<Supporting Information>

Solvent-induced Assembly of Octacyanometalates-Based Coordination Polymers with Unique cjq Topology and Magnetic Properties

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Supplementary Index

1. Topological analysis

The topologies of polymers **1** and **2** were both analyzed by program OLEX[S1] and TOPOS[S2] with the CIF files. The topological cell of OLEX shows that the short (Schläfli) symbol of the net for $\{4^{11}.6^{12}.8^{5}\}\{4^{17}.6^{10}.8\}\{4^{5}.6\}_4$, which is consistent with the result of TOPOS.

References:

S1. O. V. Dolomanov, A. J. Blake, N. R. Champness and M. Schröder, *J. Appl. Cryst.* **2003**, *36*, 1283.

S2. C. Bonneau, O. Delgado-Friederichs, M. O'Keeffe and O. M. Yaghi, *Acta Cryst. A*. **2004**, *60*, 517.

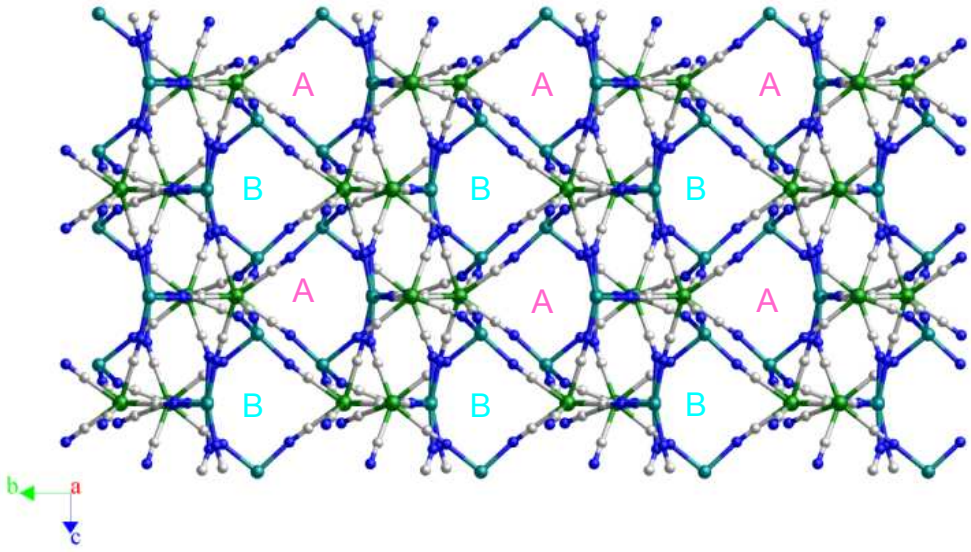

Figure S1. The packing structure of **1** and **2** viewed along *a* axis (W, Mo green, Mn cyan, C gray, N blue). Carbon, oxygen and nitrogen atoms in MeOH and water molecules and counter ions have been omitted for clarity.

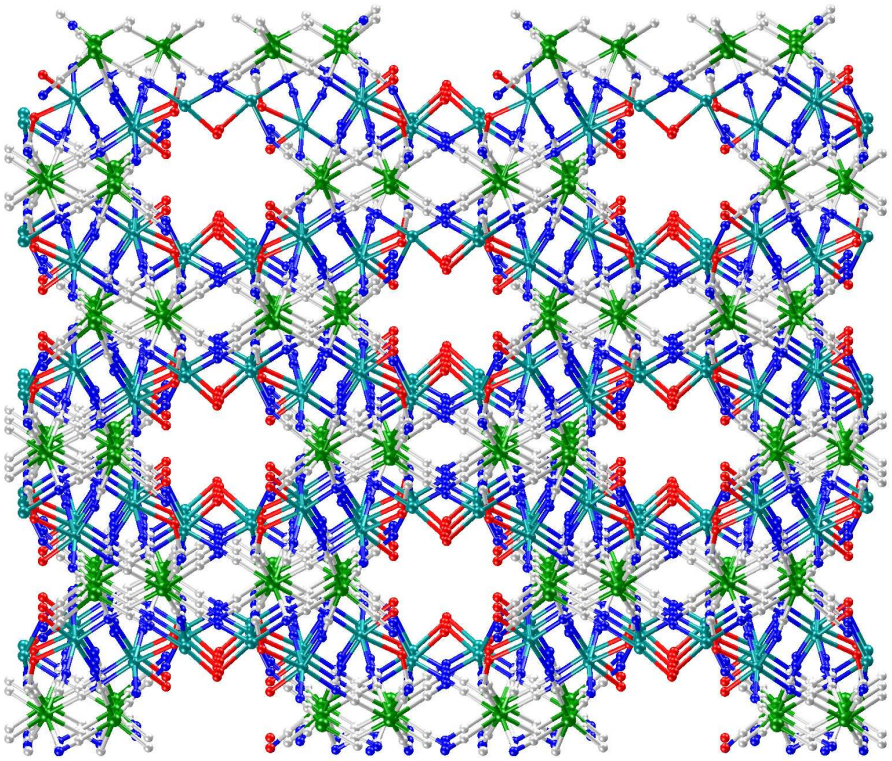

Figure S2. The packing structure of **1** and **2** viewed from 101 face (W, Mo green, Mn cyan, C gray, N blue, O red). All the hydrogen atoms and solvent MeOH and counter-ions have been omitted for clarity.

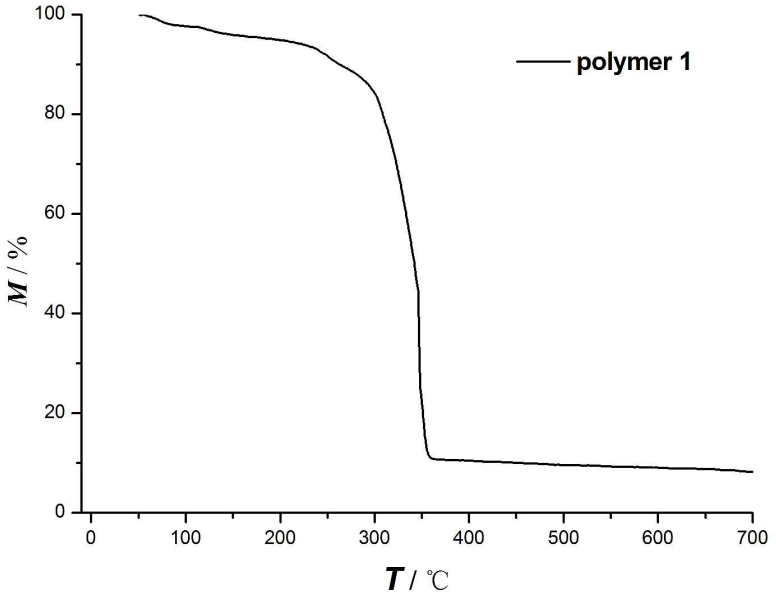

Figure S3. TG curve of polymer **1**. The TG curve shows that polymer **1** releases a methanol molecule and two water molecules per formula unit below 280°C.

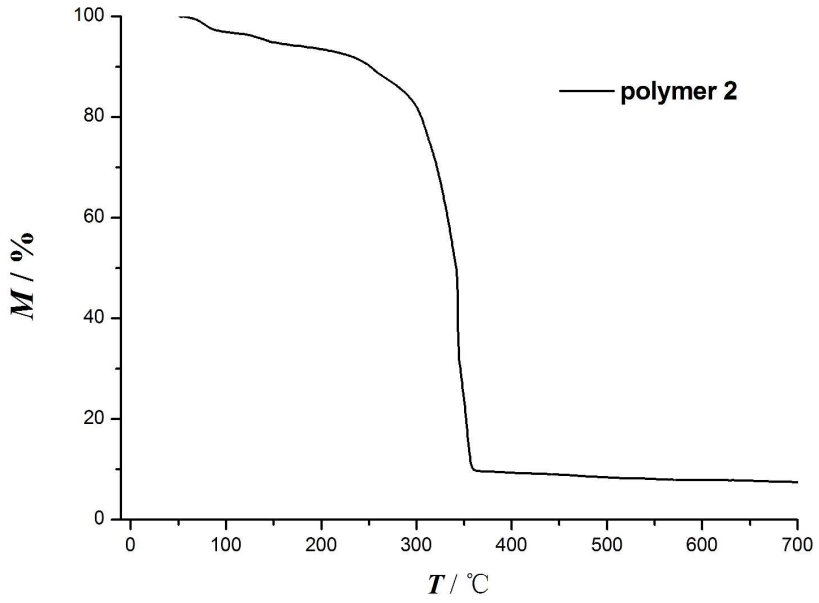

Figure S4. TG curve of polymer **2**. The TG curve shows that polymer **2** releases a methanol molecule and two water molecules per formula unit below 280°C.

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 Refinement of F^2^ against ALL reflections.    The weighted R-factor wR

and
 goodness of fit S are based on F^2^, conventional R-factors R are

based
 on F, with F set to zero for negative F^2^. The threshold expression

of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.

and is
 not relevant to the choice of reflections for refinement.    R-factors
```

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based
  on F^2^ are statistically about twice as large as those based on F,

and R-
  factors based on ALL data will be even larger.
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H8C H 0.2653 -0.1717 0.1074 0.105 Uiso 1 1 calc R . .
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H2B H 0.1296 -0.1588 0.3388 0.119 Uiso 1 1 d R . .
N6 N 0.22272(11) 0.17035(7) 0.34859(13) 0.0386(10) Uani 1 1 d R . .
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C8 0.075(5) 0.059(4) 0.092(5) 0.001(4) 0.059(4) 0.009(3)
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All esds (except the esd in the dihedral angle between two l.s.

planes)
are estimated using the full covariance matrix. The cell esds are

taken
into account individually in the estimation of esds in distances,

angles
and torsion angles; correlations between esds in cell parameters are

only
used when they are defined by crystal symmetry. An approximate

(isotropic)
treatment of cell esds is used for estimating esds involving l.s.

planes.
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Mo1 C3 2.155(4) 2_656 ?
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Mo2 C6 2.144(4) 2 ?
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Mo2 C9 2.147(4) 5 ?
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Mo2 C4 2.164(4) . ?
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 Refinement of F^2^ against ALL reflections.    The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.    R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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O1 O 0.37479(14) 0.06922(15) 0.09186(12) 0.0350(5) Uani 1 1 d . . .
O2 O 0.1946(2) 0.1672(2) 0.0000 0.0356(7) Uani 1 2 d S . .
O3 O 0.3317(2) -0.1518(2) 0.0000 0.0360(7) Uani 1 2 d S . .
N1 N 0.15094(18) -0.03783(18) 0.09223(14) 0.0303(5) Uani 1 1 d . . .
N2 N -0.0598(2) -0.24746(19) 0.19274(15) 0.0411(6) Uani 1 1 d . . .
N3 N 0.0535(3) 0.2821(3) 0.0000 0.0394(9) Uani 1 2 d S . .
N4 N 0.4007(2) 0.15591(19) 0.20796(16) 0.0398(6) Uani 1 1 d . . .
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C2 C -0.0395(2) -0.1617(2) 0.21277(16) 0.0283(6) Uani 1 1 d . . .
C3 C 0.0960(3) 0.1867(3) 0.0000 0.0303(9) Uani 1 2 d S . .
H3 H 0.0493 0.1282 0.0000 0.036 Uiso 1 2 calc SR . .
C4 C 0.4255(3) -0.1869(3) 0.0000 0.0339(10) Uani 1 2 d S . .
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C6 C 0.3697(5) -0.3721(4) 0.0000 0.119(4) Uani 1 2 d S . .
H6A H 0.2996 -0.3395 0.0000 0.179 Uiso 1 2 calc SR . .
H6B H 0.3776 -0.4160 0.0462 0.179 Uiso 0.50 1 calc PR . .
H6C H 0.3776 -0.4160 -0.0462 0.179 Uiso 0.50 1 calc PR . .
C7 C 0.1225(5) 0.3762(4) 0.0000 0.118(3) Uani 1 2 d S . .
H7A H 0.1965 0.3539 0.0000 0.178 Uiso 1 2 calc SR . .
H7B H 0.1084 0.4185 0.0462 0.178 Uiso 0.50 1 calc PR . .
H7C H 0.1084 0.4185 -0.0462 0.178 Uiso 0.50 1 calc PR . .
C8 C 0.5173(3) 0.1466(3) 0.2068(3) 0.0695(12) Uani 1 1 d . . .
H8A H 0.5394 0.1113 0.1592 0.104 Uiso 1 1 calc R . .
H8B H 0.5406 0.1052 0.2514 0.104 Uiso 1 1 calc R . .
H8C H 0.5488 0.2170 0.2091 0.104 Uiso 1 1 calc R . .
C9 C 0.3511(3) 0.2077(3) 0.2763(2) 0.0606(10) Uani 1 1 d . . .
H9A H 0.2743 0.2075 0.2702 0.091 Uiso 1 1 calc R . .
H9B H 0.3762 0.2806 0.2802 0.091 Uiso 1 1 calc R . .
H9C H 0.3702 0.1691 0.3232 0.091 Uiso 1 1 calc R . .
C10 C -0.0609(4) 0.2994(4) 0.0000 0.0504(12) Uani 1 2 d S . .
H10A H -0.0972 0.2312 0.0000 0.076 Uiso 1 2 calc SR . .
H10B H -0.0809 0.3392 -0.0462 0.076 Uiso 0.50 1 calc PR . .
H10C H -0.0809 0.3392 0.0462 0.076 Uiso 0.50 1 calc PR . .
C11 C 0.5626(4) -0.3244(4) 0.0000 0.0629(16) Uani 1 2 d S . .
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H11B H 0.5759 -0.3670 -0.0462 0.094 Uiso 0.50 1 calc PR . .
H11C H 0.5759 -0.3670 0.0462 0.094 Uiso 0.50 1 calc PR . .
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O4 O 0.4199(4) 0.4533(3) 0.2011(3) 0.1321(15) Uani 1 1 d . . .

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O1 0.0269(10) 0.0419(11) 0.0362(12) -0.0050(10) -0.0044(9) 0.0015(9)
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N5 0.0265(19) 0.0279(19) 0.081(3) 0.000 0.000 0.0056(15)
C1 0.0258(14) 0.0231(13) 0.0237(14) -0.0001(12) -0.0028(12) -0.0001(11)
C2 0.0365(16) 0.0250(15) 0.0234(15) 0.0030(12) -0.0005(13) 0.0015(12)
C3 0.038(2) 0.026(2) 0.027(2) 0.000 0.000 0.0030(17)
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C5 0.0306(15) 0.0332(16) 0.0428(19) -0.0006(15) -0.0018(15) -0.0038(12)
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C7 0.060(4) 0.022(3) 0.272(11) 0.000 0.000 0.001(3)
C8 0.048(2) 0.081(3) 0.079(3) -0.027(2) -0.028(2) 0.005(2)
C9 0.072(3) 0.060(2) 0.049(2) -0.021(2) 0.001(2) -0.016(2)
C10 0.048(3) 0.049(3) 0.053(3) 0.000 0.000 0.013(2)
C11 0.038(3) 0.039(3) 0.112(5) 0.000 0.000 0.015(2)
Cl1 0.0507(7) 0.0507(7) 0.131(2) 0.000 0.000 0.000
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
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 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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W1 C2 2.163(3) 8_556 ?
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Mn1 N1 2.229(2) 7 ?
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H8B C8 H8C 109.5 . . ?
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N4 C9 H9B 109.5 . . ?
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N4 C9 H9C 109.5 . . ?
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