Supporting Information

# Structural, thermal and topological characterization of coordination networks containing flexible aminocarboxylate ligands with a central biphenylene scaffold

Davide Balestri,[a,c] Patrick Scilabra,[b] Claudia Carraro,[a] Andrea Delledonne,[a] Alessia Bacchi,[a,c] Paolo Pio Mazzeo[a,c], Lucia Carlucci and Paolo Pelagatti*,[a]

[a]Department of Chemical Sciences, Life Sciences and Environmental Sustainability, University of Parma, Parco Area delle Scienze 17/A, 43124 Parma, Italy.

[b]Department of Chemistry, Materials and Chemistry Engineering "Giulio Natta", Politecnico di Milano, Via Mancinelli 7, 20131 Milano, Italy.

[c]Biopharmanet-TEC, Università degli studi di Parma, via Parco Area delle Scienze 27/A, 43124 Parma, Italy.

[d] Department of Chemistry, Università degli Studi di Milano, via Golgi 19, 20133, Milan, Italy

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# 1. Optical Microscope Images of MOF crystals

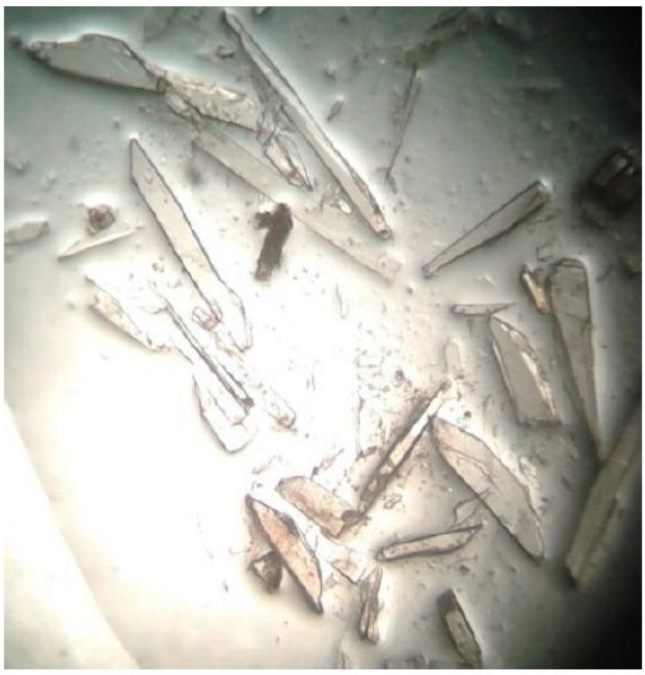

**Figure S 1** Crystals of PUM*flex*1-Zn

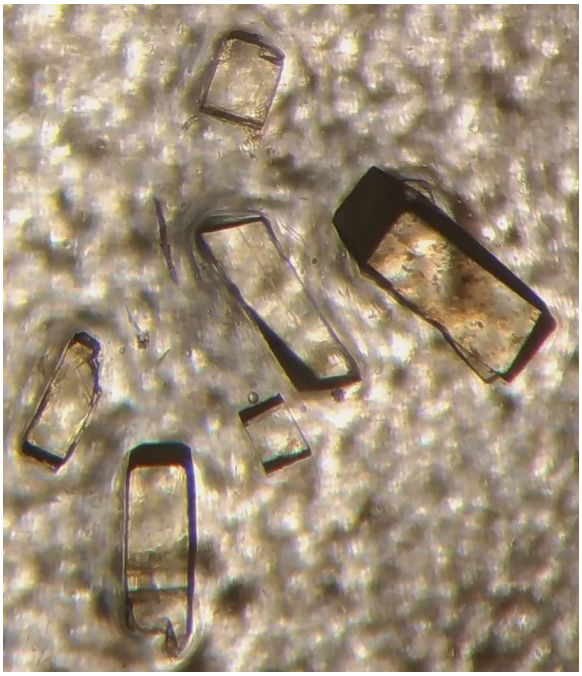

**Figure S 2** Crystals of PUM*flex*1.1-Zn

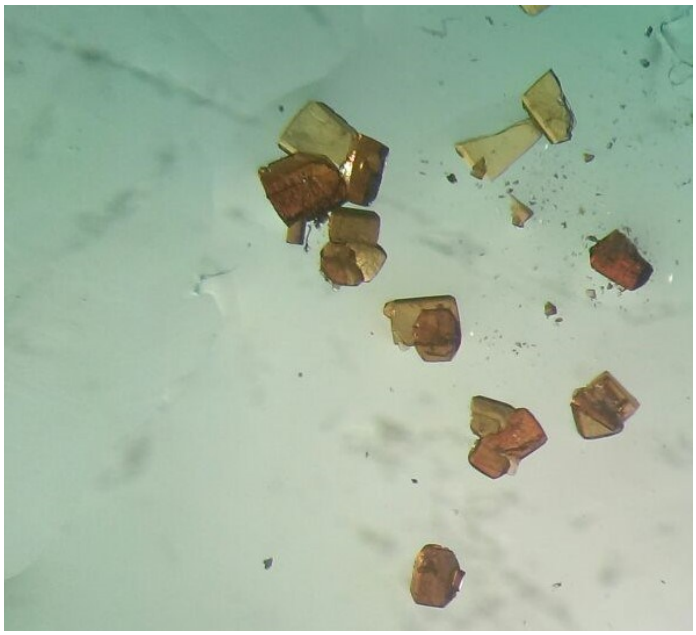

**Figure S 3** Crystals of PUM*flex*2-Cd

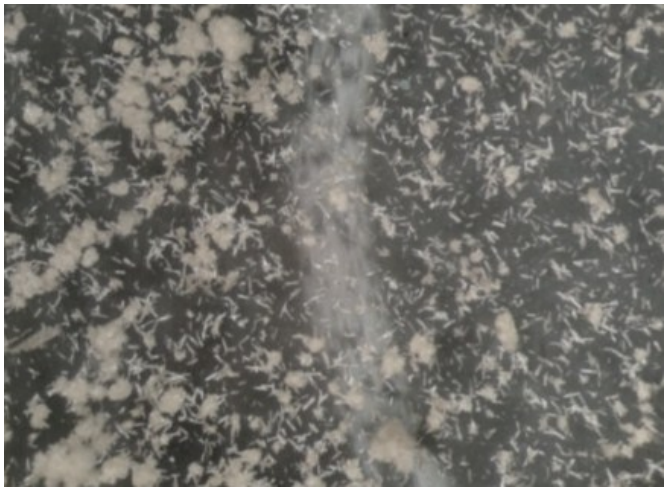

**Figure S 4** Crystals of PUM*flex*1-Zr

## 2. Additional X-Ray Figures

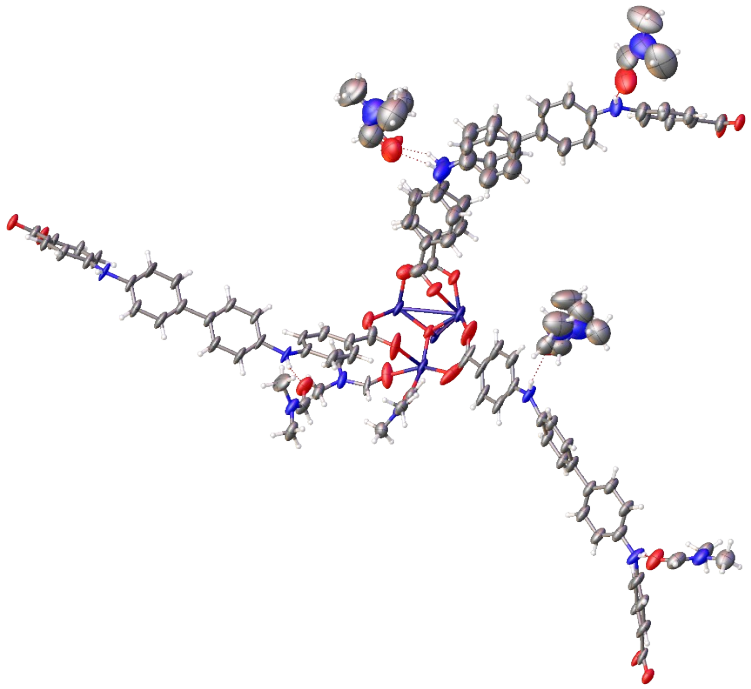

**Figure S 5** Asymmetric unit of PUM*flex*1-Zn. All non-hydrogen atoms shown as ellipsoids at the 50% probability level. H atoms (isotropically refined) are reported in ball-and-stick style for the sake of clarity.

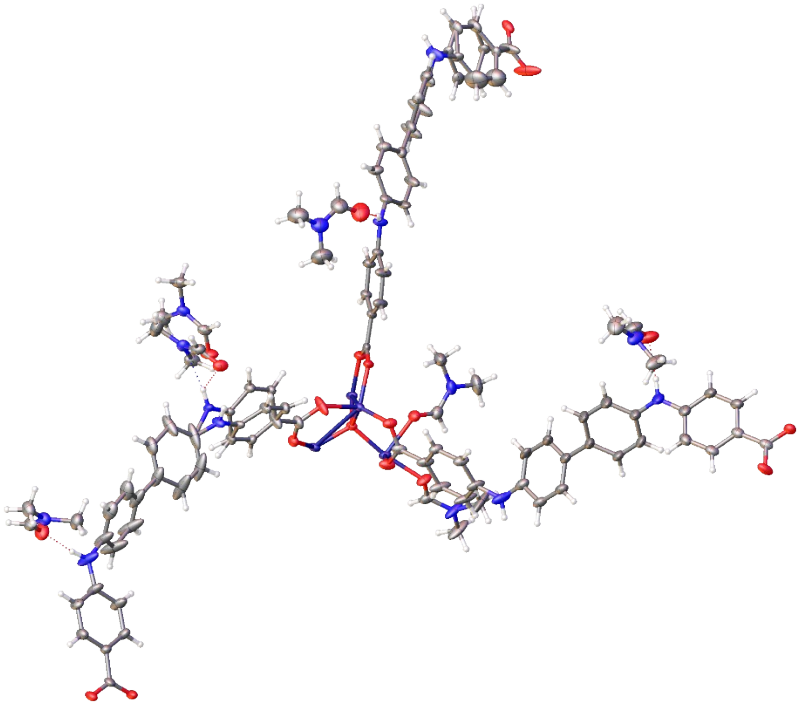

**Figure S 6** Asymmetric unit of PUM*flex*1.1-Zn. All non-hydrogen atoms shown as ellipsoids at the 50% probability level. H atoms (isotropically refined) are reported in ball-and-stick style for the sake of clarity.

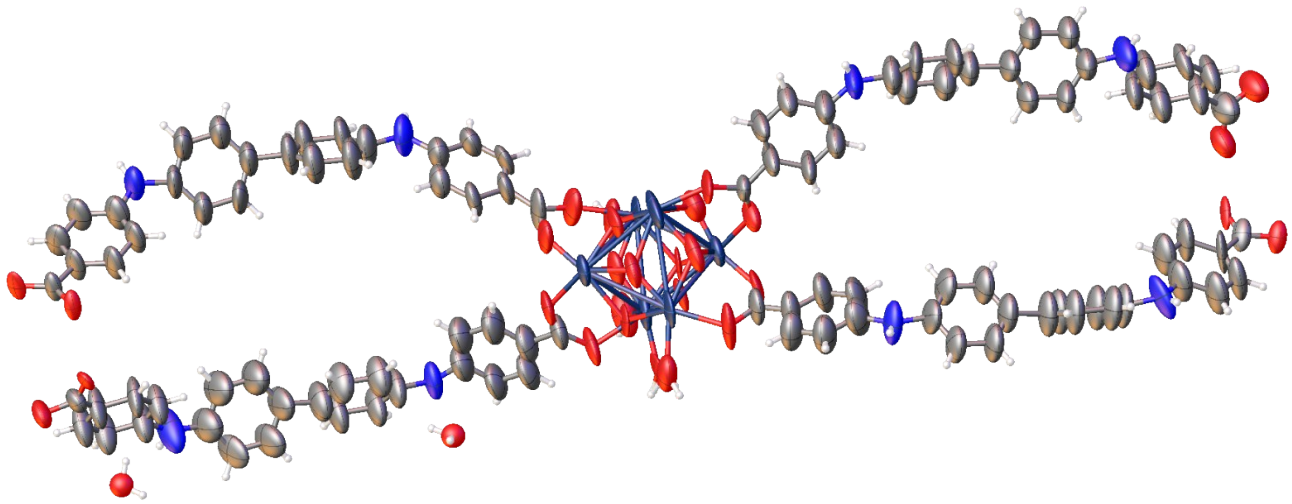

**Figure S 7**Asymmetric unit of PUM*flex*1-Zr. All non-hydrogen atoms shown as ellipsoids at the 50% probability level. H atoms (isotropically refined) are reported in ball-and-stick style for the sake of clarity.

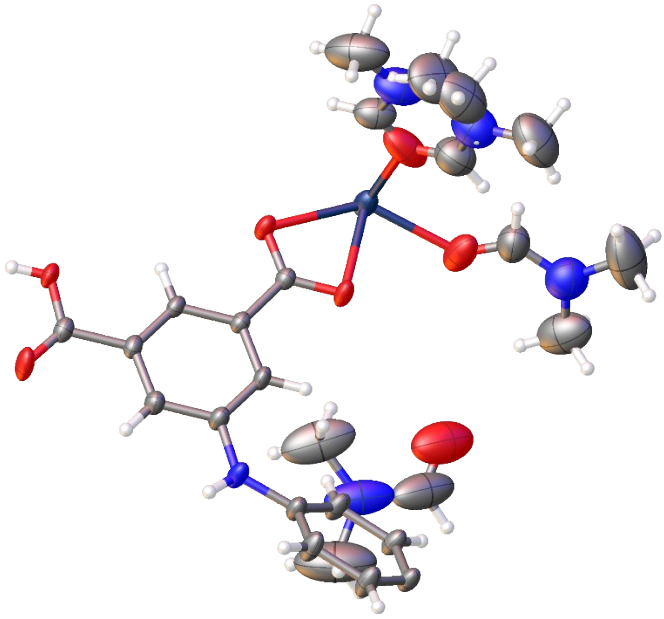

**Figure S 8** Asymmetric unit of PUM*flex*2-Cd. All non-hydrogen atoms shown as ellipsoids at the 50% probability level. H atoms (isotropically refined) are reported in ball-and-stick style for the sake of clarity

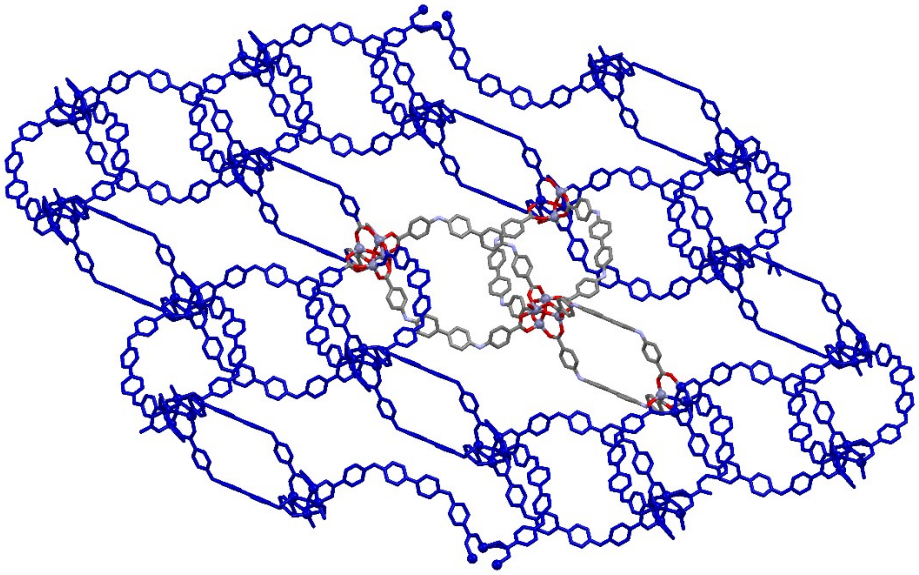

**Figure S 9** Top view of the 2D plane for PUM*flex*1-Zn

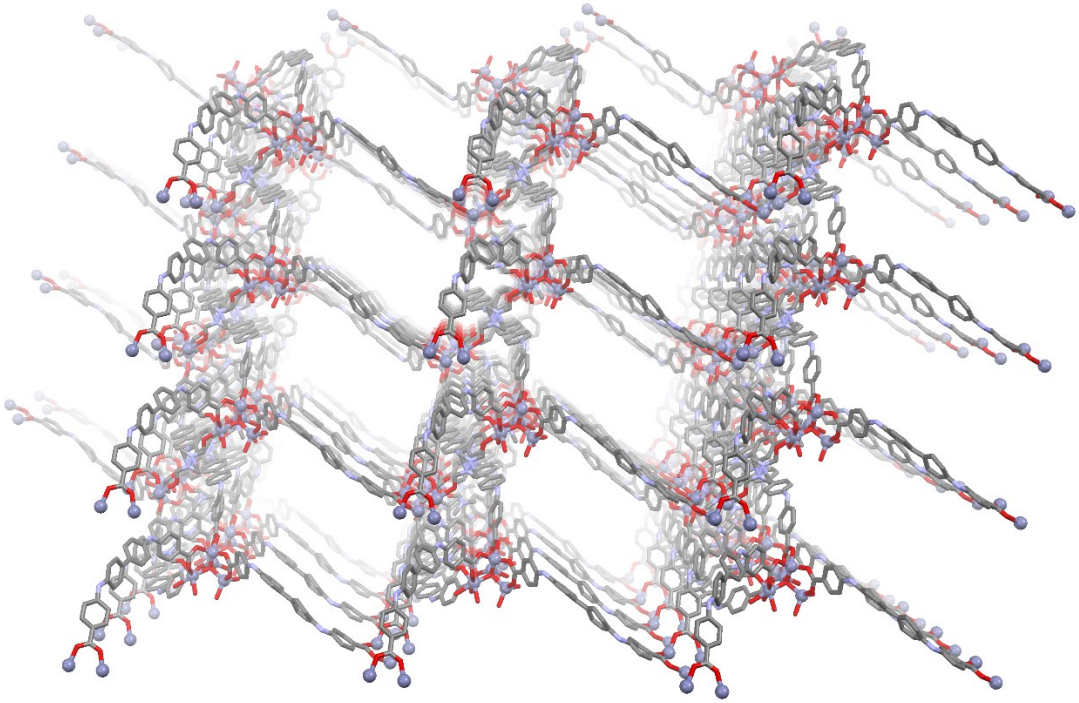

**Figure S 10** View of rectangular channels in PUM-*flex*1-Zn along the crystallographic axis b.

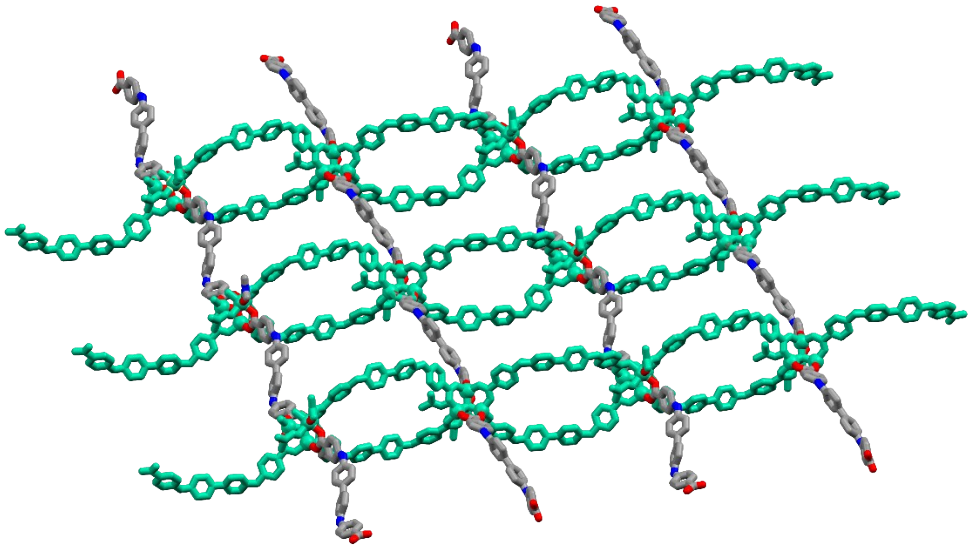

**Figure S 11** Top view of the 2D plane in PUM*flex*1.1-Zn

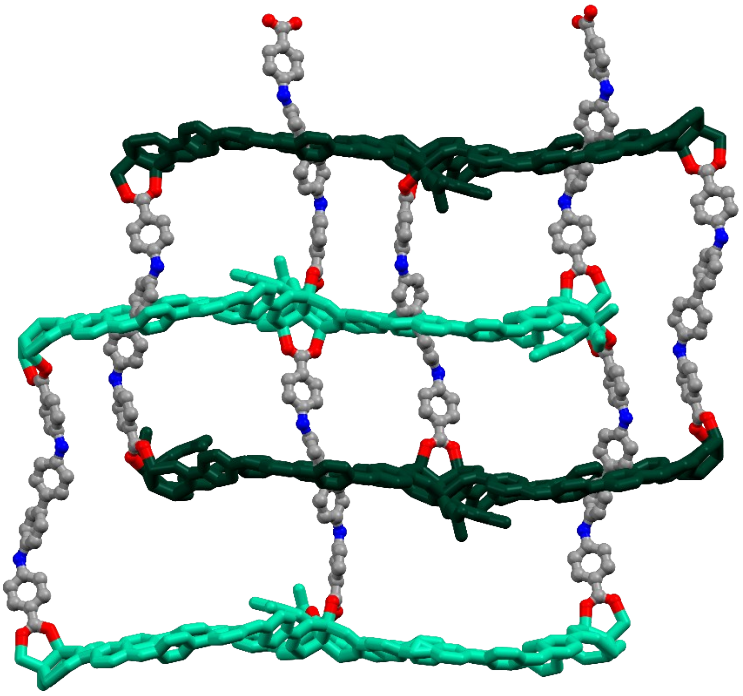

**Figure S 12** Nets interpenetration in PUM*flex*1.1-Zn

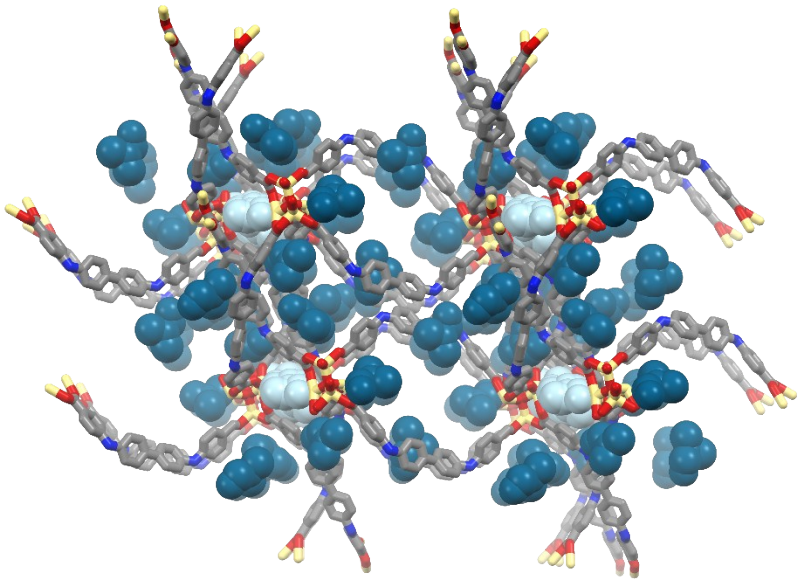

**Figure S 13** View of channels of PUM*flex*1-Zn along crystallographic axis a: light blue color for Zn-coordinated DMF molecules, dark blue color for weakly bound DMF molecules.

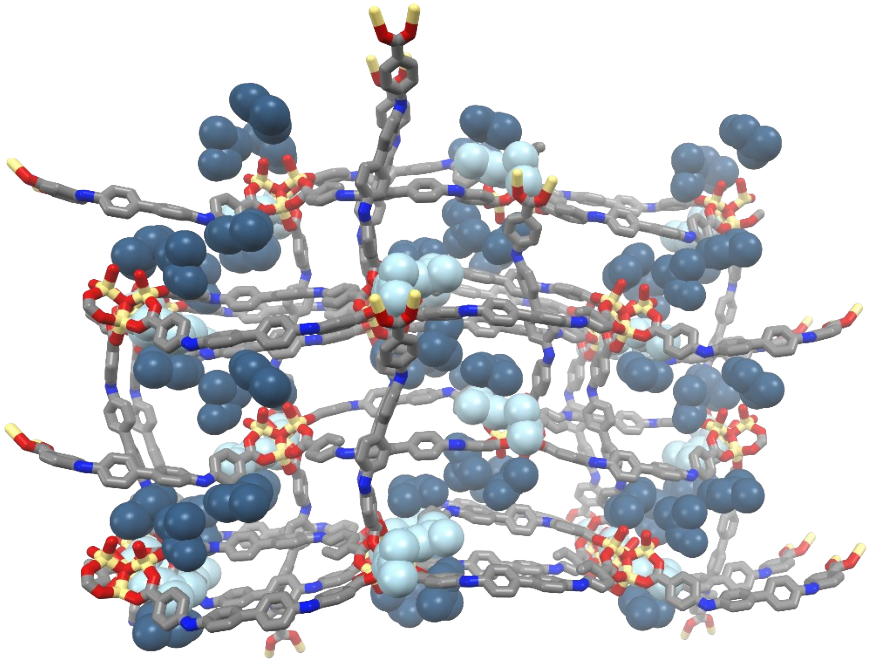

**Figure S 14** View of channels of PUM*flex*1.1-Zn along crystallographic axis a: light blue color for Zn-coordinated DMF molecules, dark blue color for weakly bound DMF molecules.

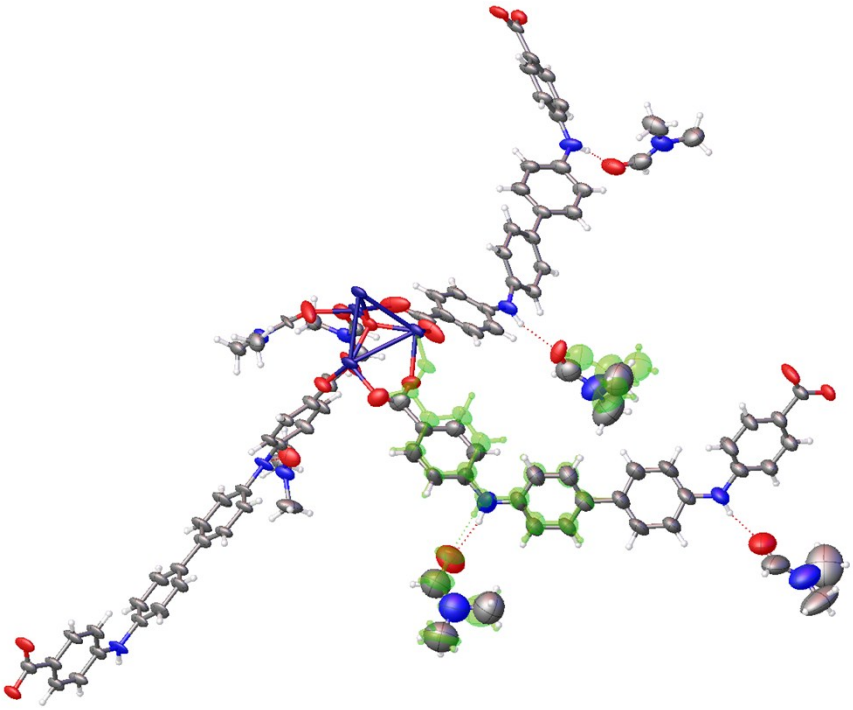

**Figure S 15** Additional view of PUM*flex*1-Zn asymmetric unit: disordered part of ligand L1 and DMF molecules ligand are highlighted

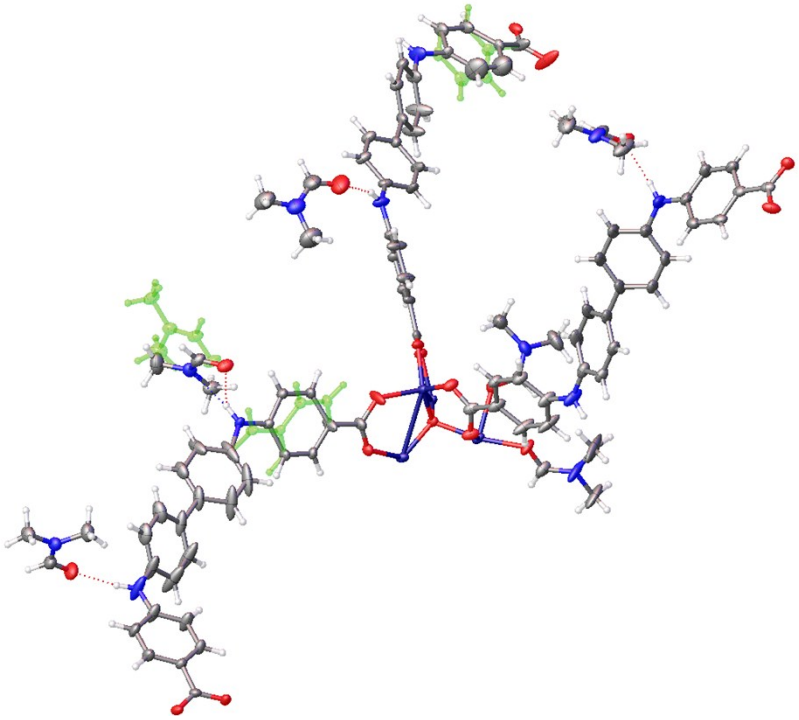

**Figure S 16** Additional view of PUM*flex*1.1-Zn asymmetric unit: disordered part of ligand L1 and DMF molecules ligand are highlighted

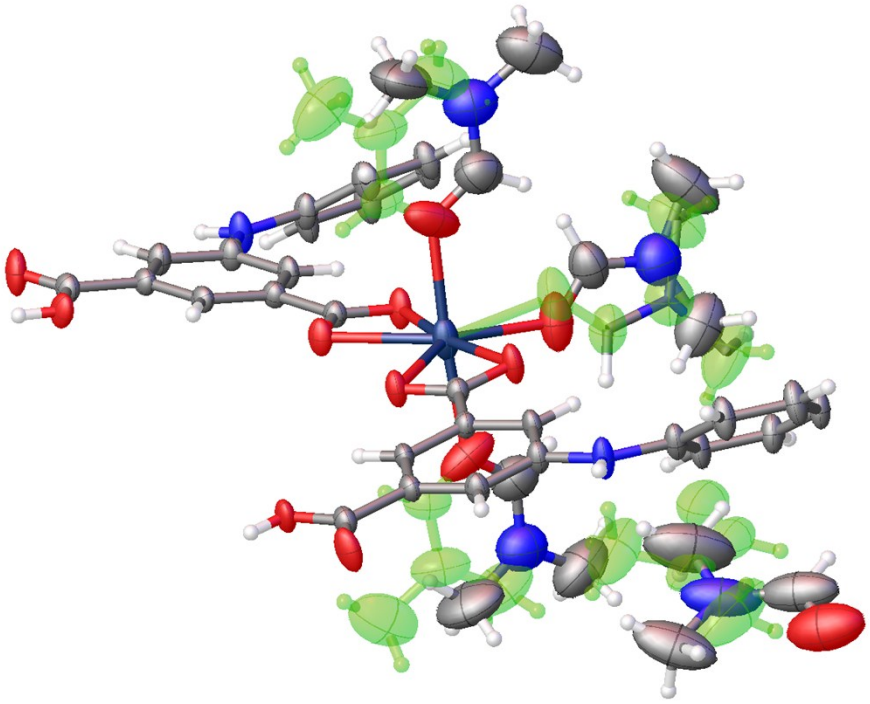

**Figure S 17** PUM*flex*2-Cd metal coordination environment: disorder of coordinated DMF molecules are highlighted.

# 3. Thermal Analysis

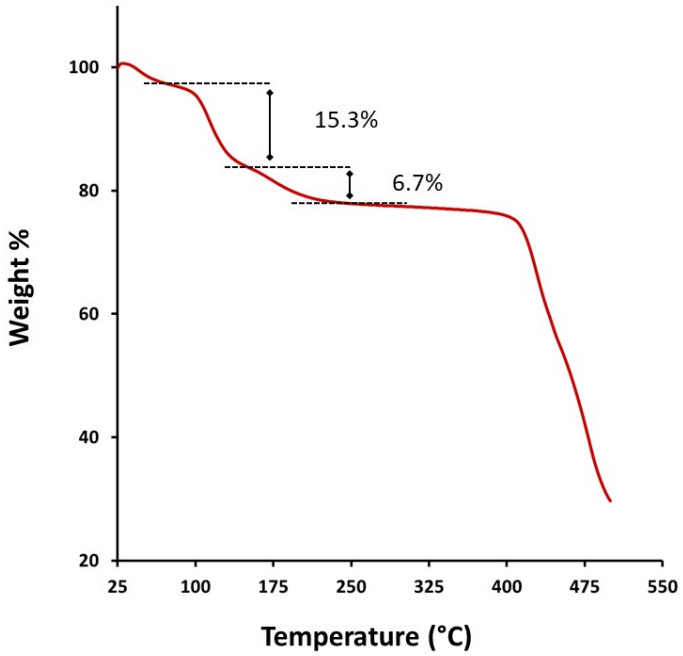


**Figure S 18** TGA trace of PUM*flex*1-Zn

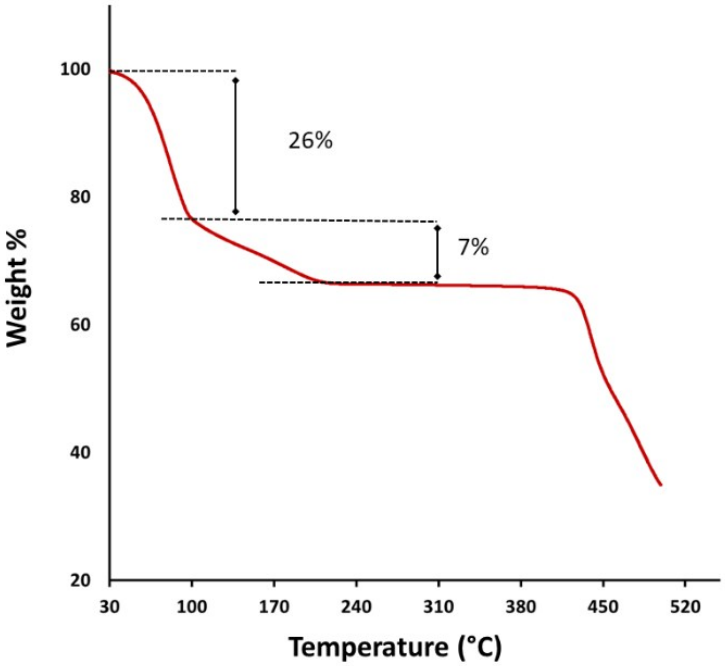


**Figure S 19** TGA trace of PUM*flex*1.1-Zn

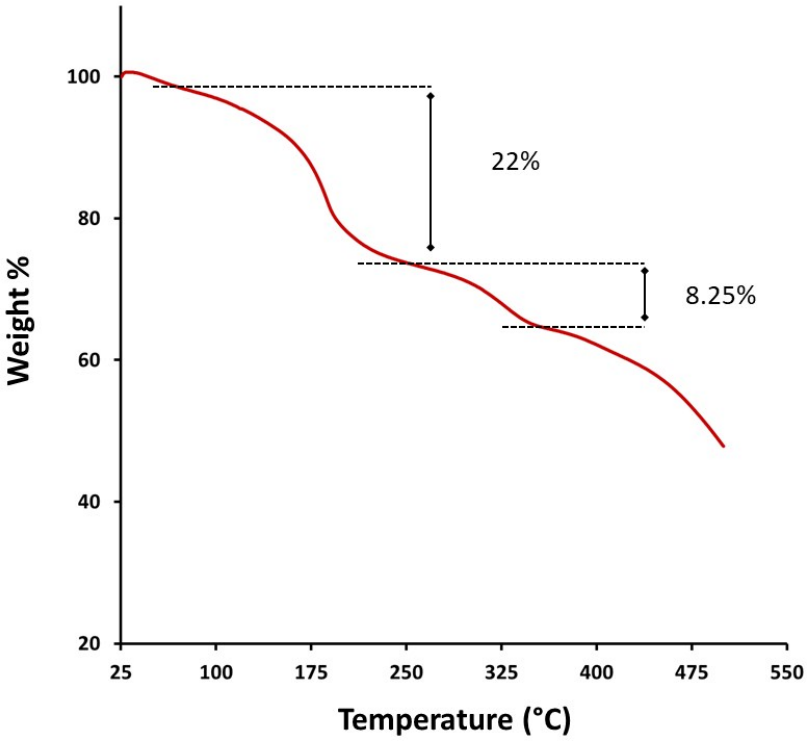


**Figure S 20** TGA trace of PUM*flex*1-Zr

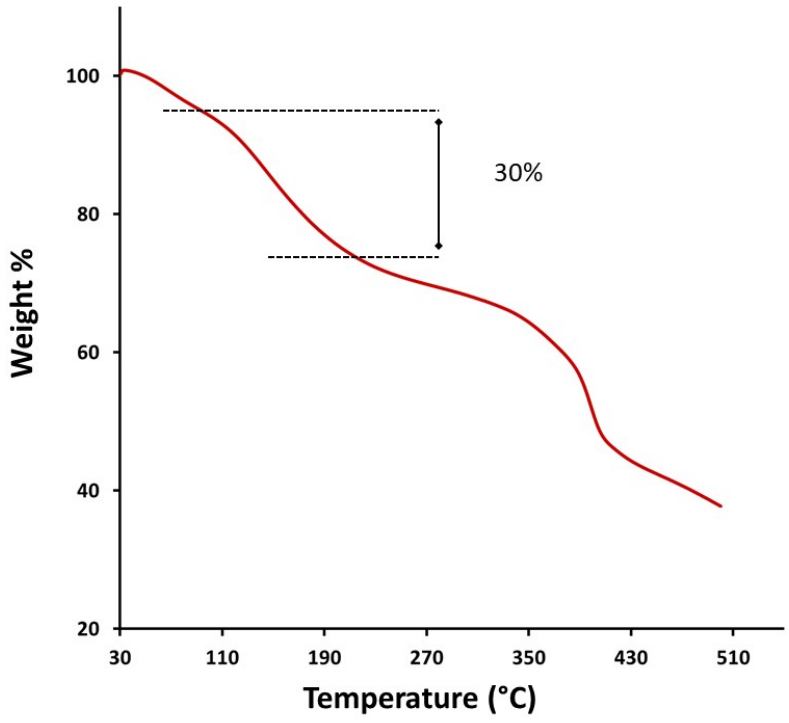


**Figure S 21** TGA trace of PUM*flex*2-Cd

# 4. FTIR (ATR) spectra

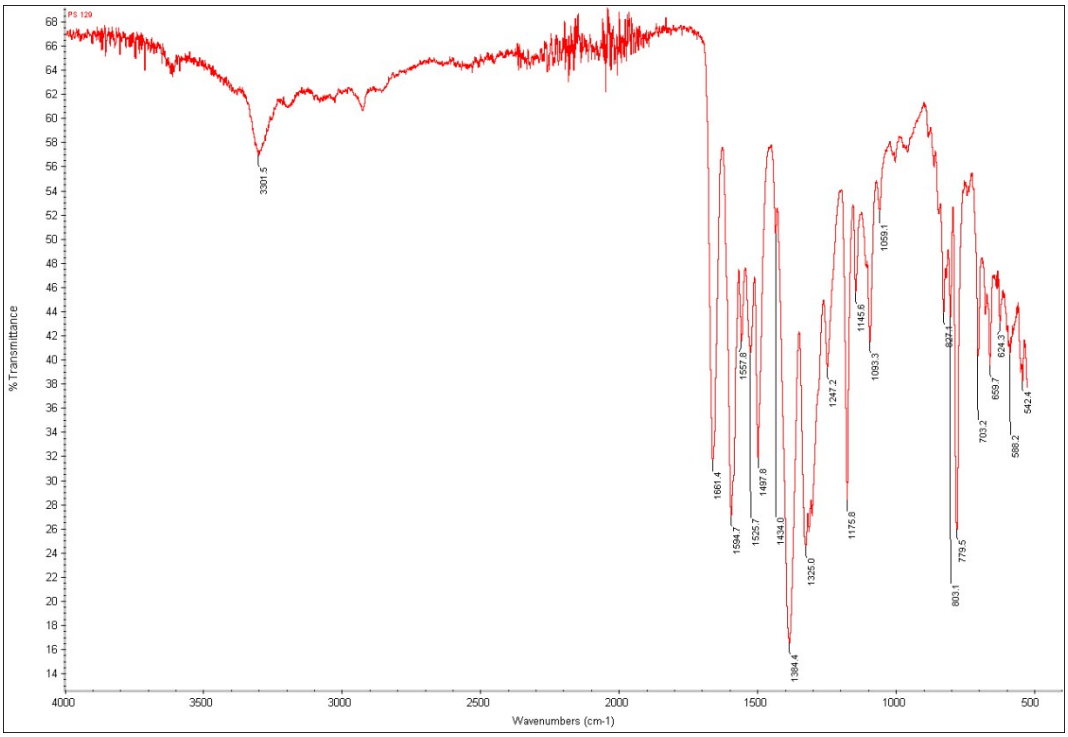


**Figure S 22** FTIR spectra of native PUM*flex*1-Zn crystals.

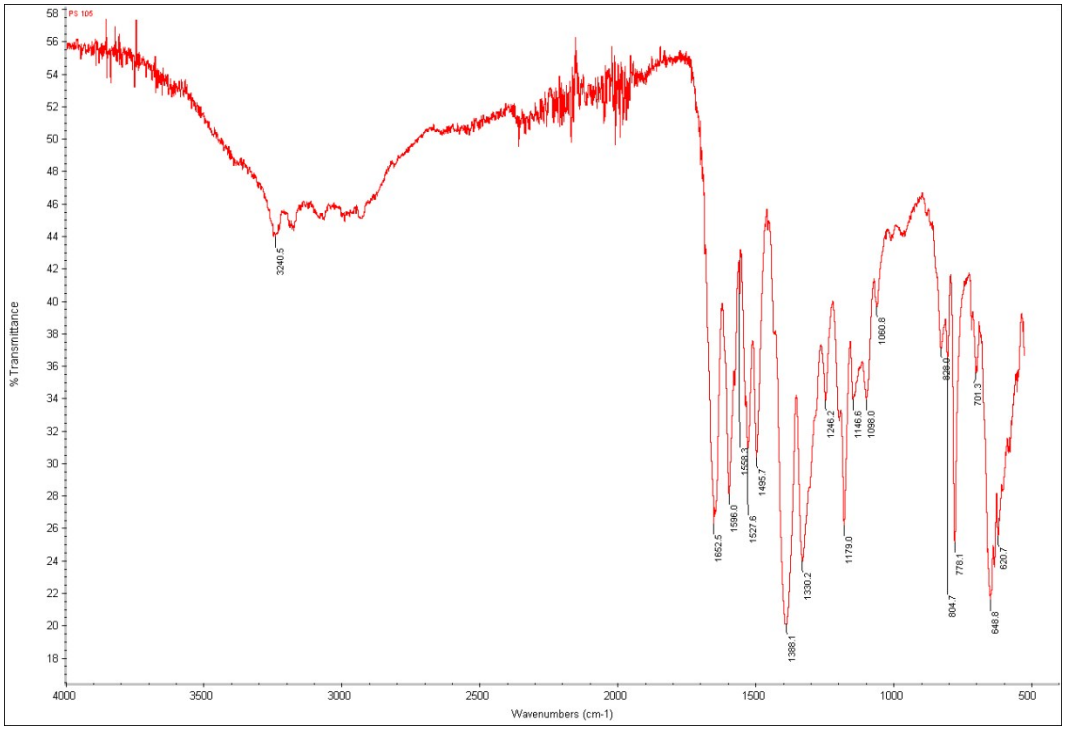


**Figure S 23** FTIR spectra of PUM*flex*1-Zr prior thermal treatment.

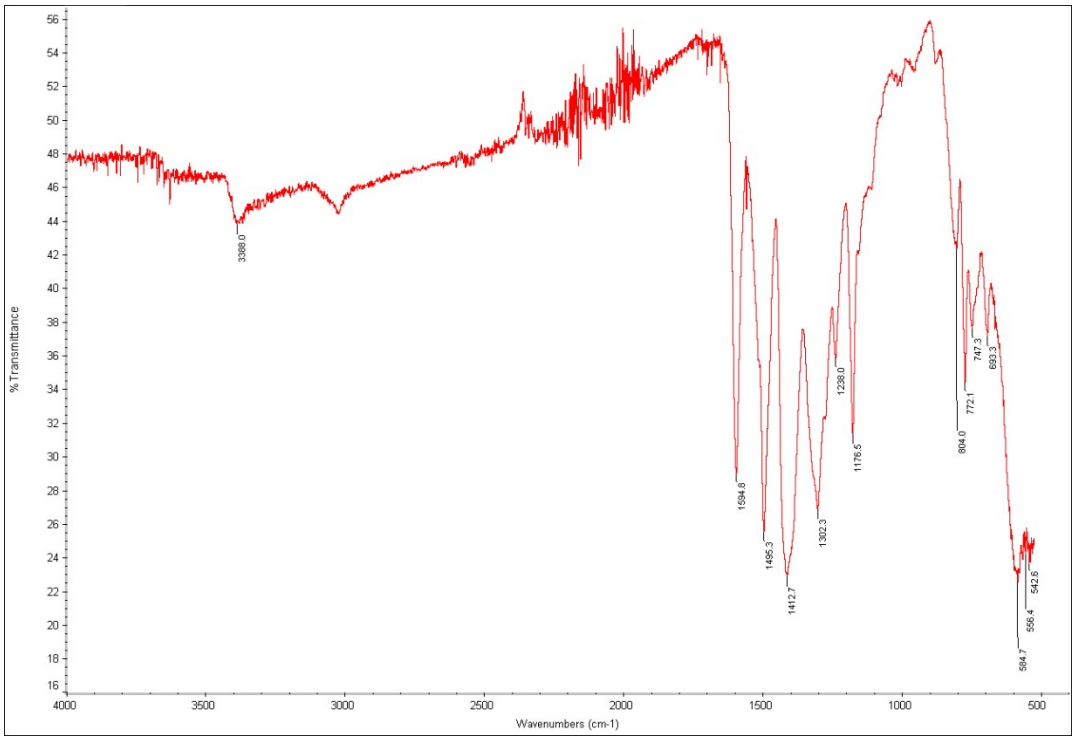


**Figure S 24** FTIR spectra of PUM*flex*1-Zr after thermal treatment.

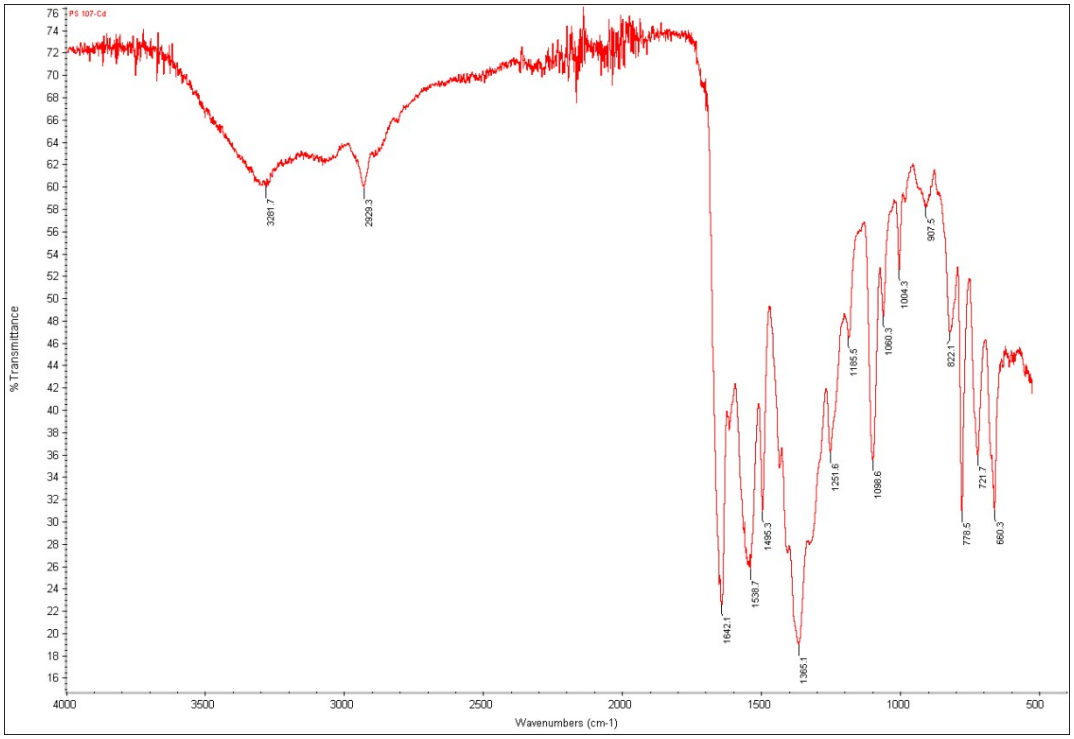


**Figure S 25** FTIR spectra of native PUM*flex*2-Cd crystals.

# 5. Additional topological Data

**Table S1**: List of structures showing 1D chains of 2,8C1 topological type.

| | Refcode | Metal | Reference |
|---|---|---|---|
| 1 | TIZLOF | Th | C.Falaise et al. Inorg.Chem.Commun. 2014, 39, 26. |
| 2 | XUKZOT | Nd | M.-L. Zhang et al. J.Coord.Chem., 2009, 62, 2347. |
| 3 | XUKZIN | Pr | M.-L. Zhang et al. J.Coord.Chem., 2009, 62, 2347. |
| 4 | XUKZAF | Gd | M.-L. Zhang et al. J.Coord.Chem., 2009, 62, 2347. |
| 5 | WURXAJ | Y | S.Mishra et al., Chem.Commun. 2010, 46, 3756. |
| 6 | URACET | U | I.Jelenic et al., Acta Crystallogr., 1964, 17, 758. |
| 7 | QEGPAU | Gd | D.John et al. Z.Naturforsch.,B:Chem.Sci. 2006, 61, 699. |
| 8 | KAHMIR | Th | O.M.Nazarenko et al., Acta Crystallogr.,Sect.C:Cryst.Struct.Commun. 2010, 66, m276. |
| 9 | AGUROK | Eu | J.-C.Rybak et al, Z.Anorg.Allg.Chem. 2010, 636, 126. |
| 10 | BEFBAS | Dy | Y.Shen, et al. Magnetochem. 2016, 2, 44. |
| 11 | TIZLUL | Th | C.Falaise et al, Inorg.Chem.Commun. 2014, 39, 26 |
| 12 | VAVFUW | Er | T.J.Boyle et al., Polyhedron, 2017, 131, 59. |
| 13 | VAVFOQ | Ho | T.J.Boyle et al., Polyhedron, 2017, 131, 59. |
| 14 | VAVFEG | Pr | T.J.Boyle et al., Polyhedron, 2017, 131, 59. |
| 15 | AKOROJ | Ce | M.A.Mansoor, New J.Chem. 2016, 40, 5177. |
| 16 | EJOZUA | Nd | Lu Pan et al., J.Mol.Struct. 2016, 1117, 57 |
| 17 | EJUBAO | Sm | Lu Pan et al., J.Mol.Struct. 2016, 1117, 57 |