E-Futures

The University Of Sheffield.

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MOFs: Metal Organic Frameworks

BY SAM RING

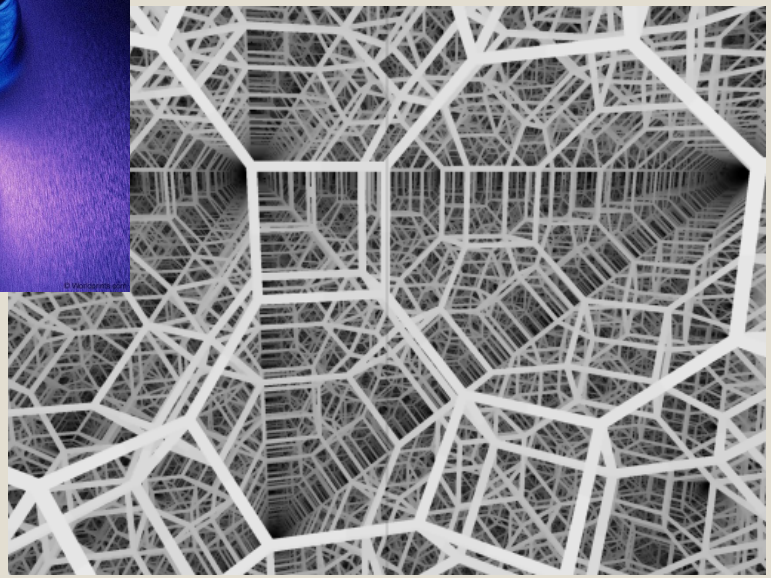
Overview

- MOFs – A quick re-cap
- Approaching the problem
- Results and analysis
- Making new MOFs
- Future work
- Acknowledgements

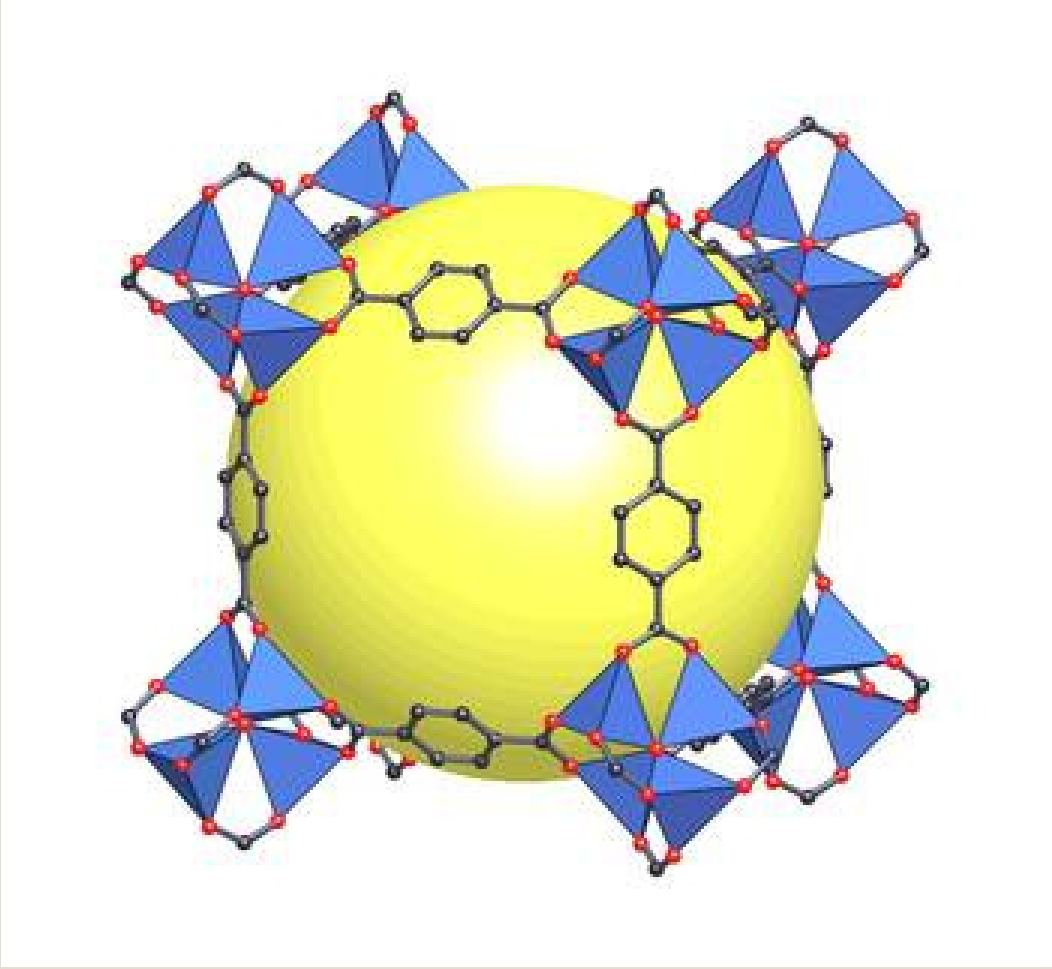
MOFs – What are they and why make them?

MOFs – Metal Organic Frameworks

"An extended framework of metal atoms or clusters connected by organic linkers"

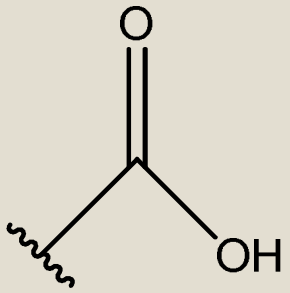


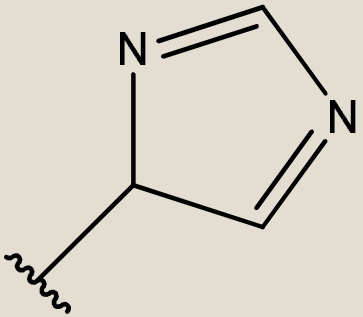
MOF-5 – A schematic view



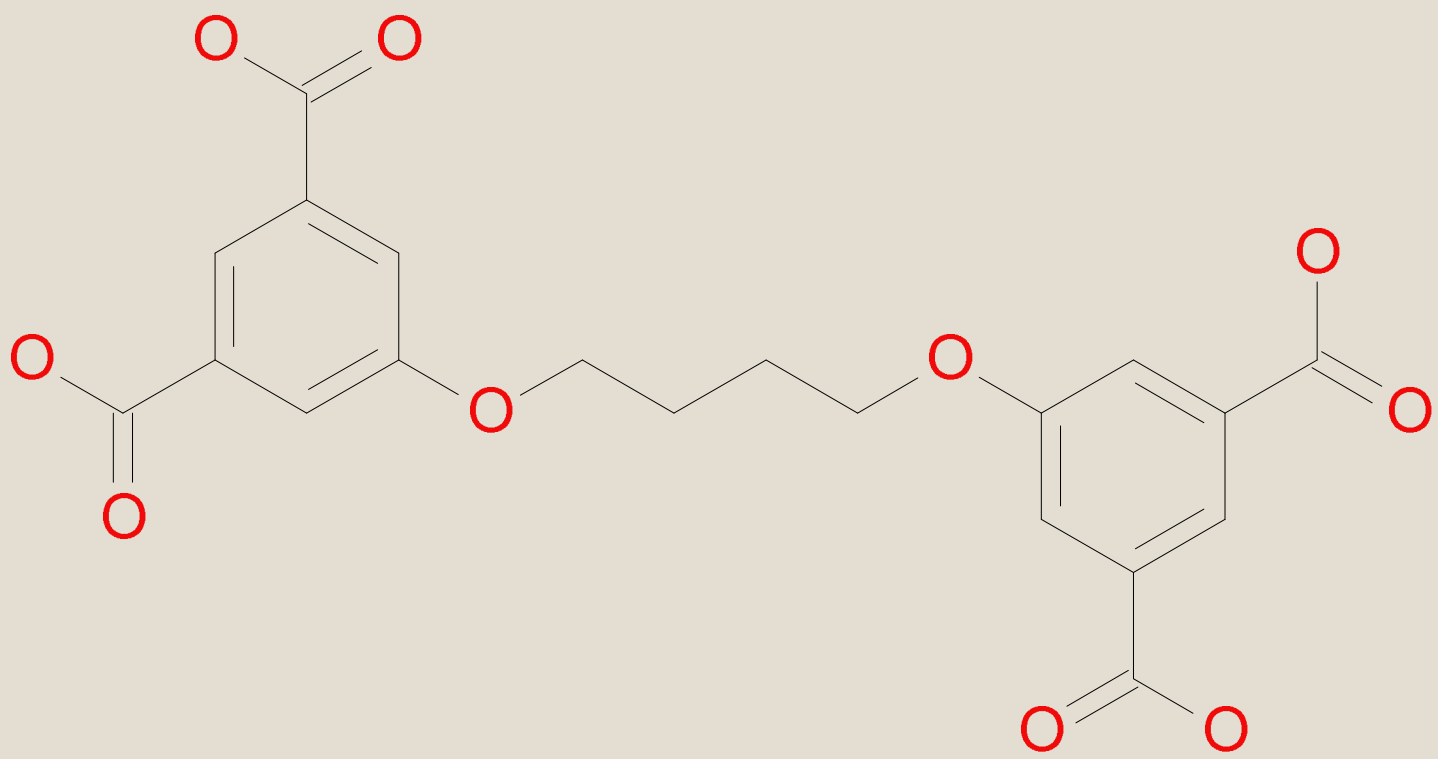
Approaching the problem

- Lots of metals, tens of thousands of potential ligands
- What makes a good ligand?
  - Co-ordinates to wide range of metals
    - Carboxylates
    - Azoles
  - Cheap and easy to make
  - Flexible/adaptive



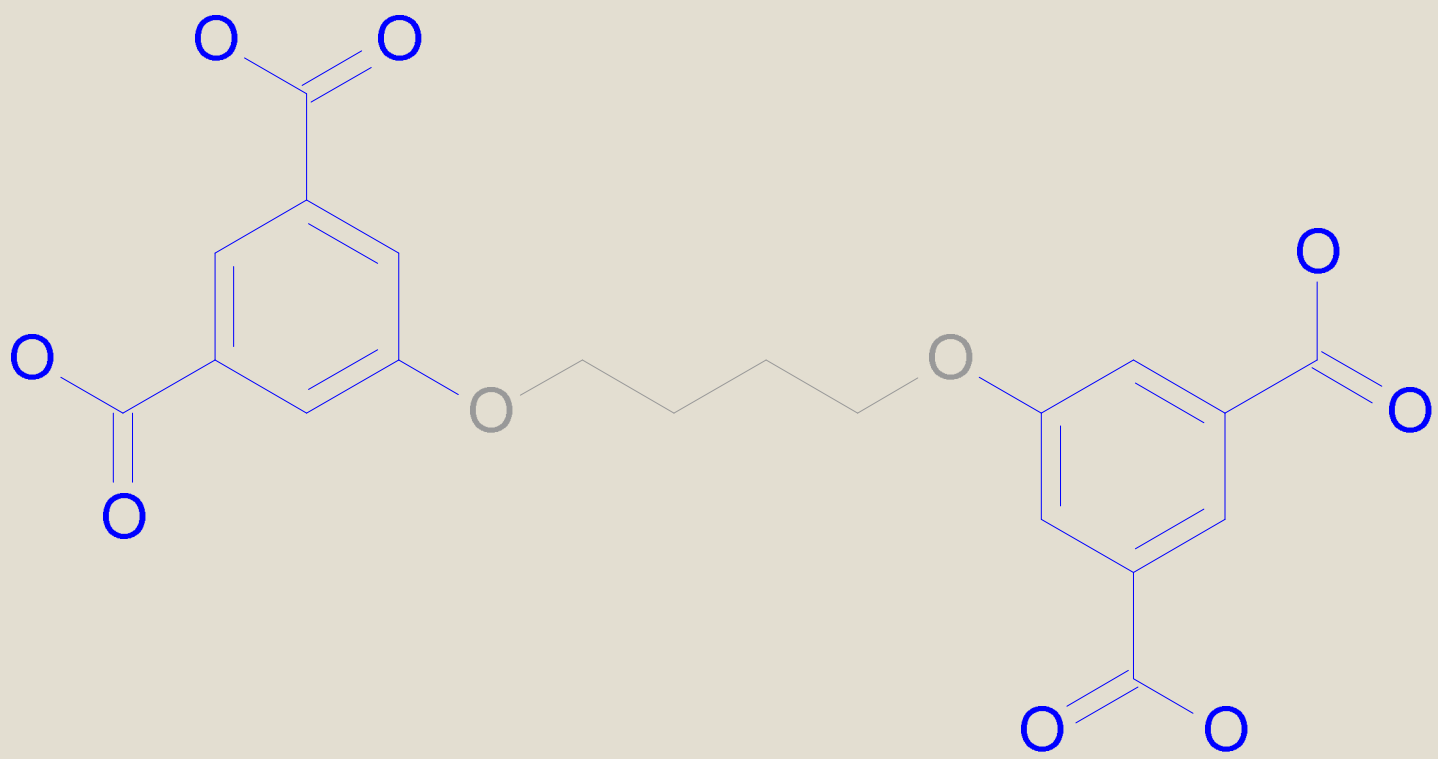


Ligands

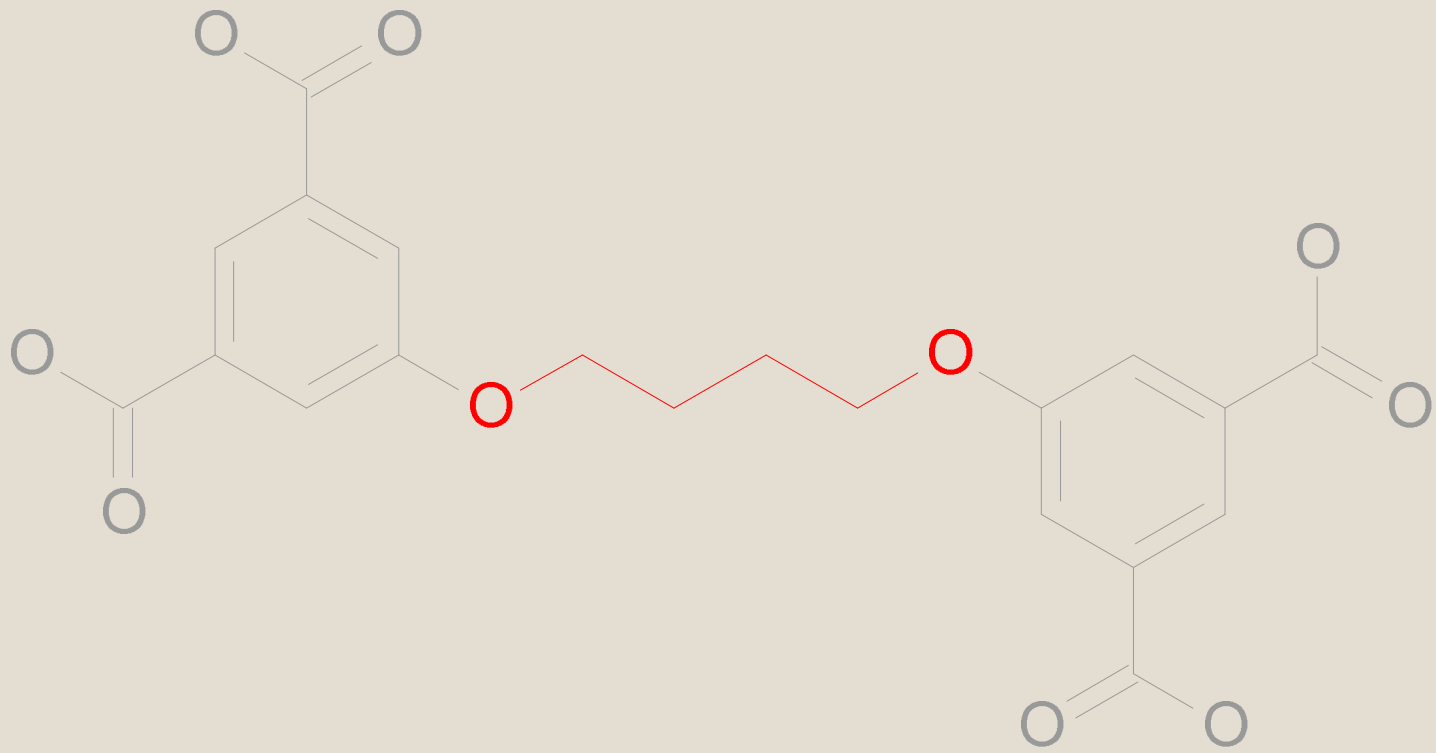


5-[4-(3,5-dicarboxylphenoxy)butoxy]benzene-1,3-dicarboxylic acid

Ligands



Ligands



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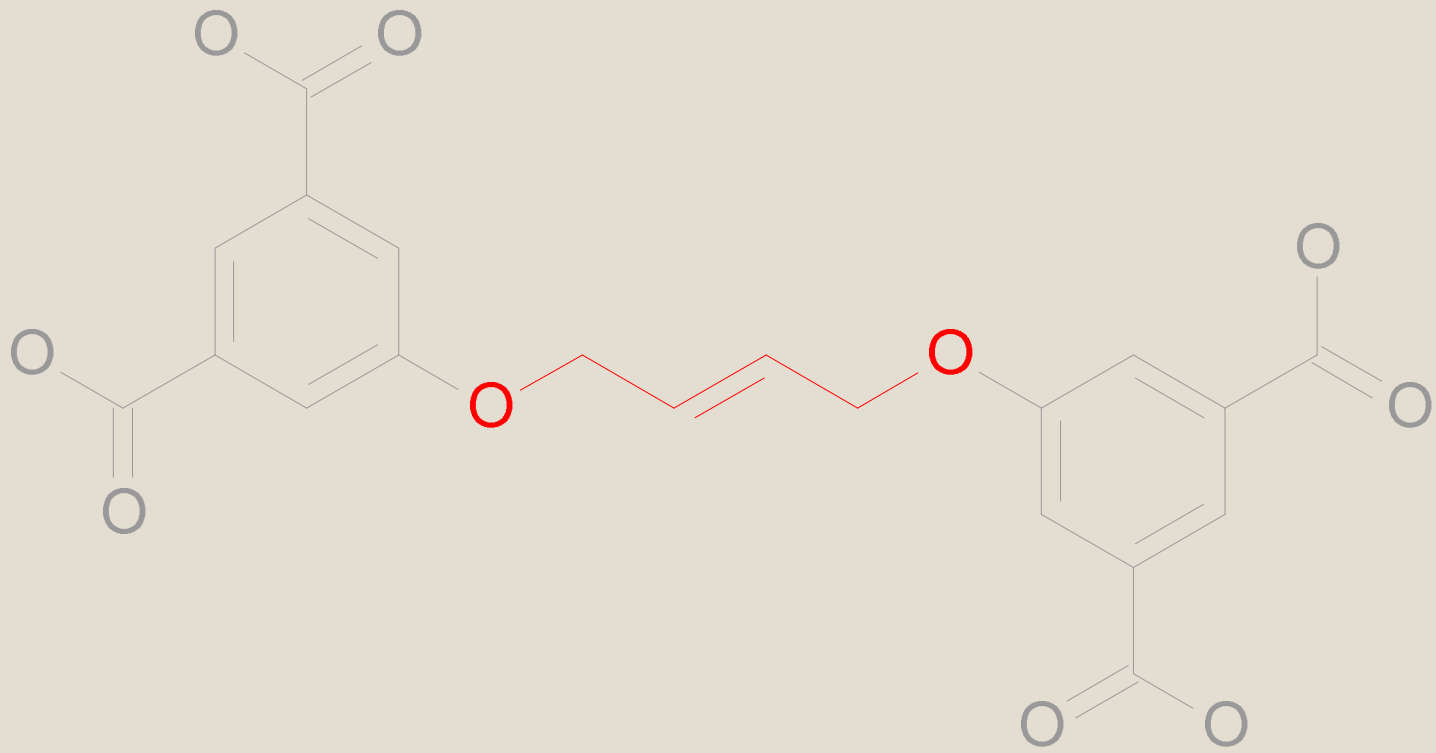

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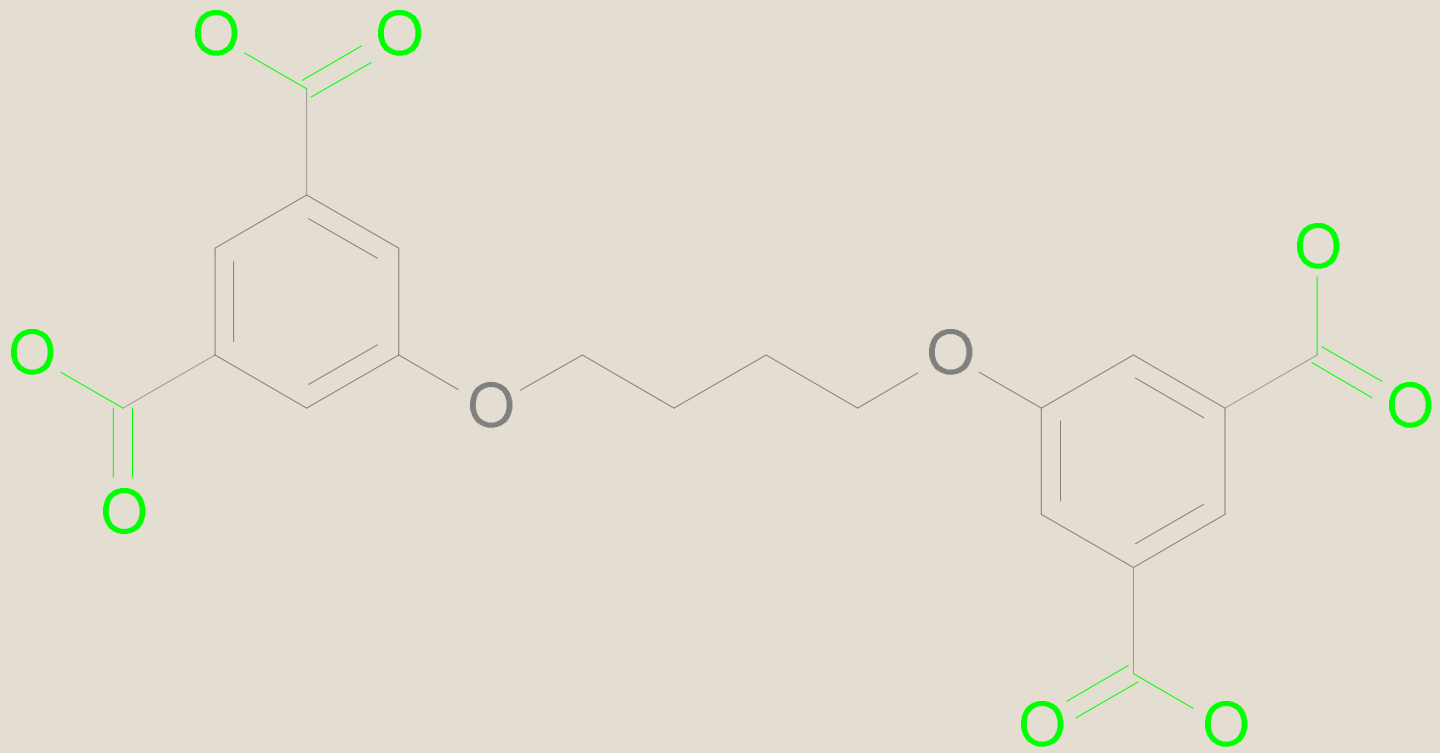

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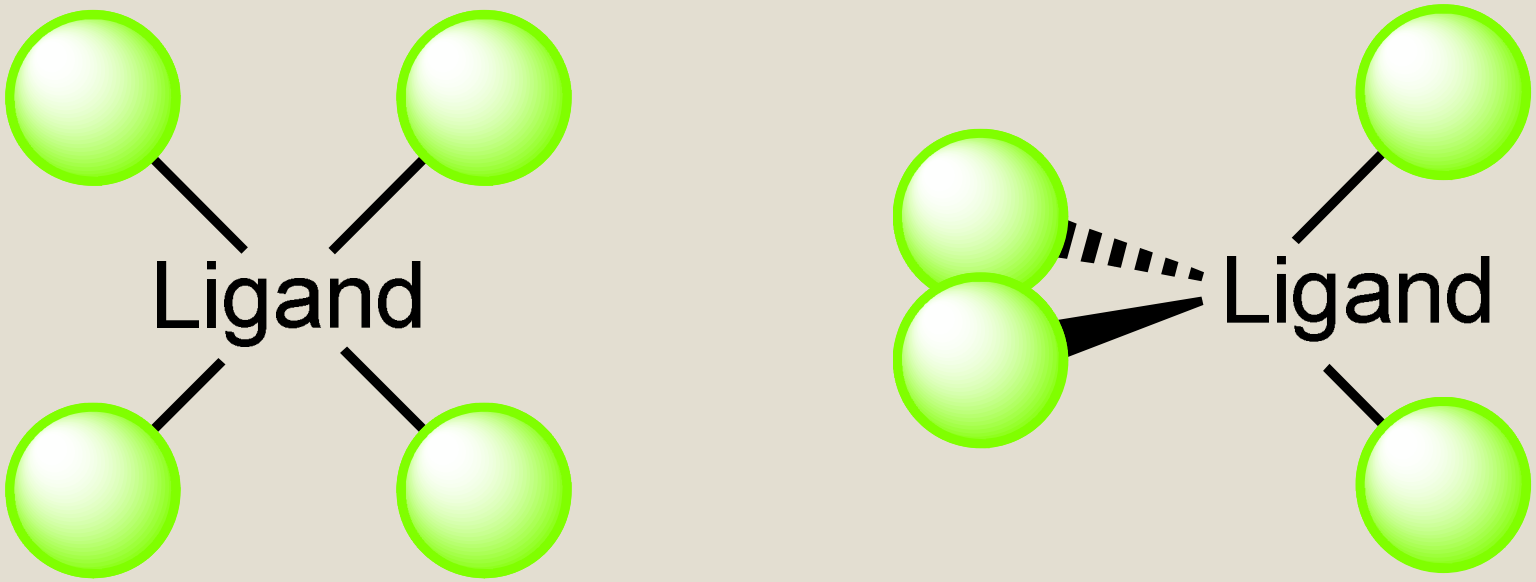


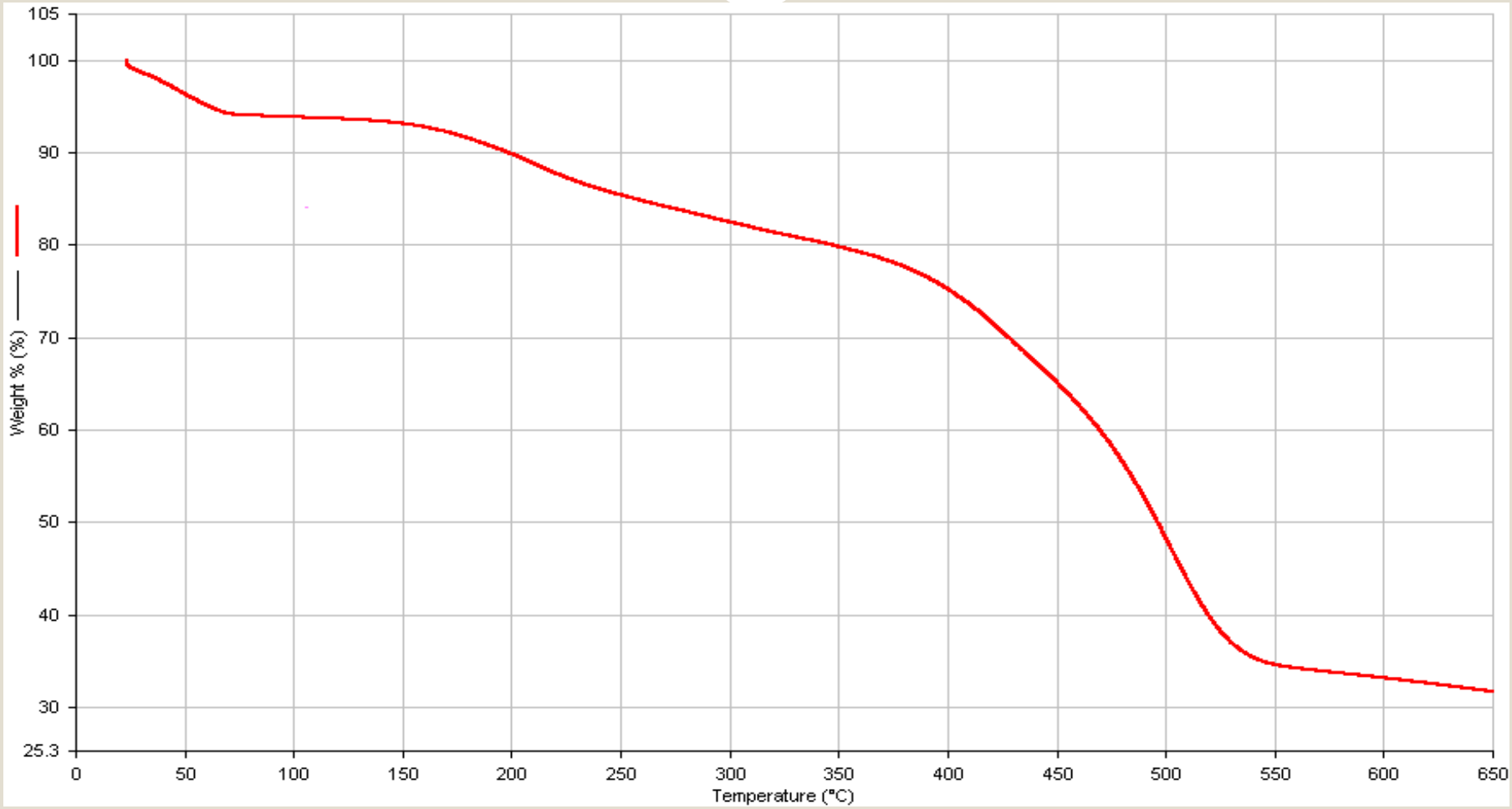
Sam Hawxwell

- Made MOFs with Zinc
  - Crystal system Monoclinic or Triclinic?
- Gas sorption potential unknown
  - Good starting point
- Initial aim to re-synthesize known MOFs for gas sorption measurements
  - Easy right?
    - Dependant on directed self-assembly – potential for problems

Results

- Butane tetra-acid
  - Product was a powder, powder diffraction pending.
  - Thermogravametric analysis (TGA)
  - Elemental analysis
- Butene tetra-acid
  - Single crystal solved
    - Triclinic, tetrahedral ligand orientation
  - Thermogravametric analysis (TGA)
  - Elemental analysis

TGA - Butane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90
80
70
60
50
40
30
25.3
Weight % (%)
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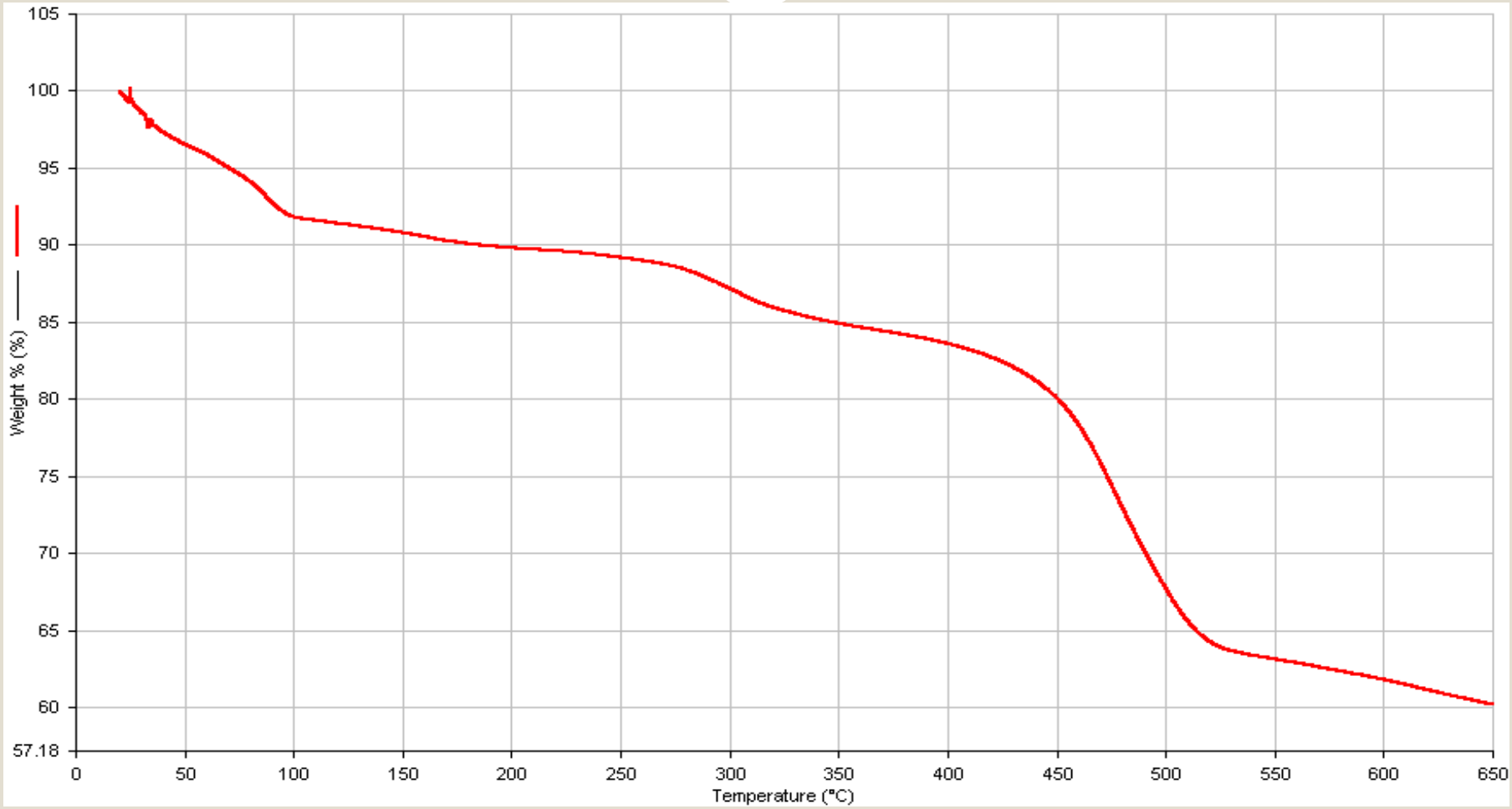
50
100
150
200
250
300
350
400
450
500
550
600
650
Temperature (°C)

TGA - Butene


105
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95
90
85
80
75
70
65
60
57.18
Weight % (%)
0
50
100
150
200
250
300
350
400
450
500
550
600
650
Temperature (°C)

Making new MOFs

- Many things to vary
  - Metals
    - Nickel, Cobalt, Manganese, Copper, Cadmium and Silver
  - Salt
    - NO_3, ClO_4, CH_3O_2H
  - Metal : Ligand ratio
  - Solvent system
    - 3:3:2 EtOH, DMF, H_2O
  - Temperature profile

- Success with $Ni(NO_3)_2$

Future work

- Large number of combinations remain for existing metal/ligand combination
- Larger, more substituted linkers including Pentaerythritol tetrabromide could be used in place of existing 1,4-dibromobutane

Acknowledgements

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- Nik Reeves, Engineering materials X-Ray powder diffraction lab manager

Questions?