Electronic Supporting Information

Anion-directed assembly of a non-interpenetrated square-grid metal–organic framework with nanoscale porosity

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Experimental Section

Self-assembly of a non-interpenetrated square grid metal–organic framework [Zn(DPNDI)₂(DMAc)₂·2ClO₄]ₙ (DPNDI = N₂N'-di(4-pyridyl)-1,4,5,8-naphthalenediimide). A solution of Zn(ClO₄)₂·6H₂O (48 mg, 0.13 mmol) and DPNDI (110 mg, 0.26 mmol) in 1:2 DMAc/MeCN mixture (40 mL) was allowed to stand at room temperature for 24 h. After that MeCN was evaporated under reduced pressure at 25 °C and small portions (5 mL each) of concentrated DMAc solutions were setup for crystallization. Upon slow Et₂O vapor diffusion into DMAc solutions, pale yellow crystals were obtained, which were used for crystallographic and thermogravimetric studies.

As-synthesized crystalline MOF was suspended in fresh Et₂O and washed (centrifugation) three times with Et₂O to exchange entrapped DMAc, MeCN, and H₂O solvents that have higher boiling points. Et₂O was easily removed under reduced pressure to obtain evacuated bulk materials as a microcrystalline off-white powder (37 mg, 11%). This material was analyzed by powder X-ray diffraction (Fig. S1).

Self-assembly of a 1D linear coordination polymer [Zn(DPNDI)₂(DMAc)(NO₃)]ₙ. A solution of Zn(NO₃)₂·6H₂O (39 mg, 0.13 mmol) and DPNDI (110 mg, 0.26 mmol) in 2:1 DMAc/MeCN (40 mL) was allowed to stand at room temperature for 24 h. After that MeCN was evaporated under reduced pressure at 25 °C and small portions (5 mL each) of concentrated DMAc solutions were setup for crystallization. Upon slow Et₂O vapor diffusion into the DMAc solutions, yellowish white crystals were obtained (50 mg, 25%), which were used for crystallographic analysis.

Crystallographic data collection and refinement. Suitable single crystals of the square-grid MOF and 1D coordination polymer were mounted on a goniometer head of a Bruker SMART APEX II diffractometer using a nylon loop with a small amount of Paratone oil (Hampton Research). Crystals were cooled to 153 K in a cold stream of N₂ gas. After finding a crystal that indexed to give a satisfactory unit cell, a full low-temperature data set at 173 K was recorded using a sample-to-detector distance of 6 cm. Diffraction data of the compound was measured with Mo Kα (λ = 0.71073 Å) radiation. Reflections were found at θ = 20° (Sinθ/λ = 0.504 < 0.550 caused an A-level alert) for the square-grid MOF crystal and at ca. 28° for the 1D coordination polymer. The Bruker suite of programs on the APEX II was used to integrate the data and SADABS was used for absorption corrections. Both structures were readily solved by direct methods and refined using the SHELXTL. The non-interpenetrated square-grid MOF crystal has very large pores (ca. 20 x 20 Å) containing disordered solvent molecules, which contributed to an A-level alert. SQUEEZE routine implemented on PLATON was used to remove electron densities corresponding to disordered solvent molecules. All atoms of the complex backbones (Zn(II), DPNDI ligands, Zn(II)-coordinated DMAc and NO₃⁻ ions, and ClO₄⁻ anions were fully accounted for. Crystallographic data has been deposited at the Cambridge Crystallographic Data Center with reference numbers CCDC 929885 and 929886. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.

Powder X-ray crystal diffraction (PXRD) analysis. PXRD analysis of the square-grid MOF was conducted on Siemens D500 powder diffractometer using Ni-filtered unmonochromated Cu Kα radiation with a graphite diffracted beam monochromater. One degree divergence apertures and 0.15 degree
receiving aperture. Scanning was done between 5θ and 65 θ, at 0.02 steps, 0.5 °/min. Samples were
dispersed on quartz zero-background holder. Data were processed using MDI Jade 6.5 software.

**Thermogravimetric analysis (TGA).** TGA of an air-dried ground sample of square-grid MOF was
conducted on a Thermogravimetric Analyzer Instrument Q50 with a heating rate of 10 °C/min under an
Ar-atmosphere. The initial 8% weight loss at 20–100 °C corresponds to loss of volatile solvents (Et₂O,
MeCN), the next 17% loss at 100–200 °C corresponds to loss of H₂O (came from Zn(ClO₄)₂·6H₂O) and
DMAc molecules. The MOF showed excellent thermal stability between 200 and 350 °C, indicating no
network collapse upon solvent evaporation. A sharp 15% weight loss from 65 to 50% occurred at 350–
400 °C. Over 45% weight was lost by 500 °C.

![Thermogravimetric analysis (TGA)](image)

**Fig. S1.** The PXRD pattern of solvent exchanged and evacuated non-interpenetrated square grid MOF.
Green bars represent simulated peaks obtained from single crystal analysis of the as-synthesized
crystalline MOF.

**References.**

S3  G. M. Sheldrick, *Shelxs97* and *Shelxl97*, Programs for Crystallographic Solution and Refinement.
Bond lengths and angles of Zn(II) coordination spheres in the square-grid MOF and 1D polymer:

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### Bond lengths and bond angles of square-grid MOF:

Table 1. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for the square-grid MOF. U(eq) is defined as one third of the trace of the orthogonalized \( U_{ij} \) tensor.

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O(41)-C(41)-C(42)  126.4(8)
N(41)-C(41)-C(42)  104.4(8)
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O(33)-Cl(31)-O(34)  113.1(5)
O(32)-Cl(31)-O(34)  108.9(5)
O(33)-Cl(31)-O(31)  110.7(7)
Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+2  #2 x-1/2,-y+1/2,z+1/2  #3 -x+1/2,y-1/2,-z+3/2
#4 -x+1/2,y+1/2,-z+3/2

Table 3. Anisotropic displacement parameters (Å² x 10³) for the square-grid MOF. The anisotropic displacement factor exponent takes the form: -2p²[h² a*²U¹¹ + ... + 2h k a* b* U¹²]

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<p>| N(41)  | 72(4) | 71(4) | 53(4) | -12(3) | 6(3) | 3(3) |
| O(41)  | 44(2) | 30(2) | 31(2) | -2(2)  | 17(2) | 1(2) |
| Zn(1)  | 38(1) | 14(1) | 36(1) | 1(1)   | 28(1) | 0(1) |
| C(1)   | 39(4) | 46(3) | 61(4) | 25(3)  | 32(3) | 6(3) |
| C(2)   | 37(3) | 56(4) | 61(4) | 25(3)  | 25(3) | 1(3) |
| C(3)   | 46(4) | 28(3) | 33(3) | -3(2)  | 25(3) | -13(2) |
| C(4)   | 50(4) | 29(3) | 32(3) | 5(2)   | 17(3) | -7(2) |
| C(5)   | 39(3) | 24(3) | 37(3) | 2(2)   | 16(3) | -3(2) |
| C(6)   | 49(3) | 31(3) | 36(3) | -6(3)  | 18(3) | -14(3) |
| C(7)   | 53(3) | 22(3) | 34(3) | -1(2)  | 20(3) | -15(2) |
| C(8)   | 40(3) | 32(3) | 25(3) | 1(2)   | 16(2) | -8(2) |
| C(9)   | 70(4) | 32(3) | 35(3) | -8(3)  | 26(3) | -25(3) |
| C(10)  | 71(4) | 43(3) | 38(4) | -2(3)  | 28(3) | -22(3) |
| C(11)  | 109(5) | 54(4) | 39(4) | -14(3) | 47(4) | -45(4) |
| C(12)  | 96(5) | 38(3) | 44(4) | -17(3) | 40(3) | -40(3) |
| C(13)  | 49(3) | 30(3) | 33(3) | -2(2)  | 15(3) | -14(2) |
| C(14)  | 34(3) | 25(3) | 38(3) | 0(2)   | 17(2) | -9(2) |
| C(15)  | 59(3) | 23(3) | 41(3) | 2(2)   | 29(3) | -13(2) |
| C(16)  | 98(5) | 39(3) | 40(3) | -8(3)  | 45(3) | -25(3) |
| C(17)  | 109(5) | 29(3) | 48(4) | -13(3) | 44(4) | -28(3) |
| C(18)  | 59(4) | 36(3) | 35(3) | -1(3)  | 29(3) | -8(3) |
| C(19)  | 40(3) | 30(3) | 46(4) | 3(3)   | 20(3) | -9(2) |
| C(20)  | 41(3) | 20(3) | 43(3) | -3(2)  | 29(3) | -8(2) |
| C(21)  | 34(3) | 32(3) | 47(3) | 7(3)   | 17(3) | -11(2) |
| C(22)  | 52(4) | 29(3) | 47(3) | 19(3)  | 20(3) | 2(3) |
| C(23)  | 28(3) | 26(3) | 60(4) | -2(3)  | 21(3) | -2(2) |
| C(24)  | 49(4) | 35(3) | 38(3) | 7(3)   | 18(3) | 3(3) |
| N(1)   | 42(3) | 24(2) | 37(3) | 2(2)   | 28(2) | -3(2) |
| N(2)   | 56(3) | 28(2) | 32(3) | -2(2)  | 25(2) | -18(2) |
| N(3)   | 45(3) | 22(2) | 36(3) | -2(2)  | 20(2) | -13(2) |
| N(4)   | 34(3) | 26(2) | 35(3) | 0(2)   | 21(2) | -2(2) |
| O(1)   | 88(3) | 40(2) | 46(2) | -9(2)  | 37(2) | -33(2) |
| O(2)   | 129(4) | 61(3) | 49(3) | -22(2) | 58(3) | -51(3) |
| O(3)   | 71(3) | 31(2) | 52(2) | -7(2)  | 33(2) | -24(2) |
| O(4)   | 104(3) | 37(2) | 55(3) | -10(2) | 56(2) | -25(2) |
| C(41)  | 71(5) | 36(3) | 65(5) | 9(3)   | 22(4) | 14(3) |
| C(42)  | 239(14) | 98(7) | 263(16) | -45(8) | 183(14) | -33(8) |
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Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^{-3}) for the square-grid MOF.

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Zn(1)-O(41)-C(41)-C(42)  4.0(10)
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C(43)-N(41)-C(41)-C(42)  11.1(9)
C(44)-N(41)-C(41)-C(42)  -172.3(9)

Symmetry transformations used to generate equivalent atoms:
#1  -x,-y,-z+2   #2  x-1/2,-y+1/2,z+1/2   #3  -x+1/2,y-1/2,-z+3/2
#4  -x+1/2,y+1/2,-z+3/2
Bond Length and Bond angle table of 1D coordination polymer

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å² x 10^3) for the 1D coordination polymer. U(eq) is defined as one third of the trace of the orthogonalized U_ij tensor.

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### Table 7. Bond lengths [Å] and angles [°] for the 1D coordination polymer.

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C(46)-N(46)-C(49)  102.8(6)
C(48)-N(46)-C(49)  108.5(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+2  #2 -x,-y+1,-z

Table 8. Anisotropic displacement parameters (Å² x 10⁶) for the 1D coordination polymer. The anisotropic displacement factor exponent takes the form: -2π² [ h² a*² U¹¹ + . . . + 2 h k a* b* U¹² ]

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Table 9. Hydrogen coordinates ($x \times 10^4$) and isotropic displacement parameters ($\AA^2 \times 10^3$) for the 1D coordination polymer

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Table 10. Torsion angles [°] for the 1D coordination polymer.

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<td>-175.5(5)</td>
<td></td>
</tr>
<tr>
<td>C(47)-C(46)-N(46)-C(48)</td>
<td>5.6(8)</td>
<td></td>
</tr>
<tr>
<td>O(46)-C(46)-N(46)-C(49)</td>
<td>-4.7(7)</td>
<td></td>
</tr>
<tr>
<td>C(47)-C(46)-N(46)-C(49)</td>
<td>176.4(2)</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+2
#2 -x,-y+1,-z