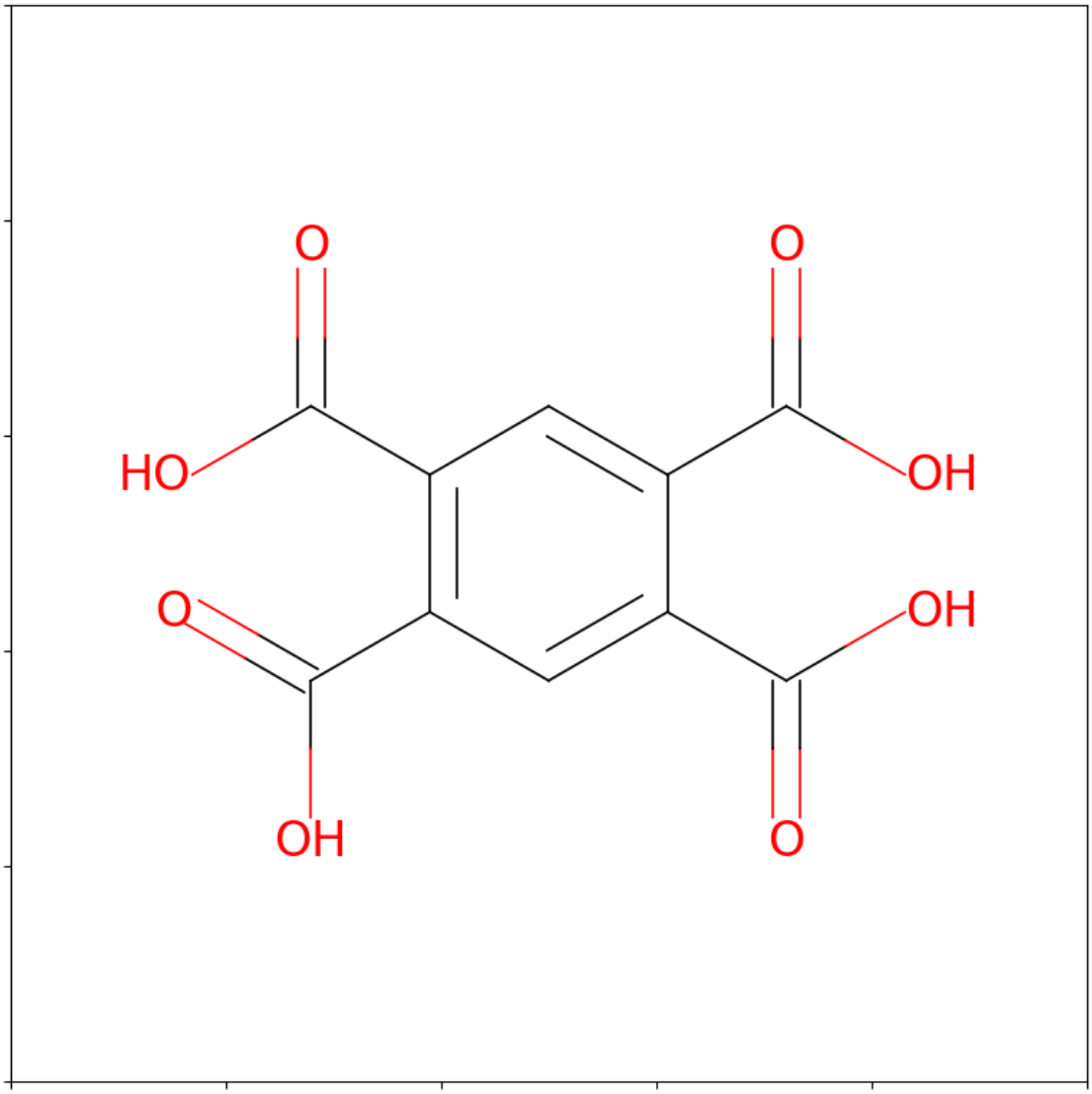
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.05
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure of the overall concentration of metal
and linker to be used in the synthesis, but relatively sure that the proposed
conditions can work for the MOF crystallization
```

```
# MOF 44
```

Here is the linker:

[189]:
```
Image('./GUCHUJ_cleansingle_linker0.png')
```

[189]:



The metal center of this MOF is ``Cu''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[190]:
```
nutils.viewer('./GUCHUJ_clean.cif')
```

[191]:
```
temperature_mof_44_Celsius  = 120 #@param {type:'number'}
time_mof_44_hours  =  48#@param {type:'number'}
```

```
first_solvent_mof_44 = 'ethanol' #@param ["None", "1-butanol",␣
↪"2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide␣
↪(DEF)", "N-methylformamide (NMF)", "pyridine", "chlorobenzene",␣
↪"cyclohexanol", "isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane",␣
↪"ethylene glycol", "diethanolamine", "acetone", "ethanol", "isopropyl␣
↪alcohol", "H2O", "chloroform", "1,2-xylene", "acetonitrile",␣
↪"dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_44 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_44 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_44 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_44 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_44_mol_per_liter  = 0.1 #@param {type:'number'}
concentration_first_linker_mof_44_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_44_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_44 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_44 =  'Not sure about the concentration,␣
↪maybe a little higher mol/L addition of metal and linker are needed, but I␣
↪think that the proposed conditions can work for the MOF crystallization'␣
↪#@param {type:'string'}
results['mof_44'] = {}
results['mof_44']['temperature']=temperature_mof_44_Celsius
```

```
results['mof_44']['time']=time_mof_44_hours
results['mof_44']['solvent1']=first_solvent_mof_44
results['mof_44']['solvent2']=second_solvent_mof_44
results['mof_44']['solvent3']=third_solvent_mof_44
results['mof_44']['additive']=additive_mof_44
results['mof_44']['counter']=counter_ion_mof_44
results['mof_44']['metal']=concentration_metal_mof_44_mol_per_liter
results['mof_44']['linker1']=concentration_first_linker_mof_44_mol_per_liter
results['mof_44']['linker2']=concentration_second_linker_mof_44_mol_per_liter
results['mof_44']['surely']=are_you_sure_about_your_selction_mof_44
results['mof_44']['additional']=what_makes_you_so_sure_or_unsure_mof_44
```

[192]:
```
nutils.print_choice(temperature_mof_44_Celsius, time_mof_44_hours,␣
↪first_solvent_mof_44,second_solvent_mof_44,third_solvent_mof_44 ,␣
↪counter_ion_mof_44, concentration_metal_mof_44_mol_per_liter,␣
↪concentration_first_linker_mof_44_mol_per_liter,concentration_second_linker_mof_44_mol_per_
↪, additive_mof_44,are_you_sure_about_your_selction_mof_44,␣
↪what_makes_you_so_sure_or_unsure_mof_44 )
```

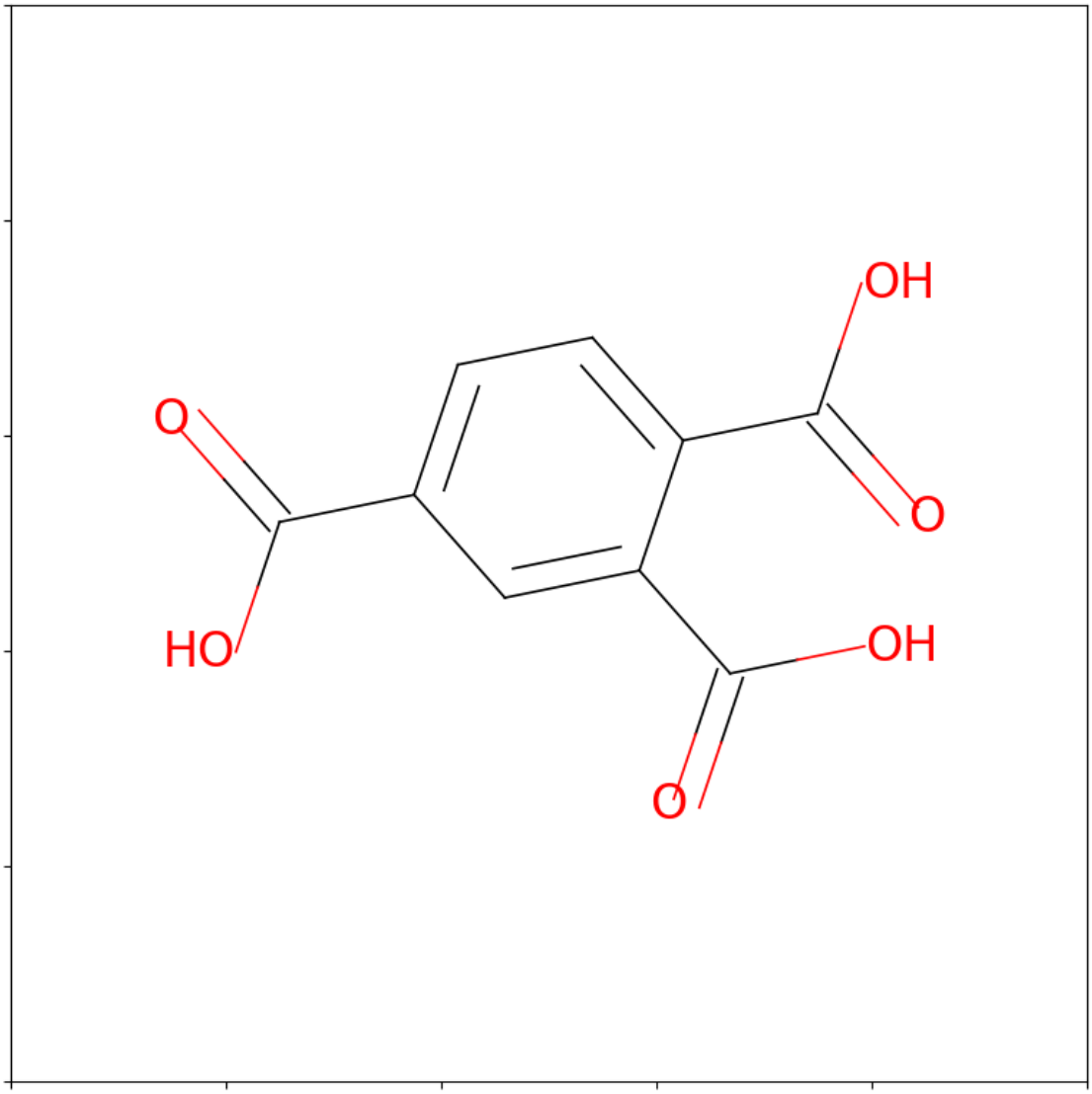
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 48
Solvent1: ethanol
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.1
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the concentration, maybe a little
higher mol/L addition of metal and linker are needed, but I think that the
proposed conditions can work for the MOF crystallization
```

```
# MOF 45
```

Here is the linker:

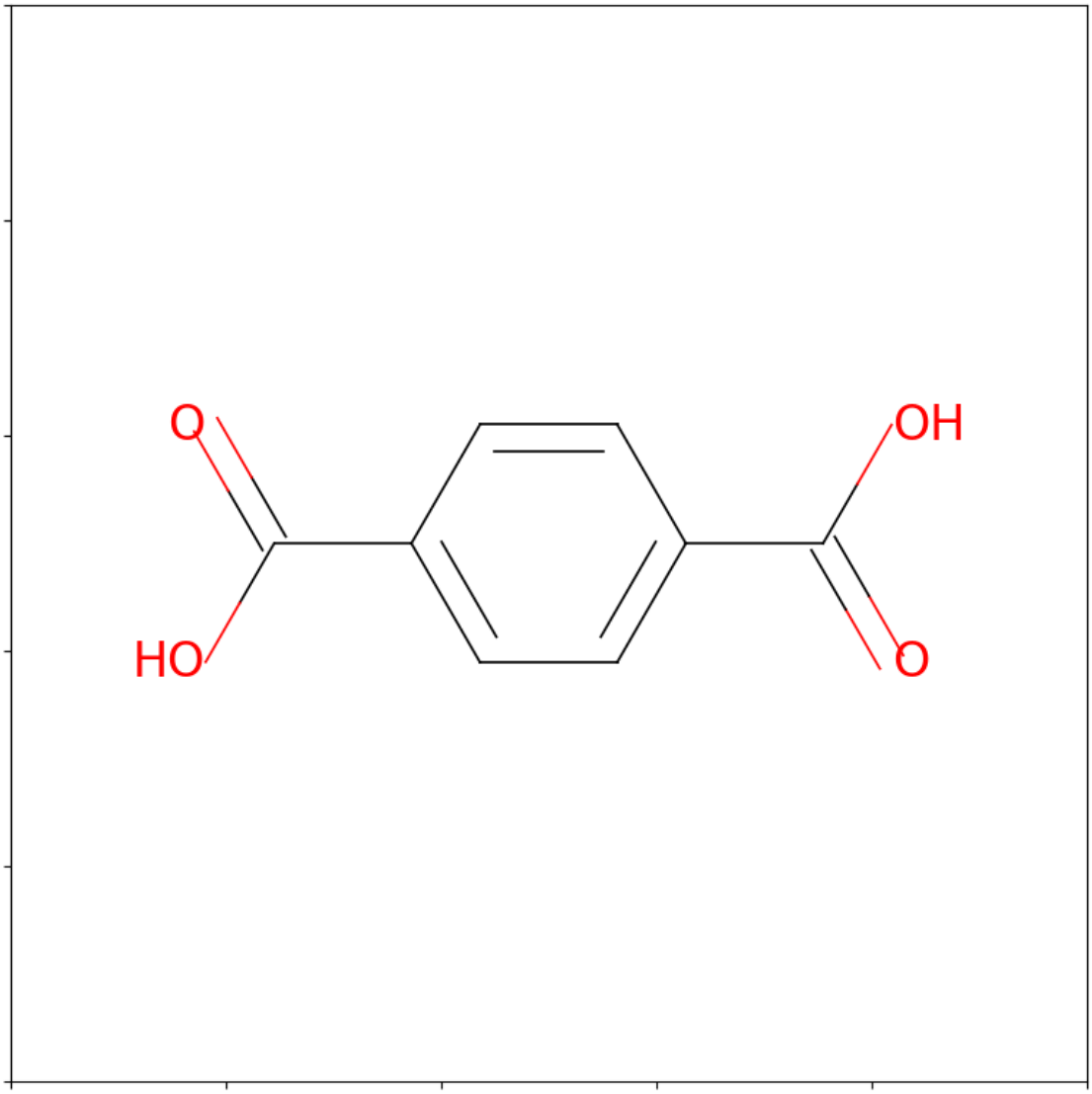
[193]:
```
Image('./GURTIX_chargedsingle_linker0.png')
```

[193]:



[194]:
```
Image('./GURTIX_chargedsingle_linker3.png')
```

[194]:



The metal center of this MOF is ``In''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[195]:
```
nutils.viewer('./GURTIX_charged.cif')
```

[196]:
```
temperature_mof_45_Celsius  = 150 #@param {type:'number'}
time_mof_45_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_45 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_45 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_45 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_45 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_45 =  'NO3'#@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_45_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_45_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_45_mol_per_liter  = 0.025 #@param {type:
↪'number'}
are_you_sure_about_your_selction_mof_45 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_45 =  "Uncertainty about the molar ratio␣
↪between the linkers\"" #@param {type:'string'}
results['mof_45'] = {}
results['mof_45']['temperature']=temperature_mof_45_Celsius
```

```
results['mof_45']['time']=time_mof_45_hours
results['mof_45']['solvent1']=first_solvent_mof_45
results['mof_45']['solvent2']=second_solvent_mof_45
results['mof_45']['solvent3']=third_solvent_mof_45
results['mof_45']['additive']=additive_mof_45
results['mof_45']['counter']=counter_ion_mof_45
results['mof_45']['metal']=concentration_metal_mof_45_mol_per_liter
results['mof_45']['linker1']=concentration_first_linker_mof_45_mol_per_liter
results['mof_45']['linker2']=concentration_second_linker_mof_45_mol_per_liter
results['mof_45']['surely']=are_you_sure_about_your_selction_mof_45
results['mof_45']['additional']=what_makes_you_so_sure_or_unsure_mof_45
```

[197]:
```
nutils.print_choice(temperature_mof_45_Celsius, time_mof_45_hours,␣
↪first_solvent_mof_45,second_solvent_mof_45,third_solvent_mof_45 ,␣
↪counter_ion_mof_45, concentration_metal_mof_45_mol_per_liter,␣
↪concentration_first_linker_mof_45_mol_per_liter,concentration_second_linker_mof_45_mol_per_
↪, additive_mof_45,are_you_sure_about_your_selction_mof_45,␣
↪what_makes_you_so_sure_or_unsure_mof_45 )
```

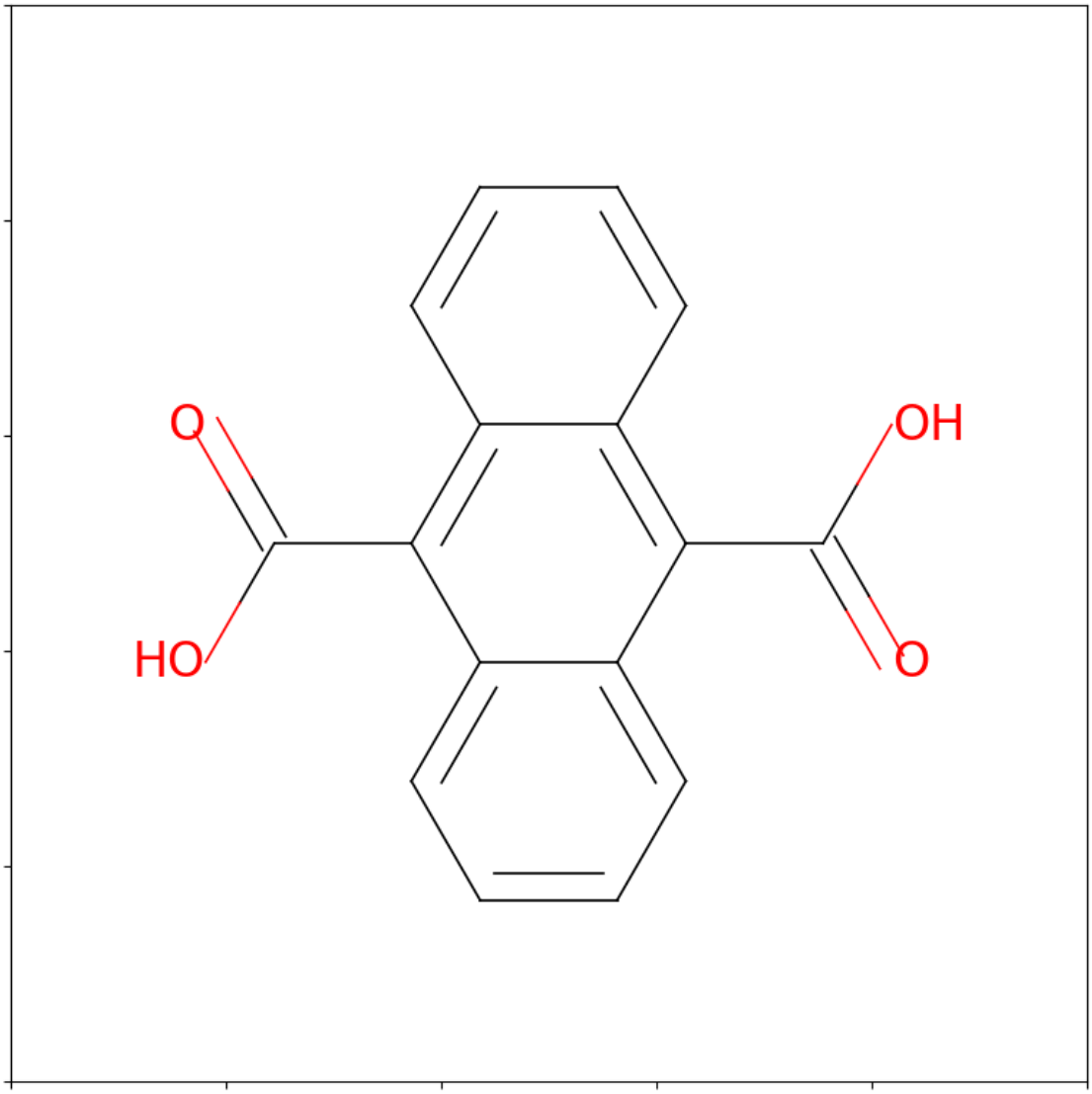
```
Thanks for your input
Your selection was:
Temperature: 150
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.075
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.025
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Uncertainty about the molar ratio between the
linkers"
```

```
# MOF 46
```

Here is the linker:

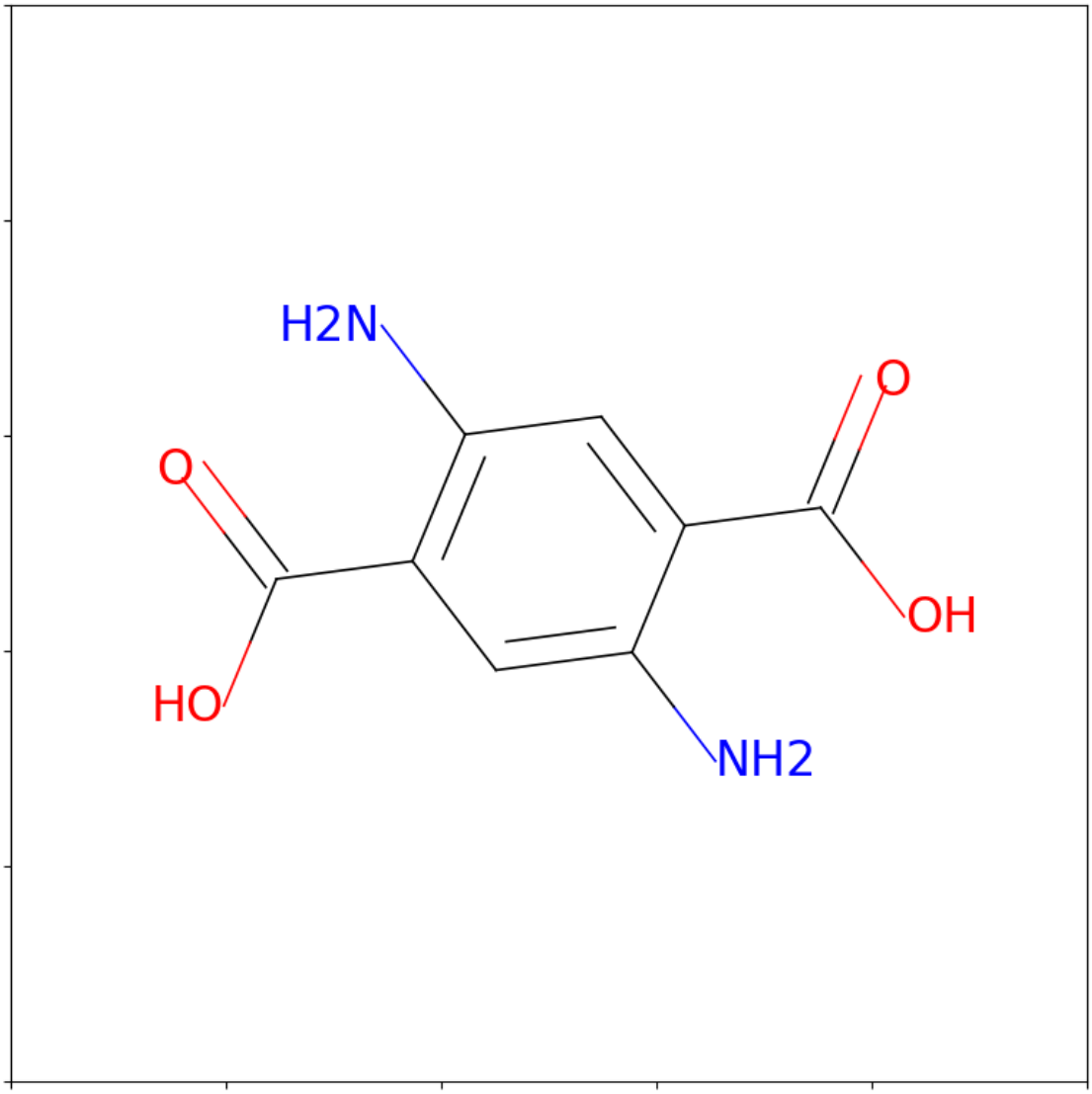
[198]:
```
Image('./IKUTOZ_cleansingle_linker0.png')
```

[198]:



[199]:
```
Image('./IKUTOZ_cleansingle_linker2.png')
```

[199]:



The metal center of this MOF is ``Dy''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[200]:
```
nutils.viewer('./IKUTOZ_clean.cif')
```

[201]:
```
temperature_mof_46_Celsius  =  135#@param {type:'number'}
time_mof_46_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_46 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_46 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_46 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_46 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_46 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_46_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_first_linker_mof_46_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_46_mol_per_liter  = 0.025 #@param {type:
↪'number'}
are_you_sure_about_your_selction_mof_46 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_46 =  'Do not know Dy chemistry, but the␣
↪proposed conditions could work since Dy is slightly less acid than Zr4, for␣
↪example ' #@param {type:'string'}
results['mof_46'] = {}
```

```
results['mof_46']['temperature']=temperature_mof_46_Celsius
results['mof_46']['time']=time_mof_46_hours
results['mof_46']['solvent1']=first_solvent_mof_46
results['mof_46']['solvent2']=second_solvent_mof_46
results['mof_46']['solvent3']=third_solvent_mof_46
results['mof_46']['additive']=additive_mof_46
results['mof_46']['counter']=counter_ion_mof_46
results['mof_46']['metal']=concentration_metal_mof_46_mol_per_liter
results['mof_46']['linker1']=concentration_first_linker_mof_46_mol_per_liter
results['mof_46']['linker2']=concentration_second_linker_mof_46_mol_per_liter
results['mof_46']['surely']=are_you_sure_about_your_selction_mof_46
results['mof_46']['additional']=what_makes_you_so_sure_or_unsure_mof_46
```

[202]:
```
nutils.print_choice(temperature_mof_46_Celsius, time_mof_46_hours,␣
↪first_solvent_mof_46,second_solvent_mof_46,third_solvent_mof_46 ,␣
↪counter_ion_mof_46, concentration_metal_mof_46_mol_per_liter,␣
↪concentration_first_linker_mof_46_mol_per_liter,concentration_second_linker_mof_46_mol_per_
↪, additive_mof_46,are_you_sure_about_your_selction_mof_46,␣
↪what_makes_you_so_sure_or_unsure_mof_46 )
```

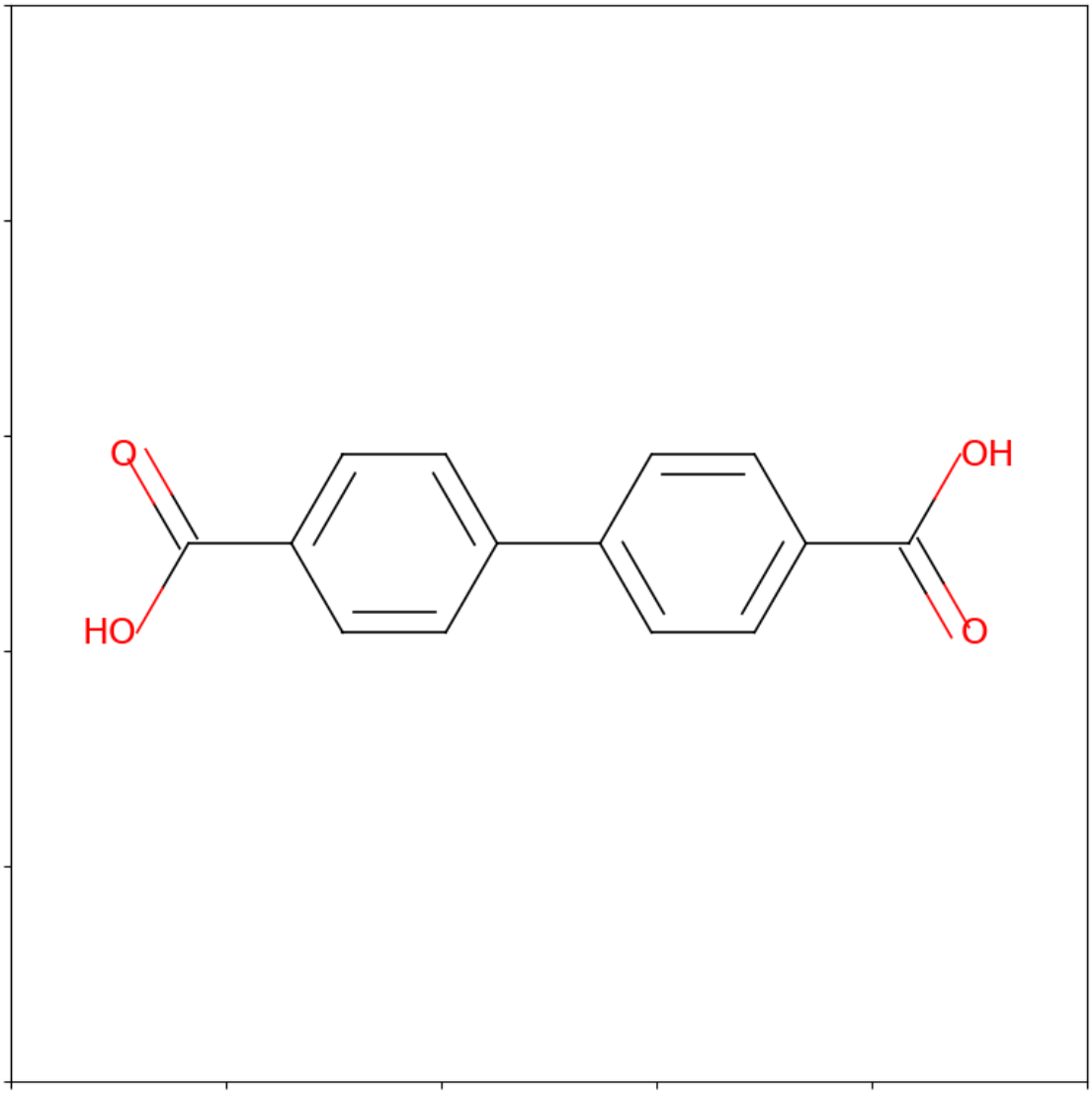
```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.075
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.025
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Do not know Dy chemistry, but the proposed
conditions could work since Dy is slightly less acid than Zr4, for example
```

```
# MOF 47
```

Here is the linker:

[203]:
```
Image('./ERULEK_cleansingle_linker0.png')
```

[203]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[204]:
```
nutils.viewer('./ERULEK_clean.cif')
```

[205]:
```
temperature_mof_47_Celsius  = 120 #@param {type:'number'}
time_mof_47_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_47 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_47 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_47 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_47 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_47 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_47_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_47_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_47_mol_per_liter  =  0#@param {type:'number'}
are_you_sure_about_your_selction_mof_47 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_47 =  'a linker is missing' #@param {type:
↪'string'}
results['mof_47'] = {}
results['mof_47']['temperature']=temperature_mof_47_Celsius
results['mof_47']['time']=time_mof_47_hours
results['mof_47']['solvent1']=first_solvent_mof_47
```

```
results['mof_47']['solvent2']=second_solvent_mof_47
results['mof_47']['solvent3']=third_solvent_mof_47
results['mof_47']['additive']=additive_mof_47
results['mof_47']['counter']=counter_ion_mof_47
results['mof_47']['metal']=concentration_metal_mof_47_mol_per_liter
results['mof_47']['linker1']=concentration_first_linker_mof_47_mol_per_liter
results['mof_47']['linker2']=concentration_second_linker_mof_47_mol_per_liter
results['mof_47']['surely']=are_you_sure_about_your_selction_mof_47
results['mof_47']['additional']=what_makes_you_so_sure_or_unsure_mof_47
```

[206]:
```
nutils.print_choice(temperature_mof_47_Celsius, time_mof_47_hours,␣
↪first_solvent_mof_47,second_solvent_mof_47,third_solvent_mof_47 ,␣
↪counter_ion_mof_47, concentration_metal_mof_47_mol_per_liter,␣
↪concentration_first_linker_mof_47_mol_per_liter,concentration_second_linker_mof_47_mol_per_
↪, additive_mof_47,are_you_sure_about_your_selction_mof_47,␣
↪what_makes_you_so_sure_or_unsure_mof_47 )
```

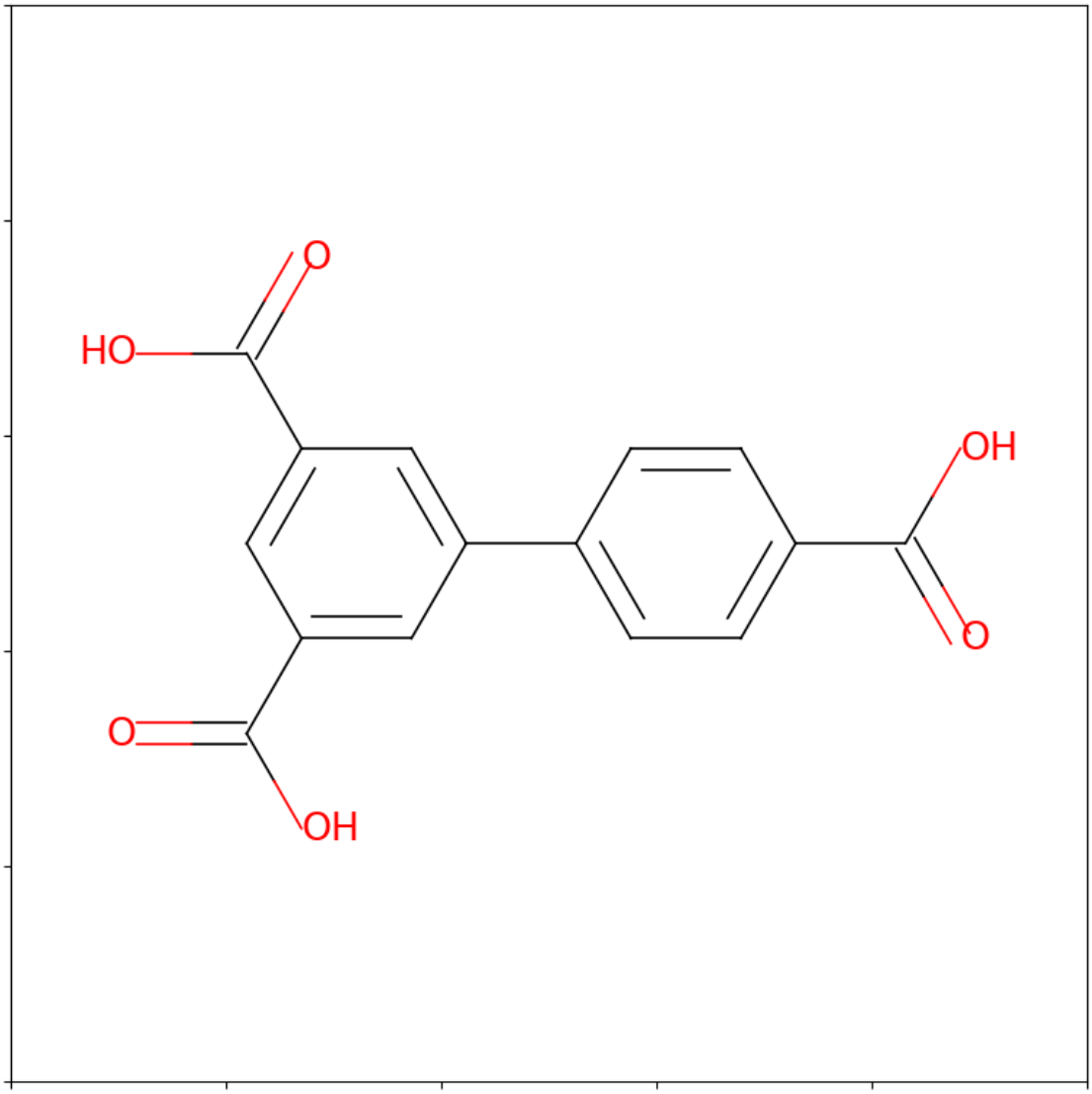
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 72
Solvent1: N,N-diethylformamide (DEF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: a linker is missing
```

```
# MOF 48
```

Here is the linker:

[207]:
```
Image('./DITTEH_cleansingle_linker1.png')
```

[207]:



The metal center of this MOF is ``Zn''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[208]:
```
nutils.viewer('./DITTEH_clean.cif')
```

[209]:
```
temperature_mof_48_Celsius  = 120.0 #@param {type:'number'}
time_mof_48_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_48 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_48 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_48 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_48 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_48 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_48_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_48_mol_per_liter  = 0.075 #@param {type:'number'}
concentration_second_linker_mof_48_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_48 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_48 =  'Not sure about the overall␣
↪concentration of the metal and linker needed ' #@param {type:'string'}
results['mof_48'] = {}
results['mof_48']['temperature']=temperature_mof_48_Celsius
results['mof_48']['time']=time_mof_48_hours
results['mof_48']['solvent1']=first_solvent_mof_48
```

```
results['mof_48']['solvent2']=second_solvent_mof_48
results['mof_48']['solvent3']=third_solvent_mof_48
results['mof_48']['additive']=additive_mof_48
results['mof_48']['counter']=counter_ion_mof_48
results['mof_48']['metal']=concentration_metal_mof_48_mol_per_liter
results['mof_48']['linker1']=concentration_first_linker_mof_48_mol_per_liter
results['mof_48']['linker2']=concentration_second_linker_mof_48_mol_per_liter
results['mof_48']['surely']=are_you_sure_about_your_selction_mof_48
results['mof_48']['additional']=what_makes_you_so_sure_or_unsure_mof_48
```

[210]:
```
nutils.print_choice(temperature_mof_48_Celsius, time_mof_48_hours,␣
↪first_solvent_mof_48,second_solvent_mof_48,third_solvent_mof_48 ,␣
↪counter_ion_mof_48, concentration_metal_mof_48_mol_per_liter,␣
↪concentration_first_linker_mof_48_mol_per_liter,concentration_second_linker_mof_48_mol_per_
↪, additive_mof_48,are_you_sure_about_your_selction_mof_48,␣
↪what_makes_you_so_sure_or_unsure_mof_48 )
```

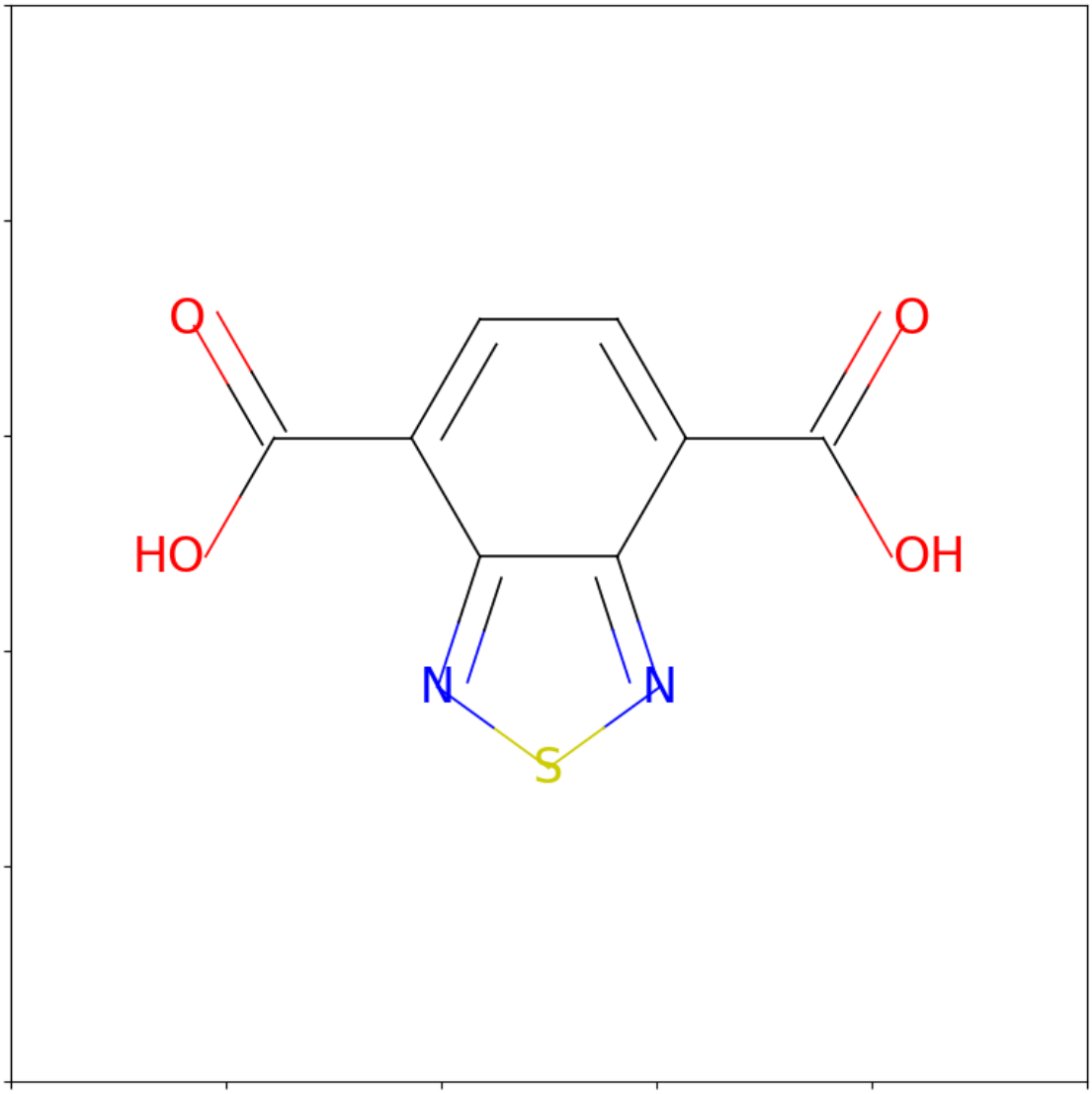
```
Thanks for your input
Your selection was:
Temperature: 120.0
Time: 72
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.075
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the overall concentration of the
metal and linker needed
```

```
# MOF 49
```

Here is the linker:

[211]:
```
Image('./LAWHUP_cleansingle_linker0.png')
```

[211]:



The metal center of this MOF is ``Cd''. The oxidation state of the metal is ``2''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[212]:
```
nutils.viewer('./LAWHUP_clean.cif')
```

[213]:
```
temperature_mof_49_Celsius  = 120 #@param {type:'number'}
time_mof_49_hours  = 72.0 #@param {type:'number'}
```

```
first_solvent_mof_49 = 'N,N-dimethylformamide (DMF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_49 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_49 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_49 = 'no additive' #@param ['no additive', 'acid', 'base']
counter_ion_mof_49 =  'Cl' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_49_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_49_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_49_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_49 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_49 =  'Not sure about the thermal&chemical␣
↪stability of the linker under the proposed crystallization conditions'␣
↪#@param {type:'string'}
results['mof_49'] = {}
results['mof_49']['temperature']=temperature_mof_49_Celsius
results['mof_49']['time']=time_mof_49_hours
```

```
results['mof_49']['solvent1']=first_solvent_mof_49
results['mof_49']['solvent2']=second_solvent_mof_49
results['mof_49']['solvent3']=third_solvent_mof_49
results['mof_49']['additive']=additive_mof_49
results['mof_49']['counter']=counter_ion_mof_49
results['mof_49']['metal']=concentration_metal_mof_49_mol_per_liter
results['mof_49']['linker1']=concentration_first_linker_mof_49_mol_per_liter
results['mof_49']['linker2']=concentration_second_linker_mof_49_mol_per_liter
results['mof_49']['surely']=are_you_sure_about_your_selction_mof_49
results['mof_49']['additional']=what_makes_you_so_sure_or_unsure_mof_49
```

[214]:
```
nutils.print_choice(temperature_mof_49_Celsius, time_mof_49_hours,␣
↪first_solvent_mof_49,second_solvent_mof_49,third_solvent_mof_49 ,␣
↪counter_ion_mof_49, concentration_metal_mof_49_mol_per_liter,␣
↪concentration_first_linker_mof_49_mol_per_liter,concentration_second_linker_mof_49_mol_per_
↪, additive_mof_49,are_you_sure_about_your_selction_mof_49,␣
↪what_makes_you_so_sure_or_unsure_mof_49 )
```

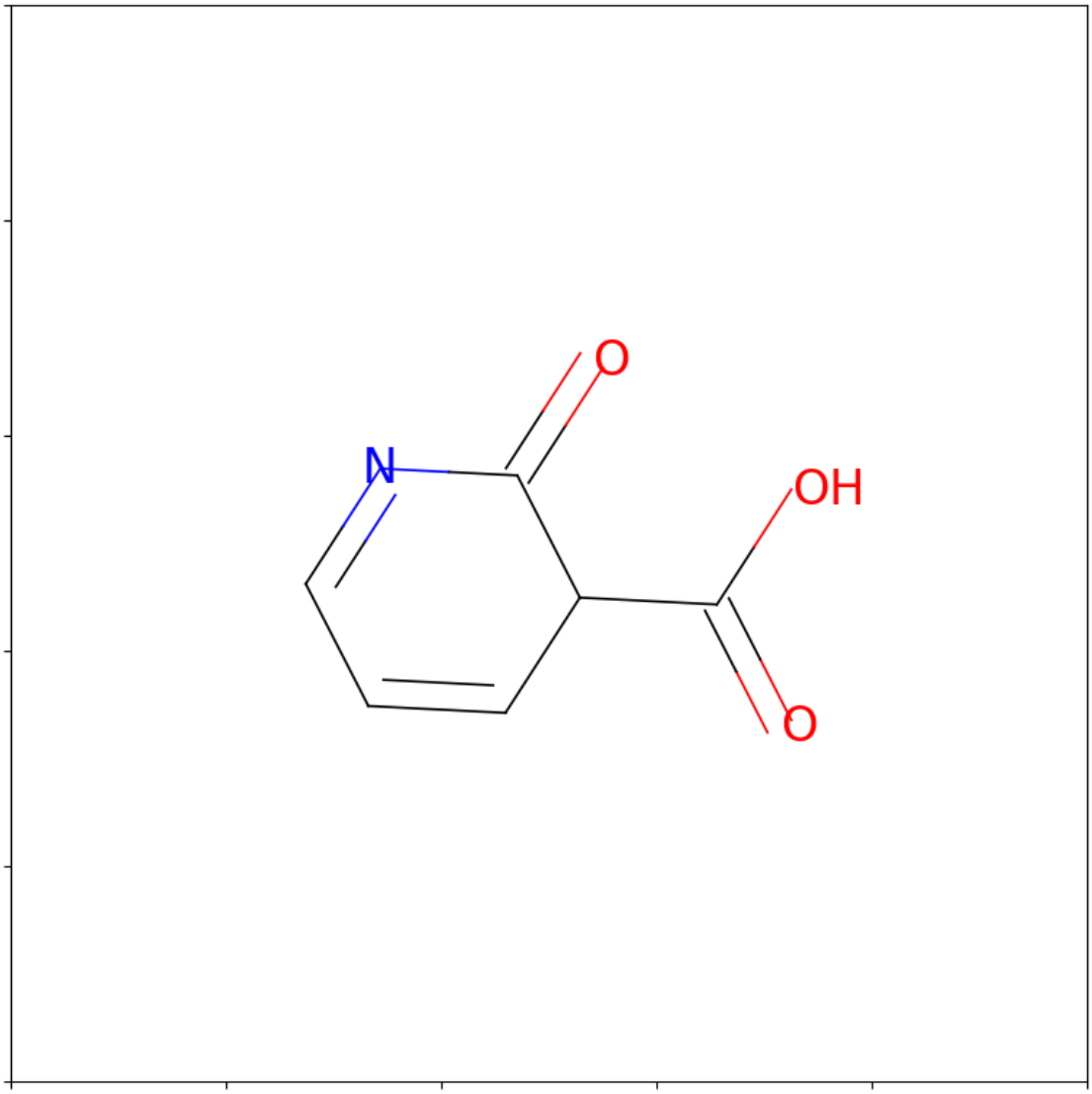
```
Thanks for your input
Your selection was:
Temperature: 120
Time: 72.0
Solvent1: N,N-dimethylformamide (DMF)
Solvent2: None
Solvent3: None
Counter Ion: Cl
Metal_Concentration: 0.05
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: no additive
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the thermal&chemical stability of
the linker under the proposed crystallization conditions
```

```
# MOF 50
```

Here is the linker:

[215]:
```
Image('./ISUGIN_cleansingle_linker0.png')
```

[215]:



The metal center of this MOF is ``Gd''. The oxidation state of the metal is ``3''.

Colour code of the atoms in the following 3D unit cell.

The 3D visualization in the next cell is interactive. You can rotate with your mouse and zoom in with the mouse wheel.

[216]:
```
nutils.viewer('./ISUGIN_clean.cif')
```

[217]:
```
temperature_mof_50_Celsius  = 135 #@param {type:'number'}
time_mof_50_hours  = 72 #@param {type:'number'}
```

```
first_solvent_mof_50 = 'N,N-diethylformamide (DEF)' #@param ["None",␣
↪"1-butanol", "2-ethoxyethanol", "N,N-dimethylacetamide (DMAc)",␣
↪"N,N-diethylformamide (DEF)", "N-methylformamide (NMF)", "pyridine",␣
↪"chlorobenzene", "cyclohexanol", "isobutanol", "methylsulfinylmethane␣
↪(DMSO)", "1,4-dioxane", "ethylene glycol", "diethanolamine", "acetone",␣
↪"ethanol", "isopropyl alcohol", "H2O", "chloroform", "1,2-xylene",␣
↪"acetonitrile", "dichloromethane (DCM)", "1-methylpyrrolidin-2-one (NMP)",␣
↪"N,N-dimethylformamide (DMF)", "1,3-butanediol", "tetrahydrofuran (THF)",␣
↪"1,3-dimethyl-1,3-diazinan-2-one (DMPU)", "benzene", "2-aminobutan-1-ol",␣
↪"toluene", "methanol", "dimethylaniline"]
second_solvent_mof_50 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
third_solvent_mof_50 = 'None' #@param ["None", "1-butanol", "2-ethoxyethanol",␣
↪"N,N-dimethylacetamide (DMAc)", "N,N-diethylformamide (DEF)",␣
↪"N-methylformamide (NMF)", "pyridine", "chlorobenzene", "cyclohexanol",␣
↪"isobutanol", "methylsulfinylmethane (DMSO)", "1,4-dioxane", "ethylene␣
↪glycol", "diethanolamine", "acetone", "ethanol", "isopropyl alcohol", "H2O",␣
↪"chloroform", "1,2-xylene", "acetonitrile", "dichloromethane (DCM)",␣
↪"1-methylpyrrolidin-2-one (NMP)", "N,N-dimethylformamide (DMF)",␣
↪"1,3-butanediol", "tetrahydrofuran (THF)", "1,3-dimethyl-1,3-diazinan-2-one␣
↪(DMPU)", "benzene", "2-aminobutan-1-ol", "toluene", "methanol",␣
↪"dimethylaniline"]
additive_mof_50 = 'acid' #@param ['no additive', 'acid', 'base']
counter_ion_mof_50 =  'NO3' #@param ["OAc", "acac", "BF4", "bpdc", "bpy", "Br",␣
↪"C2O4", "Cl", "ClO3", "ClO4", "CN", "CO3", "dien", "en", "F",␣
↪"H2SalPyMeCam", "HCOO", "MeCN", "NH4", "NO3", "O", "OH", "OiPr", "pbc",␣
↪"PF6", "PO4", "PyenH2", "S", "SO4", "meso-tetra(4-carboxyphenyl)porphyrin",␣
↪"SiO3", "NCS", "CH3CH(OH)CO2", "WO4", "NH3", "TeO3", "VO3", "tert-BuO",␣
↪"MoO4", "pztc", "Ag(CN)2"]
concentration_metal_mof_50_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_first_linker_mof_50_mol_per_liter  = 0.05 #@param {type:'number'}
concentration_second_linker_mof_50_mol_per_liter  = 0.0 #@param {type:'number'}
are_you_sure_about_your_selction_mof_50 = 'no' #@param ['no', 'yes']
what_makes_you_so_sure_or_unsure_mof_50 =  'Not sure about the coordination␣
↪chemistry and stability of the linker' #@param {type:'string'}
results['mof_50'] = {}
results['mof_50']['temperature']=temperature_mof_50_Celsius
results['mof_50']['time']=time_mof_50_hours
results['mof_50']['solvent1']=first_solvent_mof_50
```

```
results['mof_50']['solvent2']=second_solvent_mof_50
results['mof_50']['solvent3']=third_solvent_mof_50
results['mof_50']['additive']=additive_mof_50
results['mof_50']['counter']=counter_ion_mof_50
results['mof_50']['metal']=concentration_metal_mof_50_mol_per_liter
results['mof_50']['linker1']=concentration_first_linker_mof_50_mol_per_liter
results['mof_50']['linker2']=concentration_second_linker_mof_50_mol_per_liter
results['mof_50']['surely']=are_you_sure_about_your_selction_mof_50
results['mof_50']['additional']=what_makes_you_so_sure_or_unsure_mof_50
```

[218]:
```
nutils.print_choice(temperature_mof_50_Celsius, time_mof_50_hours,␣
↪first_solvent_mof_50,second_solvent_mof_50,third_solvent_mof_50 ,␣
↪counter_ion_mof_50, concentration_metal_mof_50_mol_per_liter,␣
↪concentration_first_linker_mof_50_mol_per_liter,concentration_second_linker_mof_50_mol_per_
↪, additive_mof_50,are_you_sure_about_your_selction_mof_50,␣
↪what_makes_you_so_sure_or_unsure_mof_50 )
```

```
Thanks for your input
Your selection was:
Temperature: 135
Time: 72
Solvent1: N,N-diethylformamide (DEF)
Solvent2: None
Solvent3: None
Counter Ion: NO3
Metal_Concentration: 0.05
First_Linker_Concentration: 0.05
Second_Linker_Concentration: 0.0
Additive: acid
Are_You_Sure_About_Your_Selection: no
What_Makes_You_So_Sure/Unsure: Not sure about the coordination chemistry and
stability of the linker
```

3 Let's finally save and download all results

Please run the following two cells (using ``Shift+Enter'') to generate and download your results file. Please send the file to:

[ ]:
```
nutils.save_results(results, "results.txt")
```

[ ]:
```
files.download('results.txt')
```

[ ]:
```

```