

Electronic Supplementary Information (ESI†)

Building Coordination Polymers using Dipyridone Ligands

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Supplementary Information

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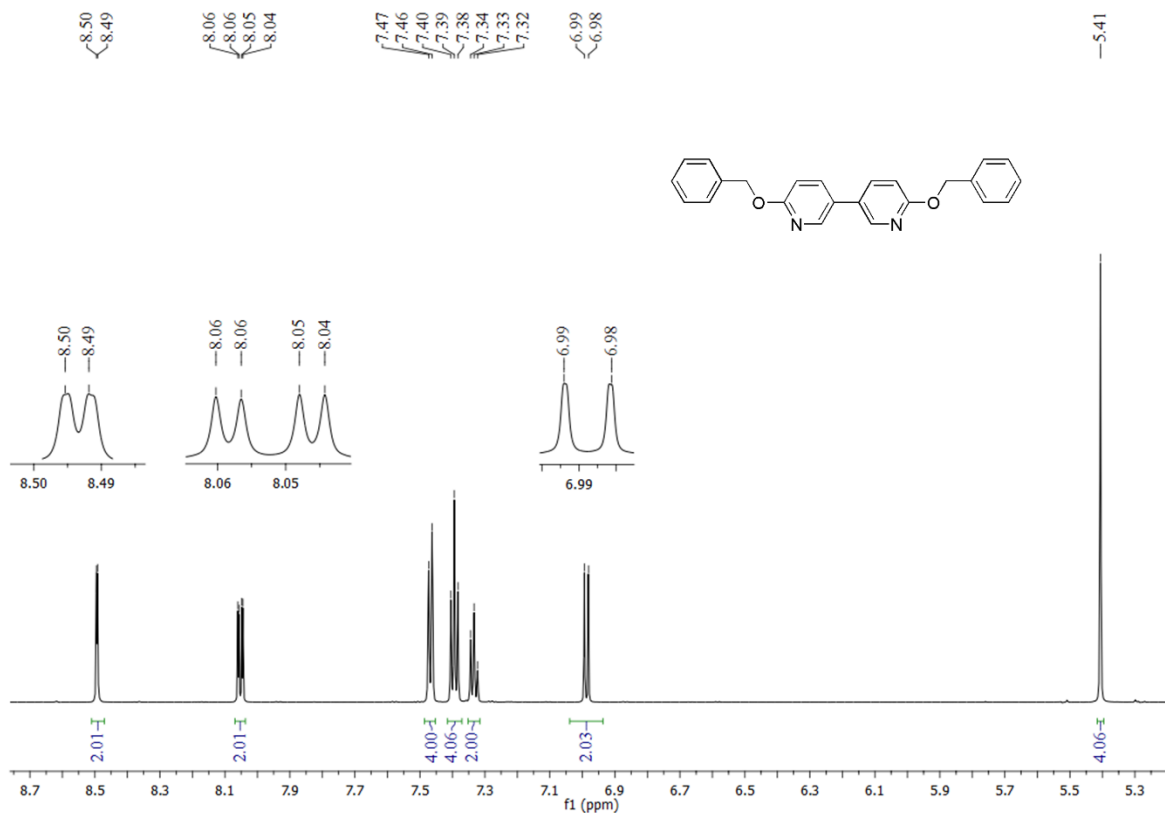


Fig. S1. ¹H-NMR spectrum of **2** recorded in DMSO-*d*₆ solution.

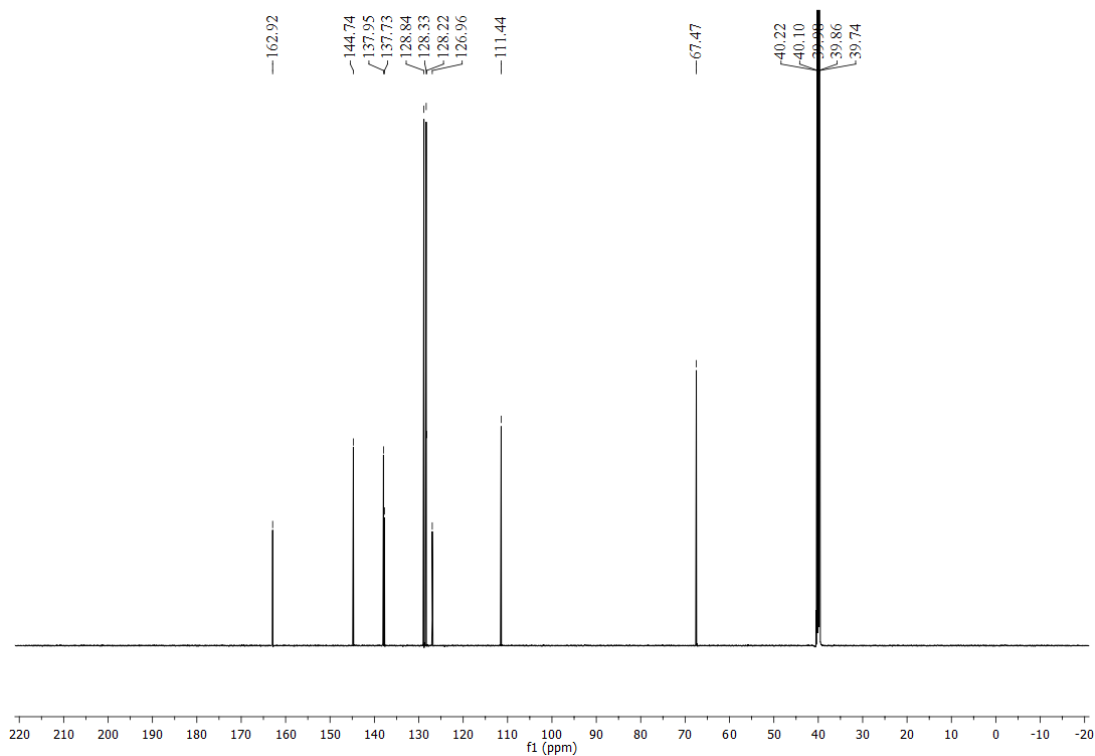


Fig. S2. ¹³C-NMR spectrum of **2** recorded in DMSO-*d*₆ solution.

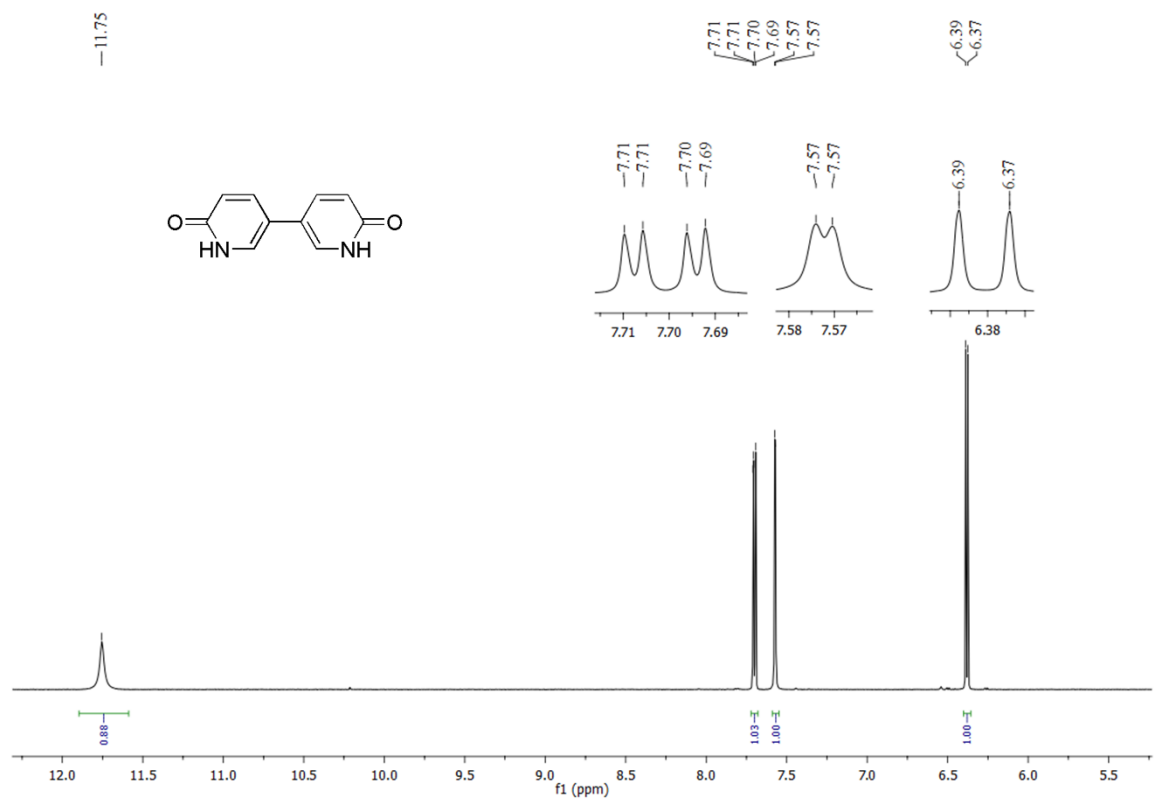


Fig. S3. ¹H-NMR spectrum of **1** recorded in DMSO-*d*₆ solution.

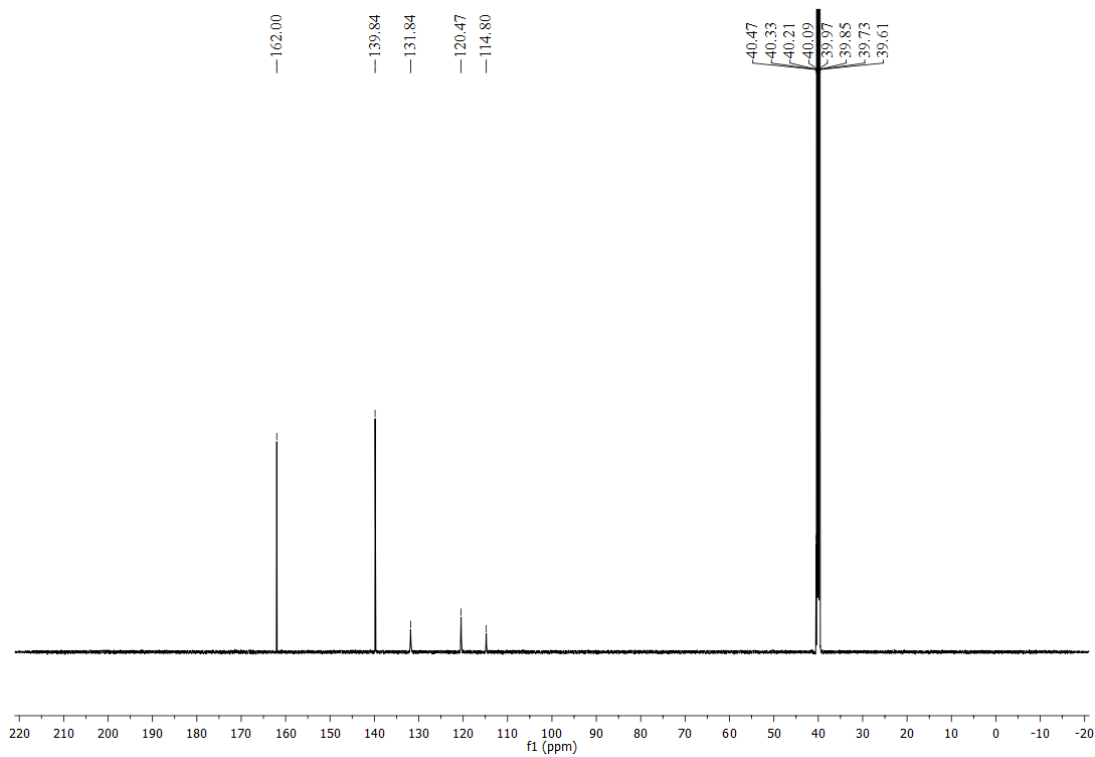


Fig. S4. ¹³C-NMR spectrum of **1** recorded in DMSO-*d*₆ solution.

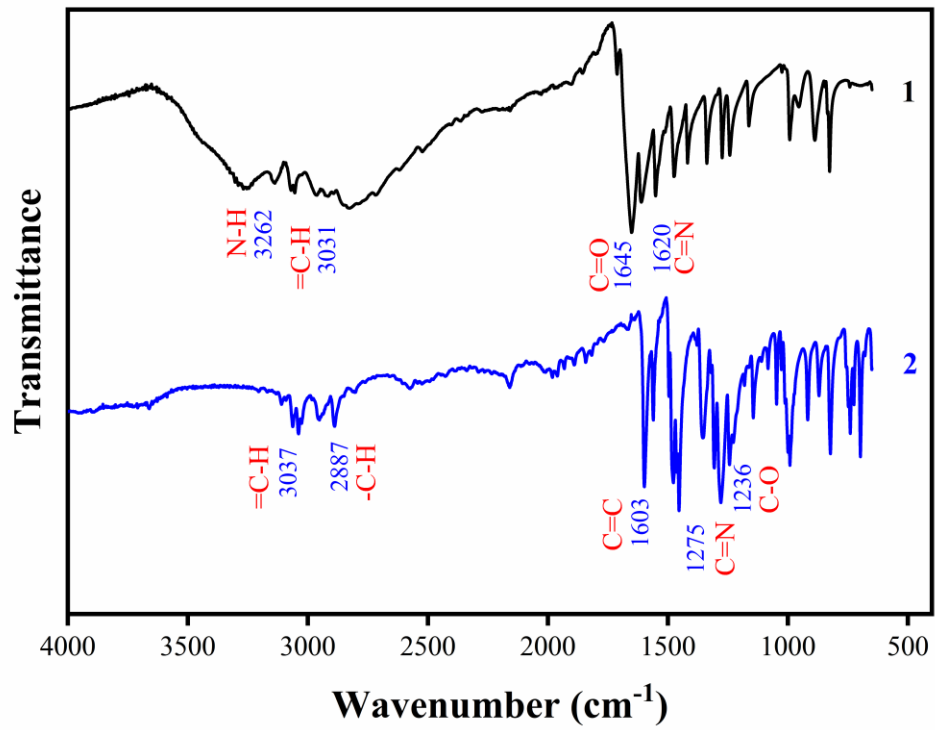


Fig S5. FTIR of compounds **1** (black) and **2** (blue).

Crystallographic data

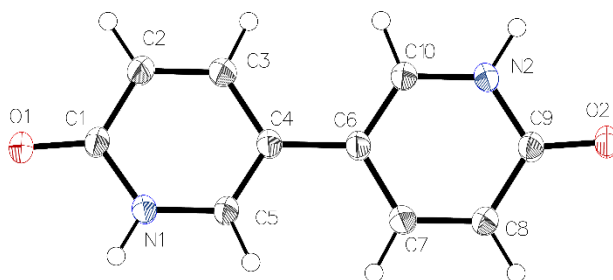


Fig. S6 Thermal atomic displacement ellipsoid plot of **1a** crystallized at 80 °C in EtOH/DMF. The ellipsoids of non-hydrogen atoms are drawn at 50% probability level, hydrogen atoms are represented by a sphere of arbitrary size.

Table S1. Hydrogen bond geometry (Å, °) of **1a** crystallized in EtOH/DMF

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1···O2 ⁱ	0.941 (19)	1.800 (19)	2.7287 (14)	168.6 (17)
N2—H2···O1 ⁱⁱ	0.963 (19)	1.764 (19)	2.7053 (14)	164.7 (16)

Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+3/2, y-1/2, -z+1/2$.

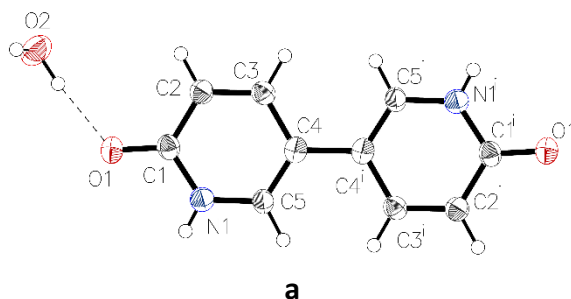


Fig. S7 Thermal atomic displacement ellipsoid plot of **1b** crystallized in DMSO/H₂O. The ellipsoids of non-hydrogen atoms are drawn at 50% probability level, hydrogen atoms are represented by a sphere of arbitrary size.

Table S2. Hydrogen bond geometry (Å, °) of **1b** crystallized in DMSO/H₂O

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O1 ⁱ	0.79 (5)	2.00 (5)	2.782 (5)	174 (4)
O2—H2A...O2 ⁱⁱ	0.87 (1)	1.94 (1)	2.788 (5)	166 (5)
O2—H2B...O1	0.87 (1)	1.91 (2)	2.753 (4)	164 (6)

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1/2, y+1/2, -z+1/2$.

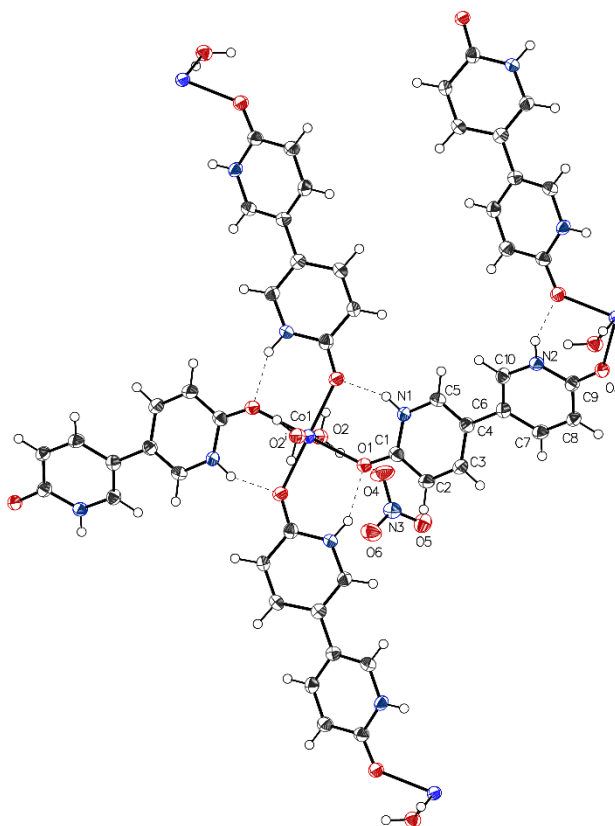


Fig. S8 Thermal atomic displacement ellipsoid plot of **CP-671** crystallized at 80 °C in EtOH/DMF. The ellipsoids of non-hydrogen atoms are drawn at 50% probability level, hydrogen atoms are represented by a sphere of arbitrary size, and hydrogen bonds are represented by dotted lines.

Table S3. Hydrogen bond geometry (Å, °) observed in **CP-671**

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O3 ⁱ	0.88	1.89	2.720 (4)	157
C2—H2...O5 ⁱⁱ	0.95	2.38	3.278 (6)	158
O2—H2A...O4	0.89	1.85	2.690 (5)	158
O2—H2B...O4 ⁱⁱⁱ	0.88	1.85	2.692 (5)	159
N2—H2C...O1 ^{iv}	0.88	1.94	2.759 (5)	154
C5—H5...O6 ^v	0.95	2.36	3.295 (6)	167
C8—H8...O6 ^{vi}	0.95	2.54	3.309 (6)	138
C10—H10...O5 ^v	0.95	2.39	3.304 (6)	162

Symmetry codes: (i) $x, -y+3/2, z+1/2$; (ii) $x+1/2, y, -z+1/2$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+2, y+1/2, -z+1/2$; (v) $-x+3/2, y+1/2, z$; (vi) $-x+3/2, -y+1, z-1/2$.

Table S4. Bond angles (°) observed in **CP-671**

Atoms	Angle (°)	Atoms	Angle (°)
O1 ⁱ Co1 O1	180.0	C3 C2 C1	120.4 (5)
O2 Co1 O1 ⁱ	89.51 (12)	C10 N2 C9	124.7 (4)
O2 ⁱ Co1 O1	89.51 (12)	C4 C3 C2	122.1 (5)
O2 Co1 O1	90.49 (12)	C9 O3 Co1 ^{iv}	137.5 (3)
O2 ⁱ Co1 O1 ⁱ	90.49 (12)	C5 C4 C3	116.4 (4)
O2 ⁱ Co1 O2	180.0	C6 C4 C3	121.3 (4)
O3 ⁱⁱ Co1 O1	90.49 (12)	C6 C4 C5	122.3 (4)
O3 ⁱⁱ Co1 O1 ⁱ	89.51 (12)	C4 C5 N1	121.3 (4)
O3 ⁱⁱⁱ Co1 O1 ⁱ	90.49 (12)	C7 C6 C4	120.8 (4)
O3 ⁱⁱⁱ Co1 O1	89.51 (12)	C10 C6 C4	122.1 (4)
O3 ⁱⁱ Co1 O2 ⁱ	90.44 (13)	C10 C6 C7	117.1 (4)
O3 ⁱⁱ Co1 O2	89.56 (13)	C8 C7 C6	120.9 (4)
O3 ⁱⁱⁱ Co1 O2 ⁱ	89.56 (13)	C9 C8 C7	120.7 (4)
O3 ⁱⁱⁱ Co1 O2	90.44 (13)	O3 C9 N2	120.0 (4)
O3 ⁱⁱ Co1 O3 ⁱⁱⁱ	180.0	C8 C9 N2	116.0 (4)
N1 C1 O1	119.8 (4)	C8 C9 O3	124.0 (4)
C2 C1 O1	124.5 (5)	C6 C10 N2	120.6 (4)
C2 C1 N1	115.7 (4)	O5 N3 O4	119.2 (4)
C1 O1 Co1 ⁱ	133.6 (3)	O6 N3 O4	118.7 (4)
C5 N1 C1	124.1 (4)	O6 N3 O5	122.1 (4)

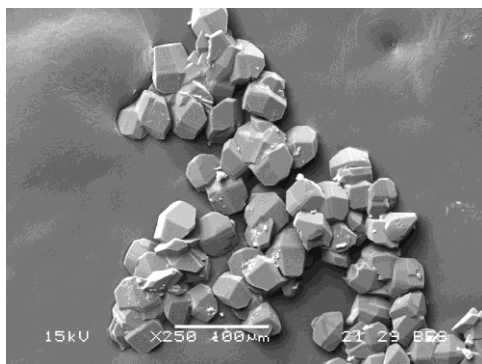
Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, -y+3/2, z+1/2$; (iii) $-x+2, y-1/2, -z+1/2$; (iv) $-x+2, y+1/2, -z+1/2$.

Table S5. Bond lengths (Å) observed in **CP-671**

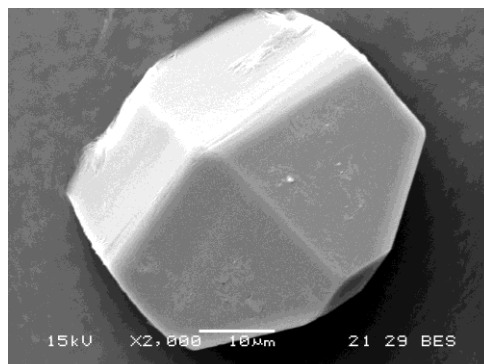
Atoms	Bond Lengths (Å)	Atoms	Bond Lengths (Å)
Co1 O1	2.109 (3)	N2 C10	1.354 (6)
Co1 O1 ⁱ	2.109 (3)	C3 C4	1.408 (7)
Co1 O2	2.044 (3)	O3 C9	1.278 (5)
Co1 O2 ⁱ	2.044 (3)	C4 C5	1.367 (6)
Co1 O3 ⁱⁱ	2.118 (3)	C4 C6	1.481 (6)
Co1 O3 ⁱⁱⁱ	2.118 (3)	C6 C7	1.425 (6)
C1 O1	1.270 (5)	C6 C10	1.360 (6)
C1 N1	1.368 (6)	C7 C8	1.363 (7)
C1 C2	1.413 (7)	C8 C9	1.411 (7)
N1 C5	1.357 (6)	N3 O4	1.263 (5)
C2 C3	1.370 (7)	N3 O5	1.240 (5)
N2 C9	1.352 (6)	N3 O6	1.235 (5)

Symmetry codes: (i) -x+2, -y+1, -z+1; (ii) x, -y+3/2, z+1/2; (iii) -x+2, y-1/2, -z+1/2.

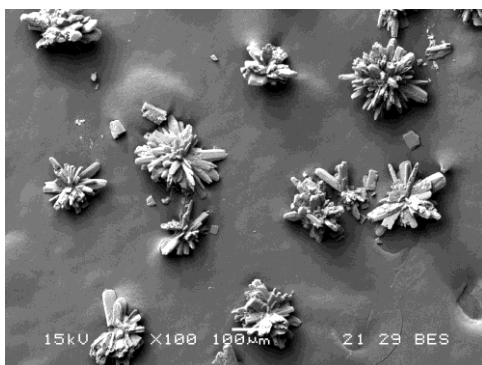
Additional SEM images



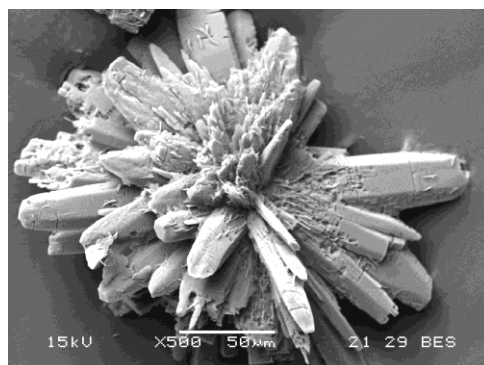
a



b



c



d

Fig. S9 (a), (c) SEM images of **1a** and **CP-671** respectively and (b), (d) Crystal morphologies of **1a** and **CP-671** respectively.