Electronic Supplementary Information (ESI) for

Structural diversity of zinc(II) coordination polymers with octafluorobiphenyl-4,4’-dicarboxylate based on mononuclear, paddle wheel and cuboidal units

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Identification codes

(1) – [Zn(eg)$_3$](oFBPDC)
(2) – [Zn(H_2O)(ur)(oFBPDC)]
(3) – [Zn(CH_3OH)($CH_3OCH_2CH_2OH$)(oFBPDC)]
(4) – [Zn_2(CH_3CN)$_2$(oFBPDC)$_2$]·2C_6H_6·2CH_3CN
(5) – [Zn_2(H_2O)$_2$(oFBPDC)$_2$]·4$(CH_3)_2CO$
(6) – [{Zn_4(μ_3-OCH_3)$_4$}(CH_3OH)$_4$(oFBPDC)$_2$]·[{Zn_4(μ_3-OCH_3)$_4$}(H_2O)(CH_3OH)$_3$(oFBPDC)$_2$]·13CH_3OH

H_2oFBPDC – octafluorobiphenyl-4,4’-dicarboxylic acid
eg – ethylene glycol
ur – urotropine, hexamethylenetetramine

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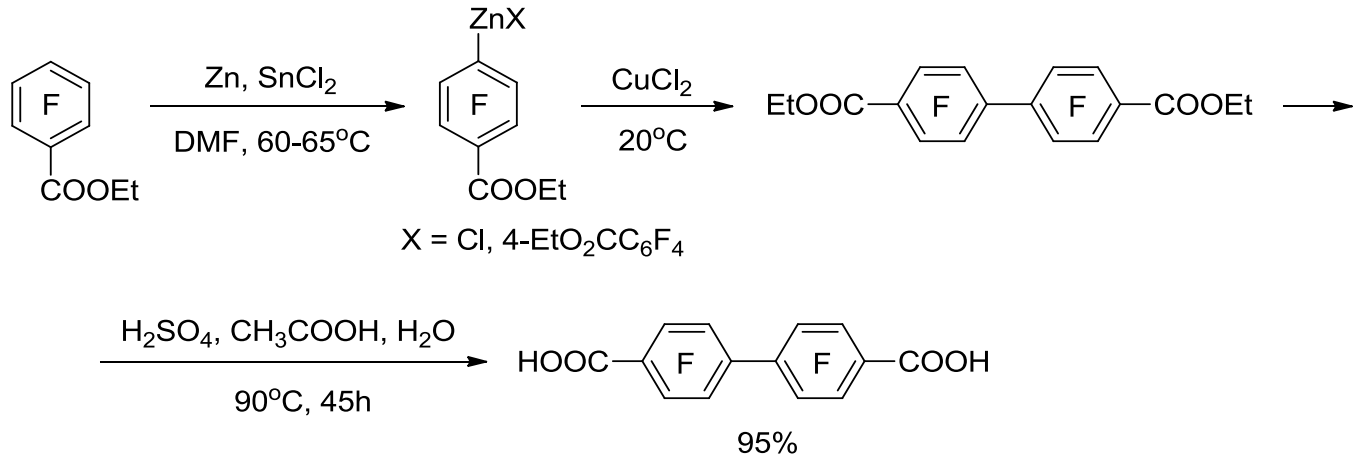
Ligand synthesis



Scheme S1. The synthesis of H_2oFBPDC.

^{19}F and ^{1}H NMR spectra were recorded on a Bruker AV 300 instrument (282.4 and 300 MHz) using $(CD_3)_2CO$ + CCl_4 as a solvent. The chemical shifts of the ^{1}H and ^{19}F NMR spectra were referenced to internal solvent resonances (2.05 from TMS) and C_6F_6 (–162.9 ppm from CCl_3F).

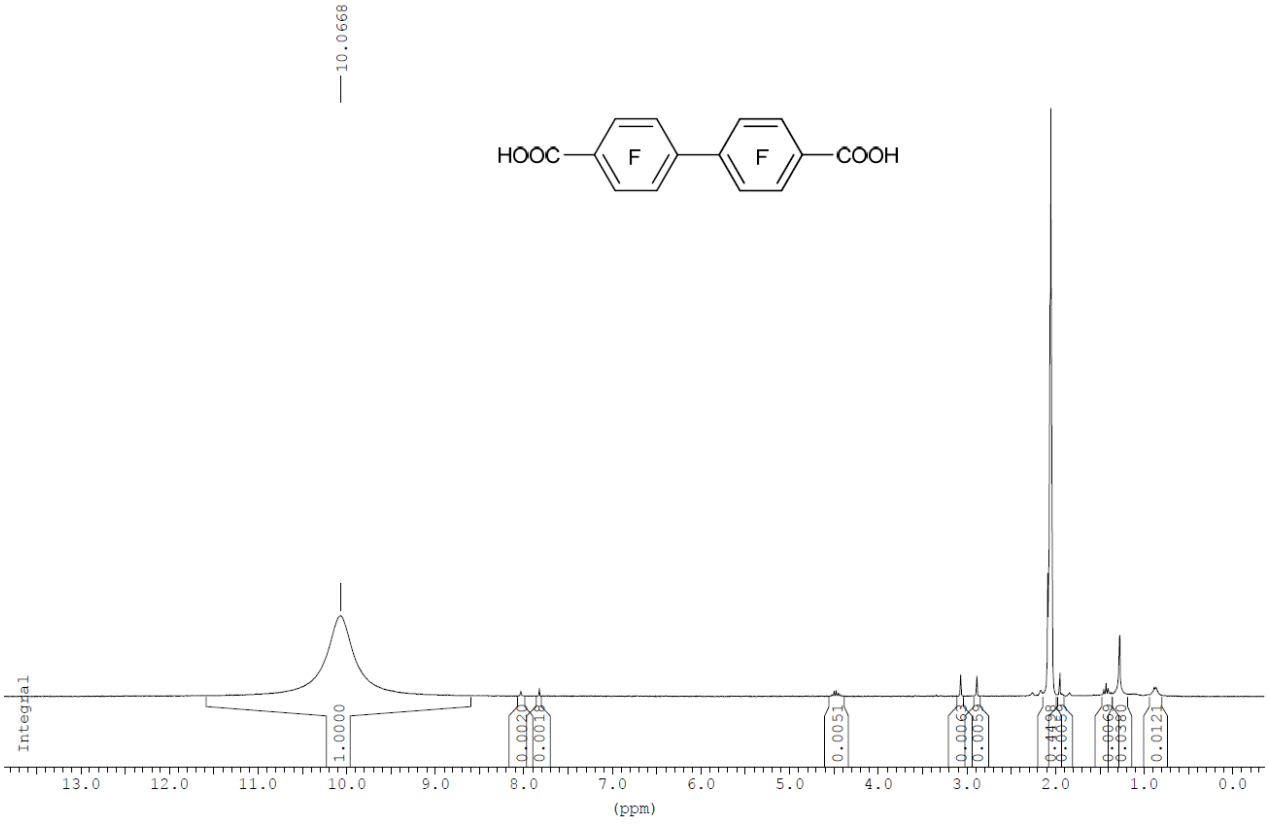


Fig. S1. ^{1}H NMR spectrum of H_2oFBPDC.

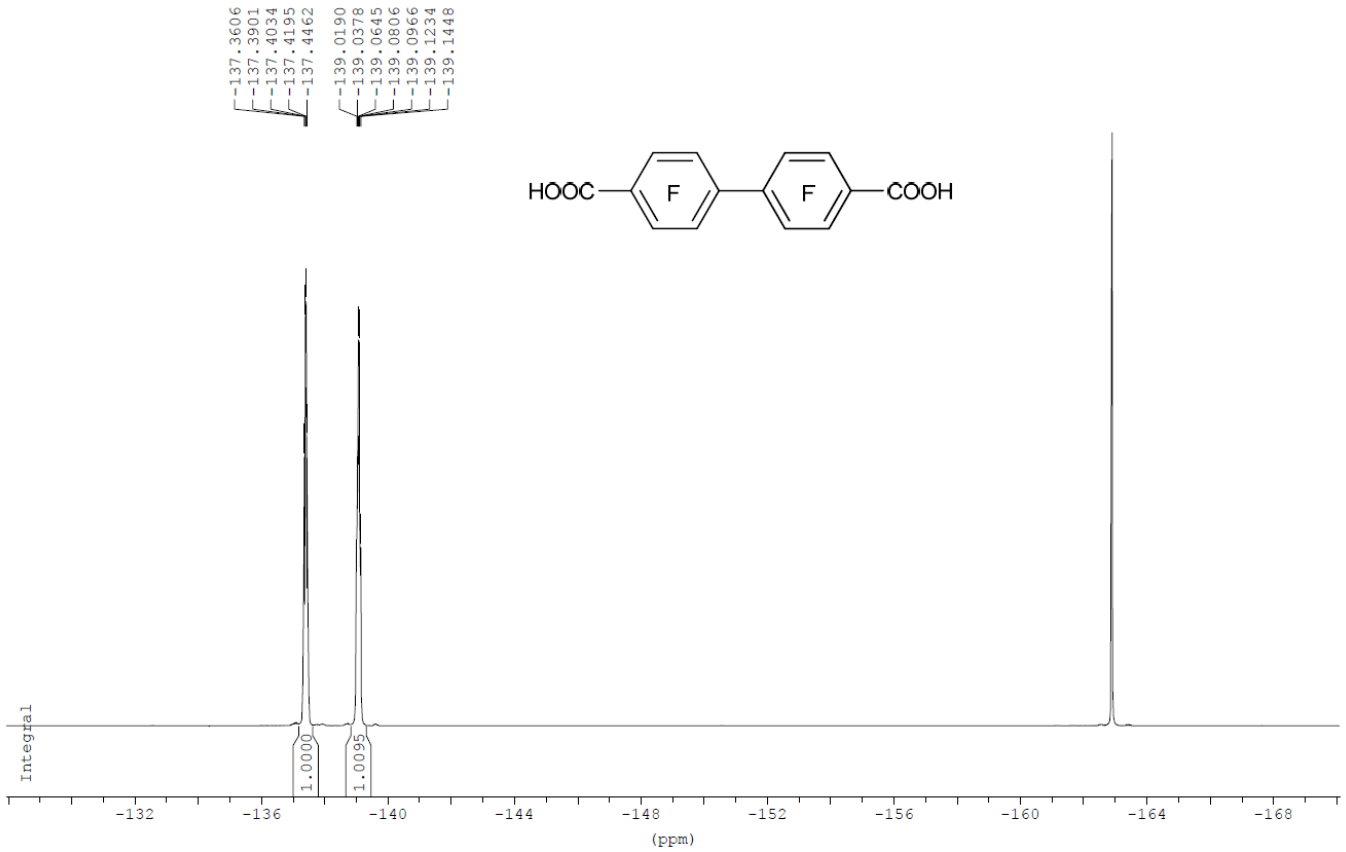


Fig. S2. ^{19}F NMR spectrum of H_2oFBPDC.

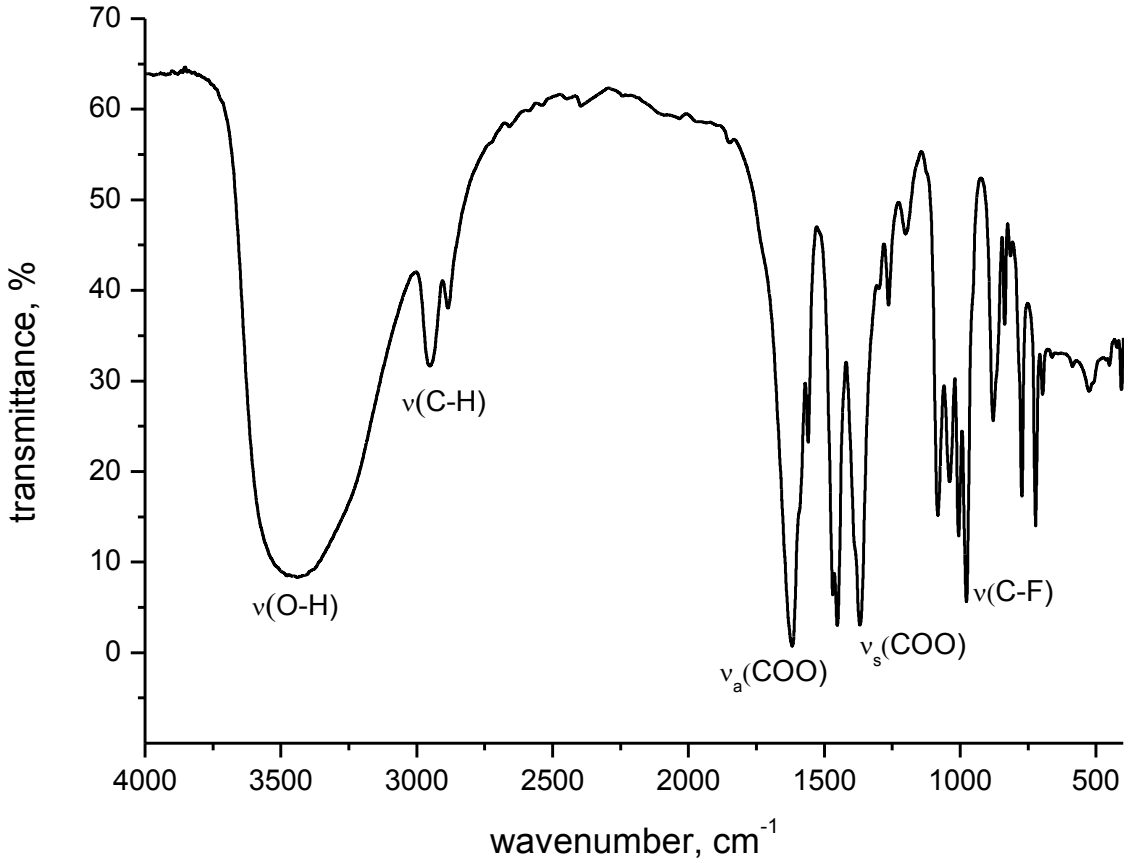


Fig. S3. The FT-IR spectrum of **1**.

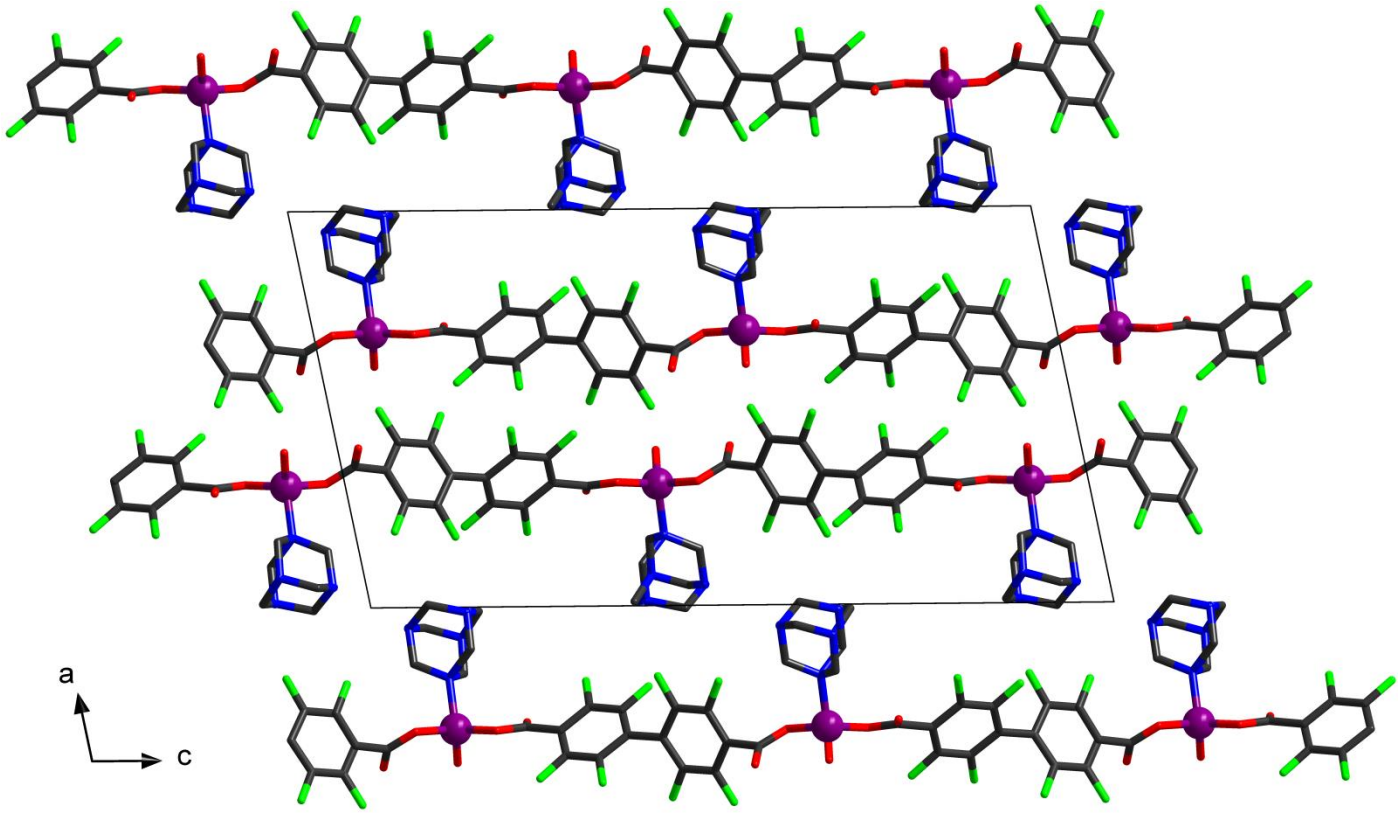


Fig. S4. Packing of the chains in **2.** View along the b axis. Hydrogen atoms are omitted for clarity.

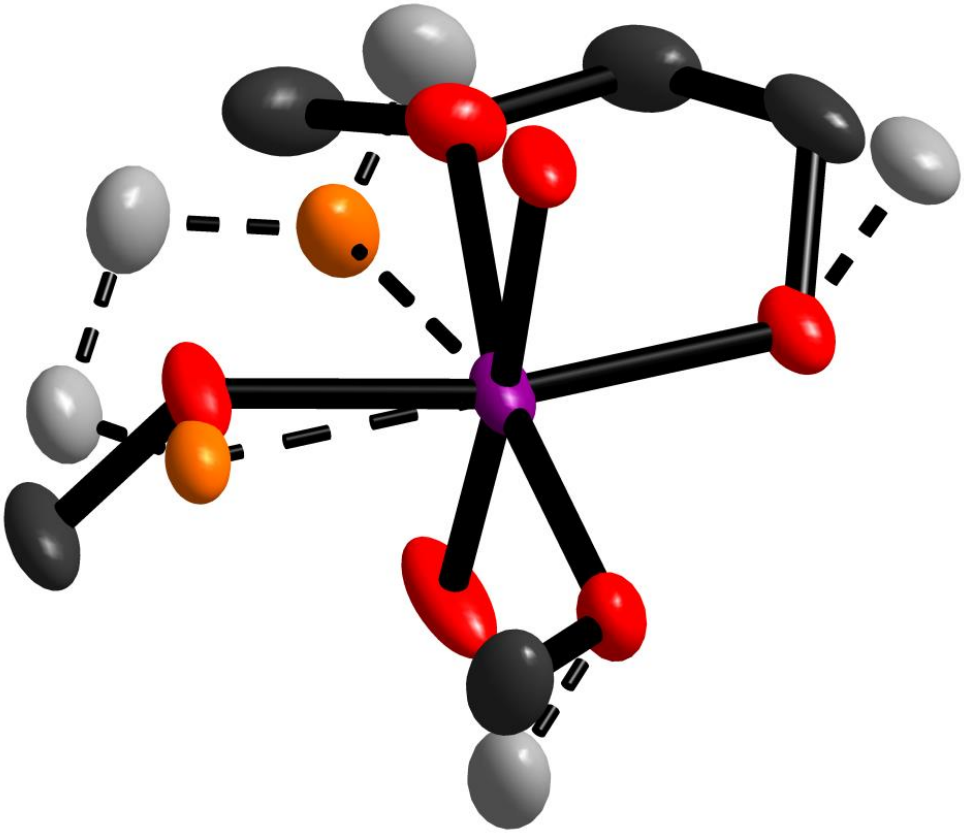


Fig. S5. Coordination environment of Zn(II) cations in the structure **3** (50% probability ellipsoids). Hydrogen atoms are omitted for clarity. The alternative orientation of disordered 2-methoxyethanol and methanol are shown with dashed lines.

Fig. S6. The single crystals of **4** of a few millimeters in size.

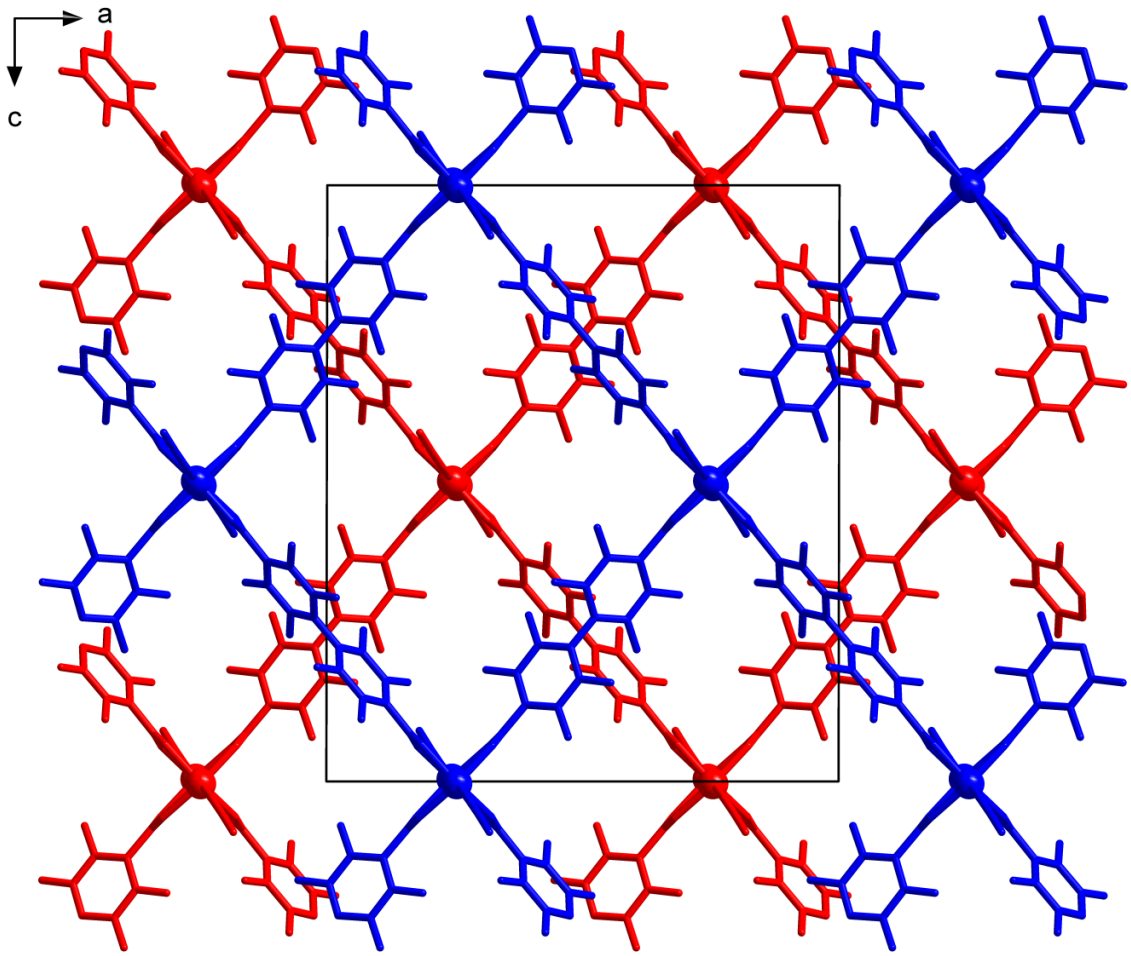


Fig. S7. Packing of the layers in **4**. View along the *b* axis. Guest molecules of benzene and acetonitrile and hydrogen atoms are omitted for clarity.

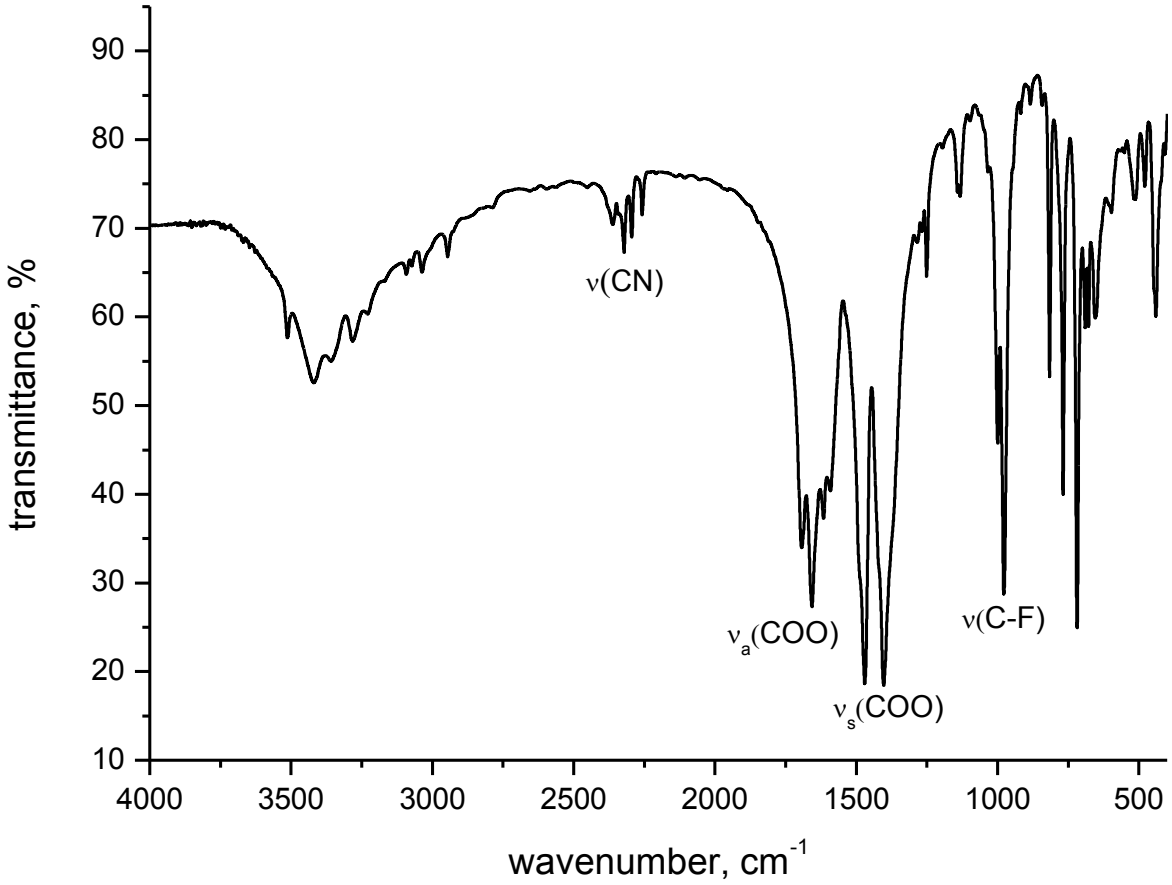


Fig. S8. The FT-IR spectrum of complex **4**.

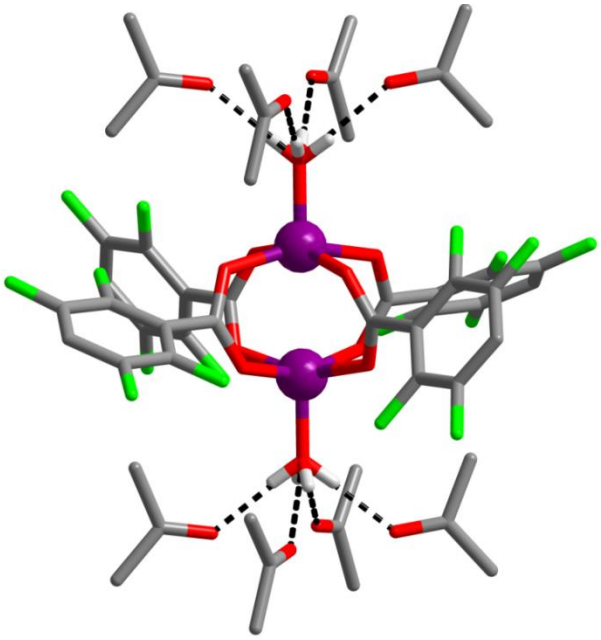


Fig. S9. Coordination environment of Zn(II) cations in the structure **5**. Hydrogen atoms are omitted for clarity. Hydrogen bonds are shown with dashed lines.

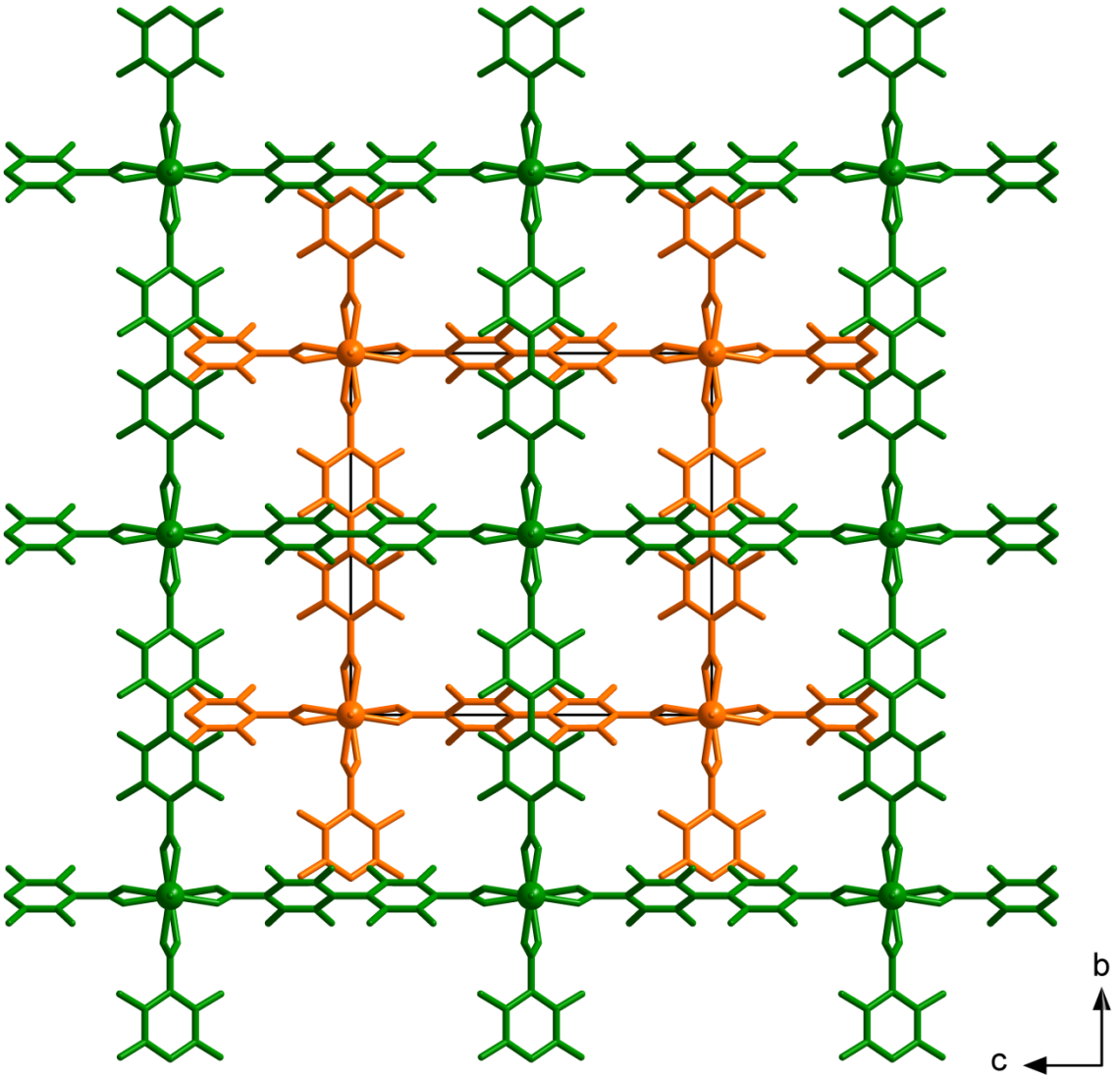


Fig. S10. Packing of the layers in **5**. View along the *a* axis. Guest molecules of acetone and hydrogen atoms are omitted for clarity.

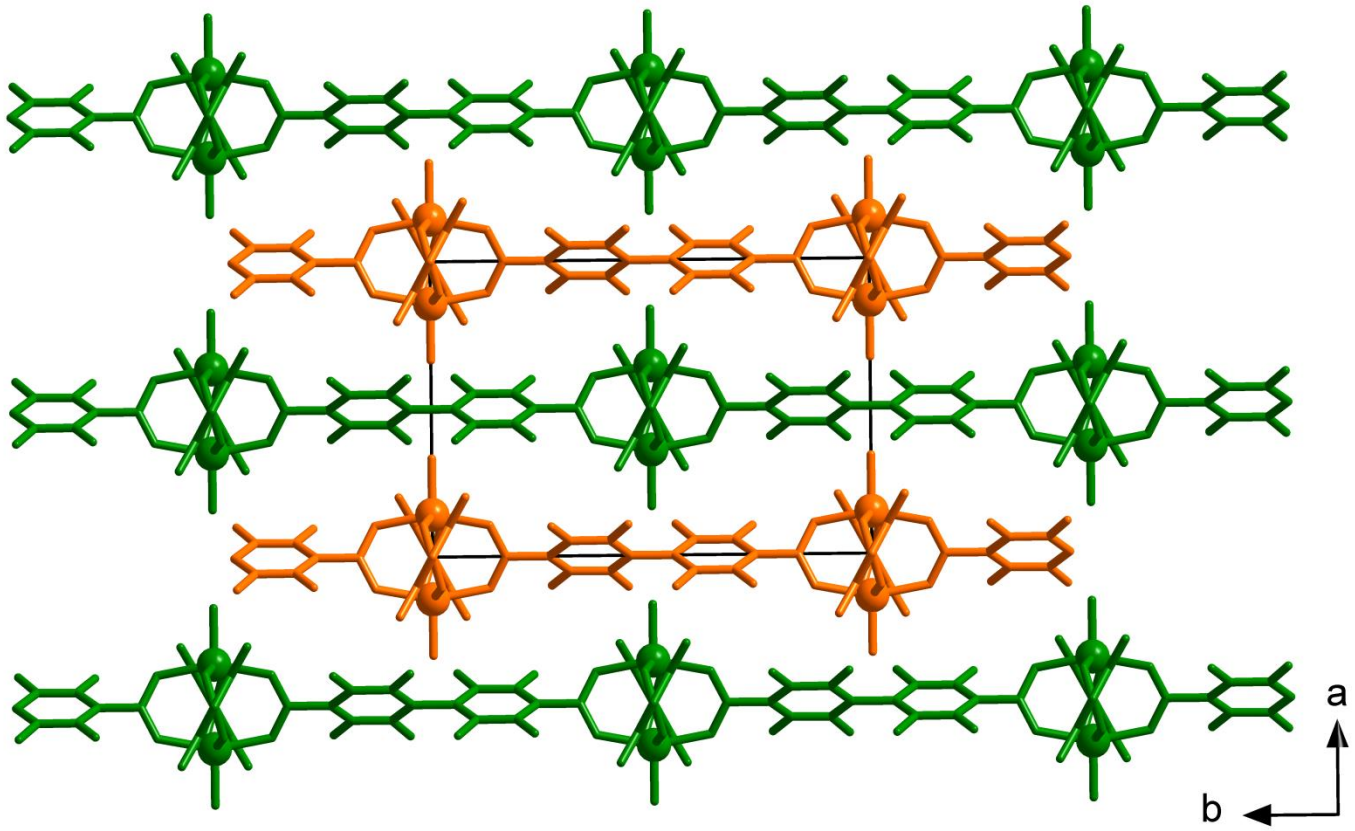


Fig. S11. Packing of the layers in **5**. View along the *c* axis. Guest molecules of acetone and hydrogen atoms are omitted for clarity.

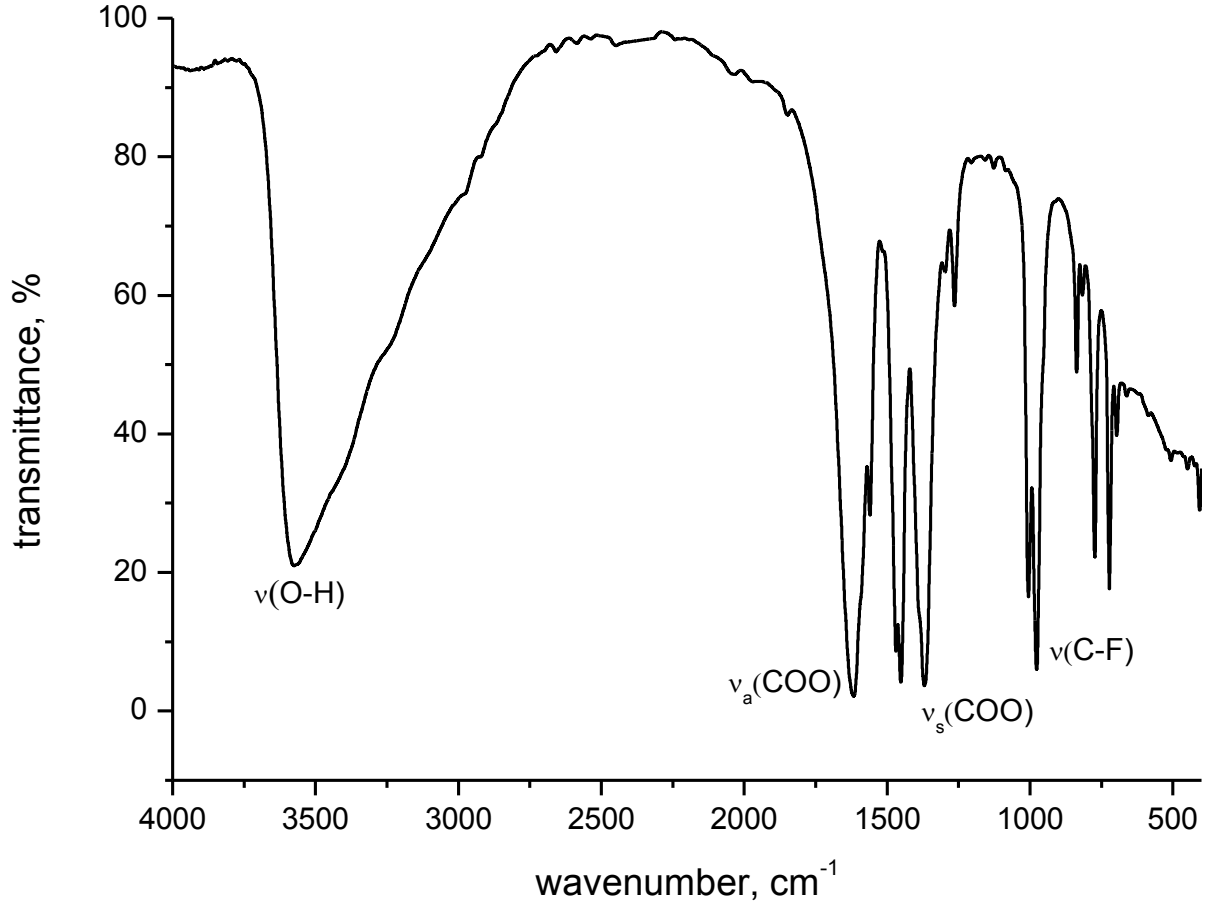


Fig. S12. The FT-IR spectrum of complex $[Zn_2(H_2O)_2(oFBPDC)_2]\cdot 1.3(CH_3)_2CO$.

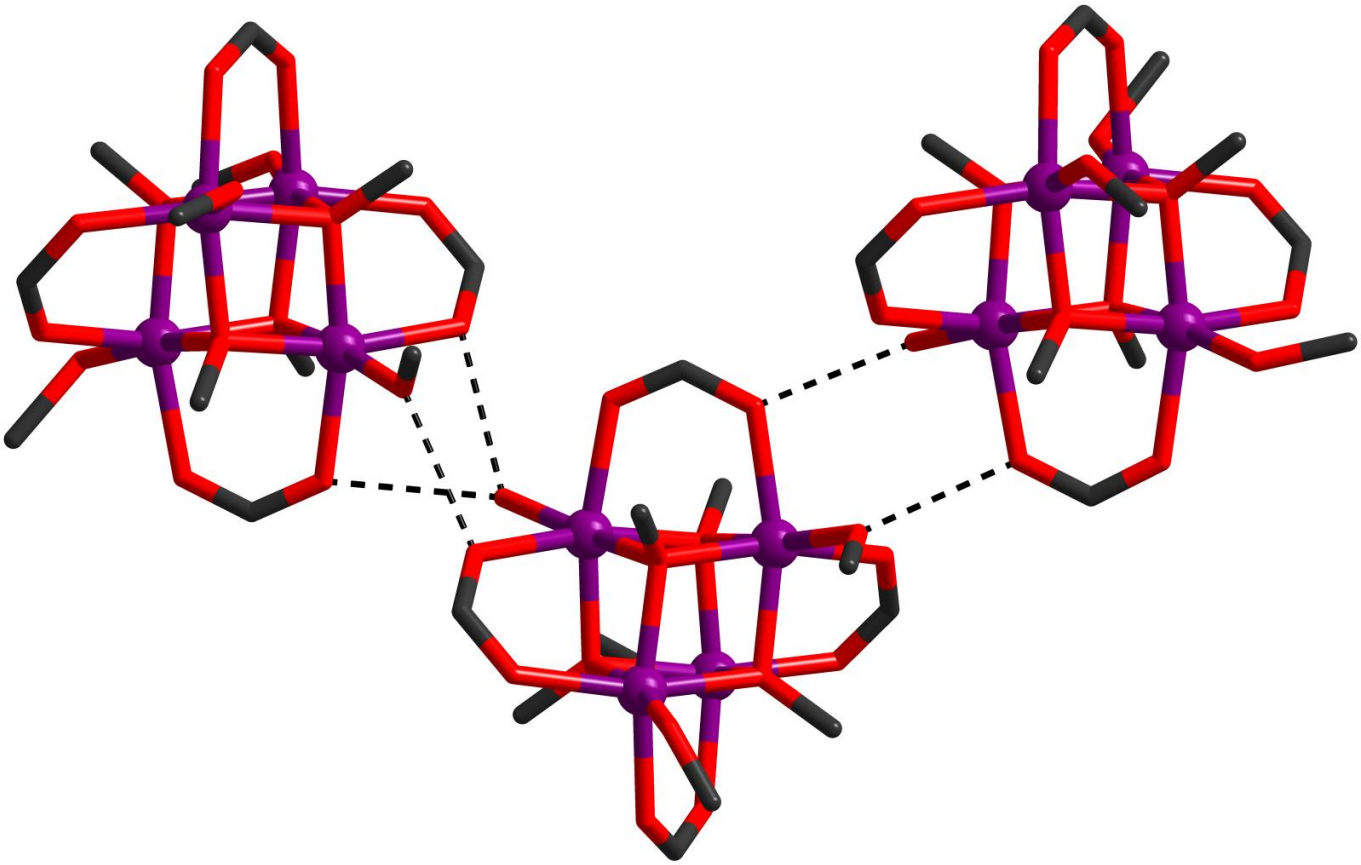


Fig. S13. The system of hydrogen bonds (shown with dashed lines) in structure **6**.

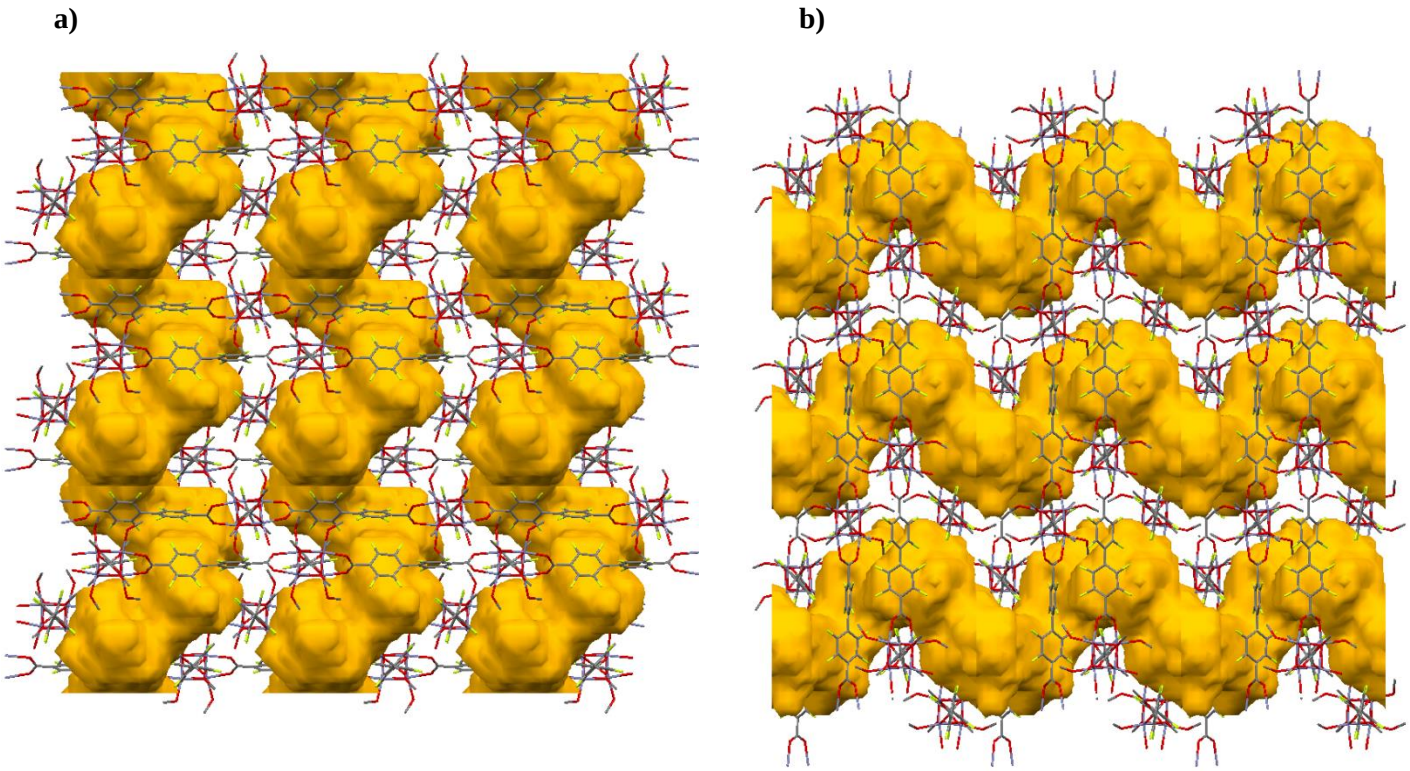


Fig. S14. Representation of the free solvent accessible void volume in crystal structure **6**: **a)** view along *c* axis; **b)** view along *a* axis.

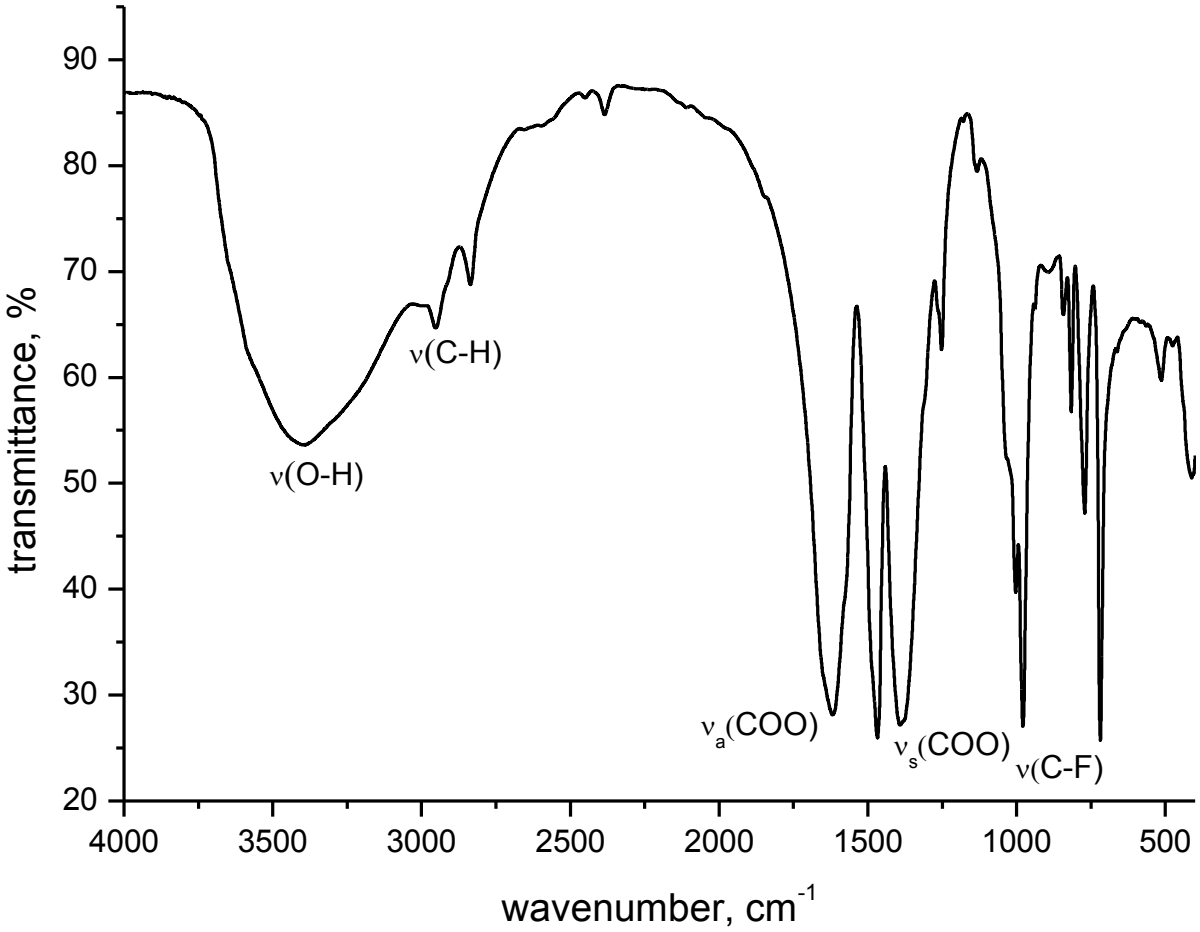


Fig. S15. The FT-IR spectrum of complex **6**.

Thermal analysis

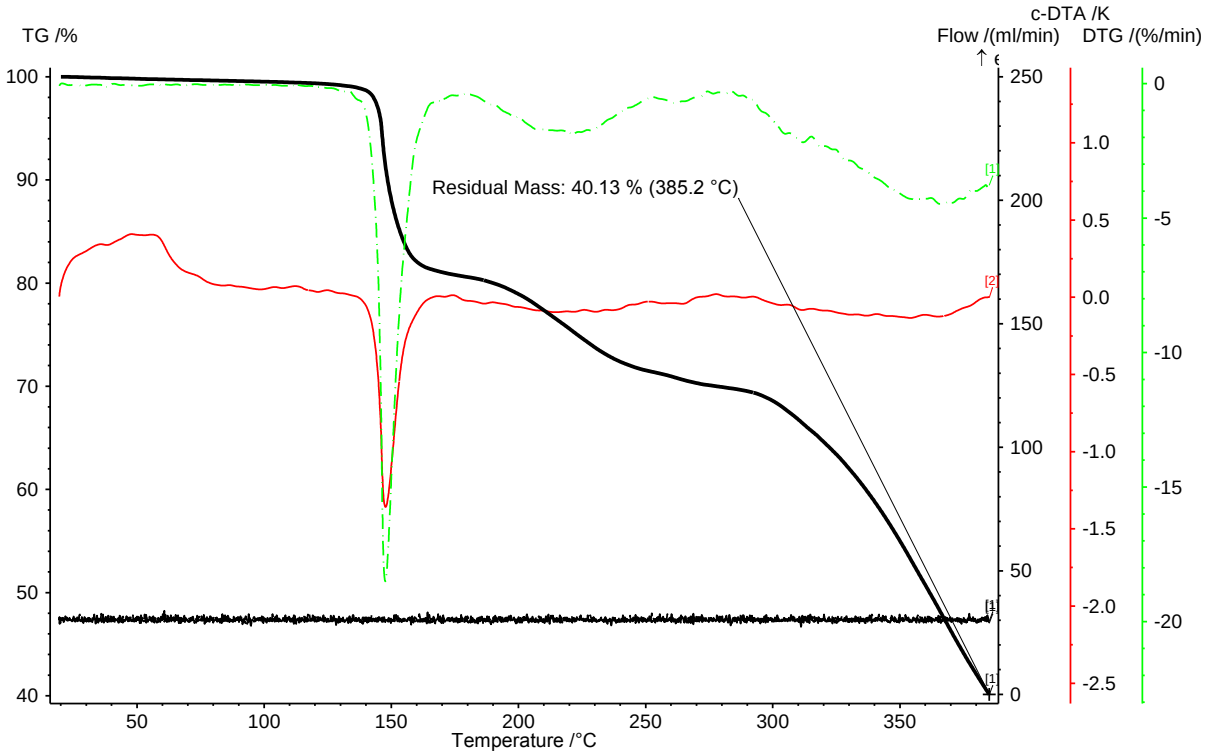


Fig. S16. TG curve of complex **1**.

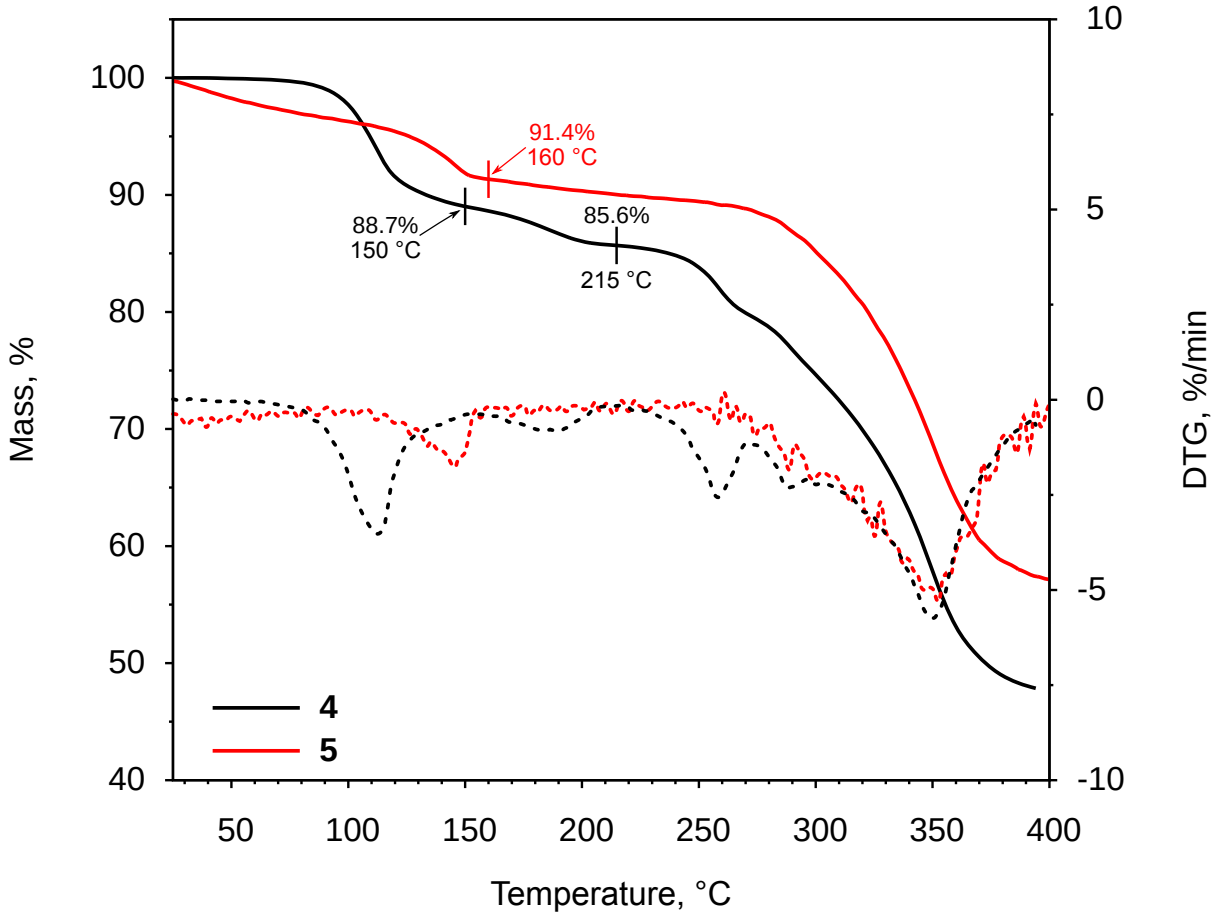


Fig. S17. TG (solid) and DTG (dashed) curves of complexes **4** (black) and **5** (red).

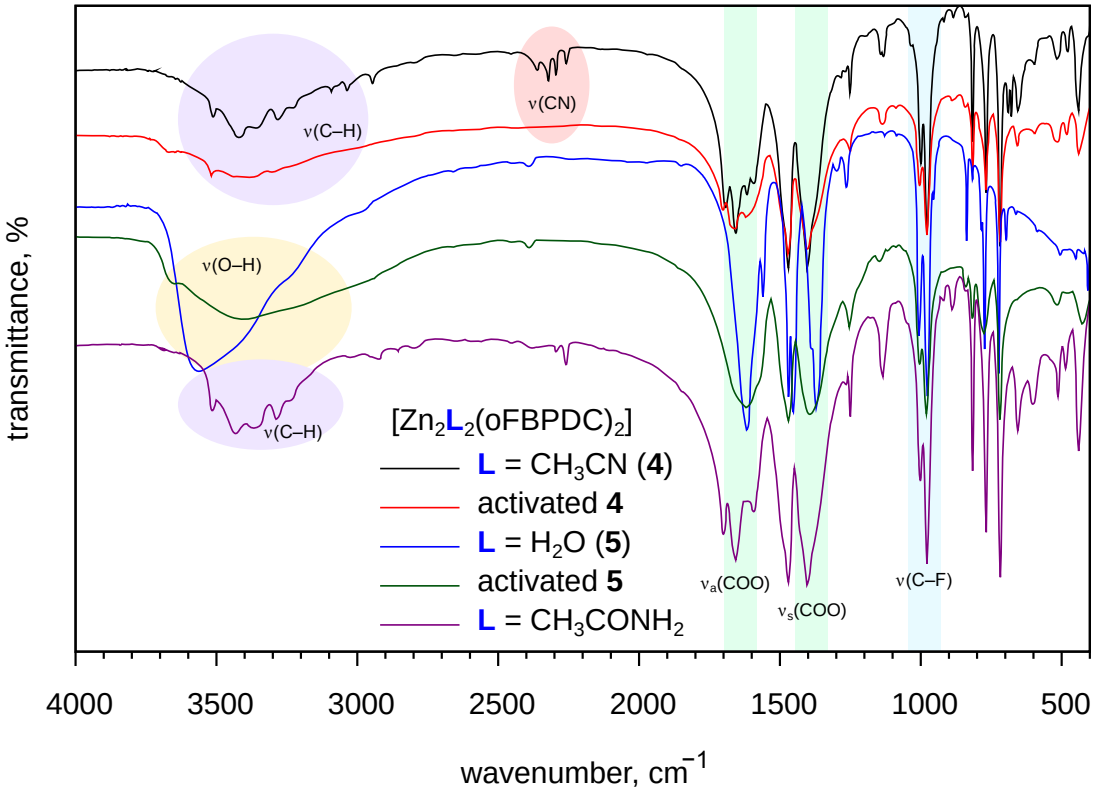


Fig. S18. The comparison of FT-IR spectra of pristine and activated compounds **4** and **5** as well as $[Zn_2(CH_3CONH_2)_2(oFBPDC)_2]$.

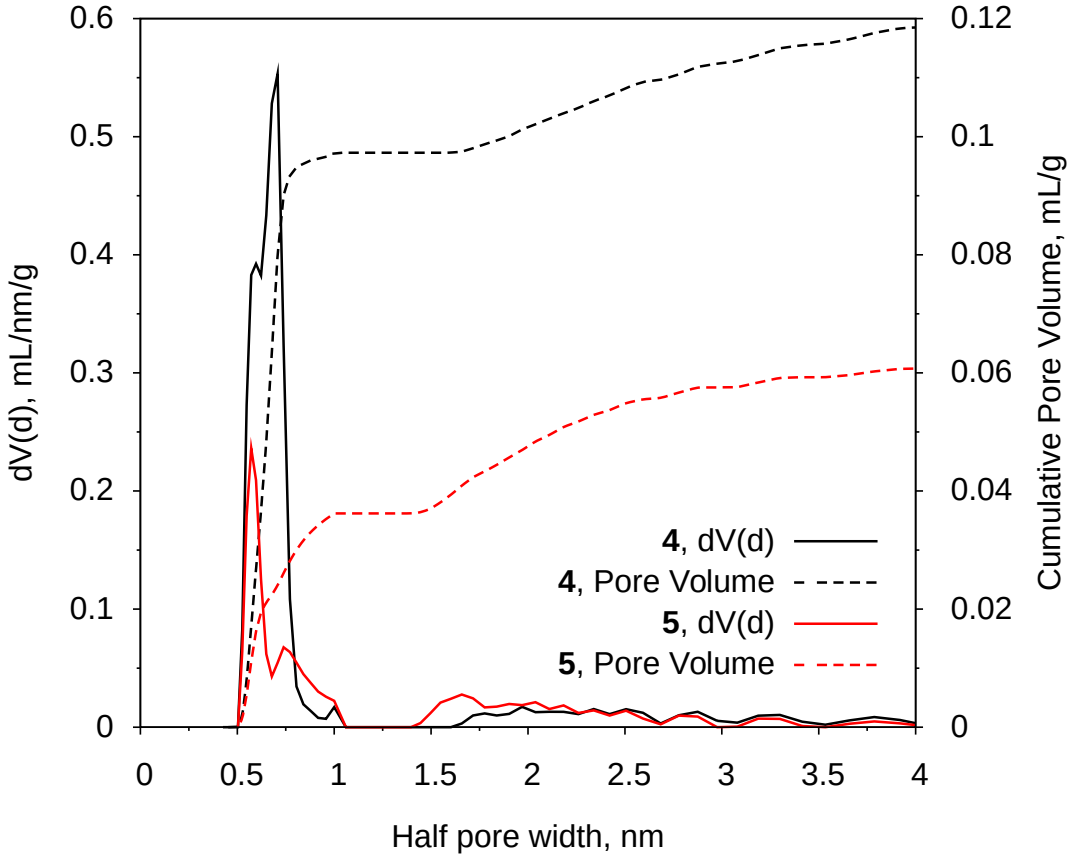


Fig. S19. Pore size distribution for activated **4** and **5**.