Supporting Information for:

Three new 3D coordination polymers constructed from semirigid tri-carboxylate V-shaped ligand, synthesis, characterization and magnetic properties

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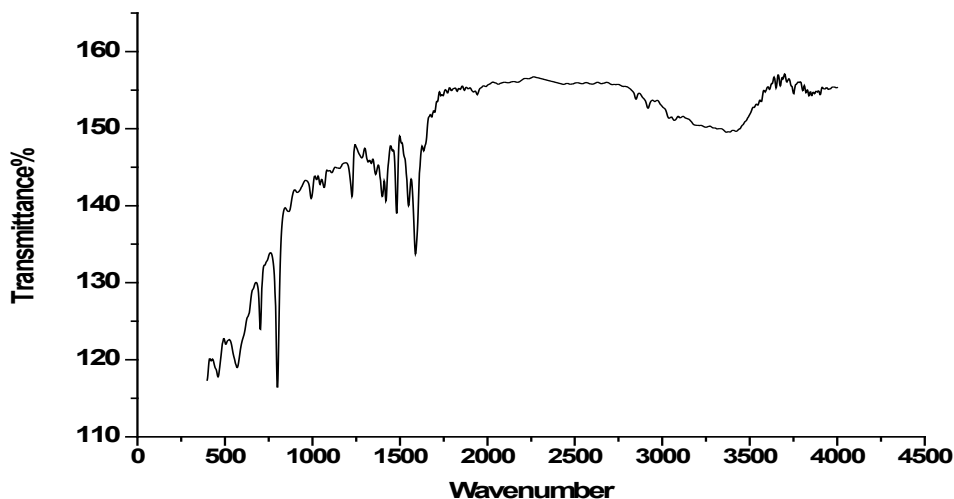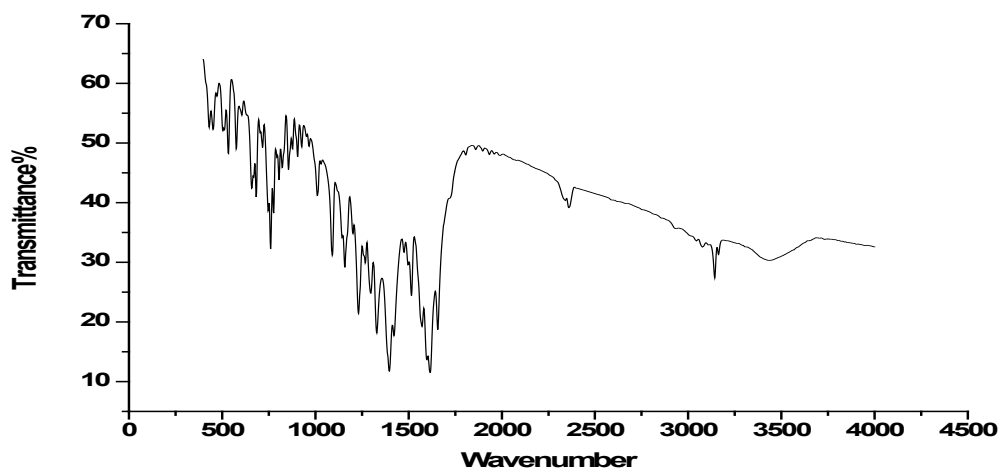
Figure S1. IR spectra for complex 1
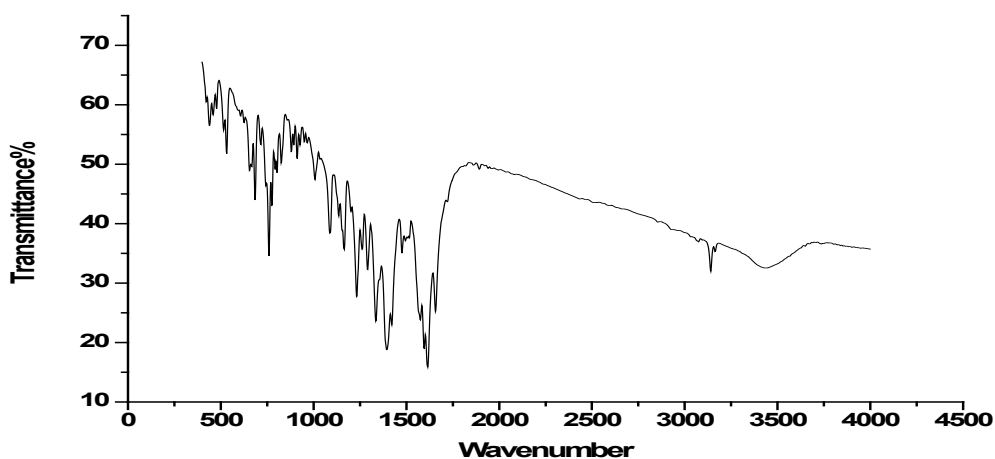
Figure S2. IR spectra for complex 2

Figure S3. IR spectra for complex

A. Supplementary data

CCDC **1578309** to **1578311**, contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/conts/retrieving.html. The specific information may be obtained free of charge from the director, CCDC, 12 Union Road, Cambridge, CB21EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.com.ac.uk).

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20150508lzz1_0m

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: 20150508lzz1_0m

```
Bond precision:    C-C = 0.0031 A            Wavelength=0.71073

Cell:              a=20.943(4)     b=16.165(3)          c=16.293(3)
                   alpha=90        beta=102.144(3)      gamma=90
Temperature:       296 K

                   Calculated                Reported
Volume             5392.5(17)                5392.4(18)
Space group        C 2/c                     C2/c
Hall group         -C 2yc                    ?
                   C62 H42 Mn3 N4 O16, 2(H2
Moiety formula                               ?
                   O)
Sum formula        C62 H46 Mn3 N4 O18        C62 H46 Mn3 N4 O18
Mr                 1299.85                   1299.85
Dx,g cm-3          1.601                     1.601
Z                  4                         4
Mu (mm-1)          0.776                     0.776
F000               2660.0                    2660.0
F000'              2665.31
h,k,lmax           24,19,19                  24,19,19
Nref               4760                      4760
Tmin,Tmax          0.811,0.843               0.818,0.848
Tmin'              0.811

Correction method= # Reported T Limits: Tmin=0.818 Tmax=0.848
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.000

R(reflections)= 0.0304( 4187)      wR2(reflections)= 0.0821( 4760)

S = 1.076                  Npar= 398
```

The following ALERTS were generated. Each ALERT has the format
 test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🟡 Alert level C
```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of        O1 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
              C62 H42 Mn3 N4 O16
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.595          5 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....         1 Check
```

⚪ Alert level G
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         6 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF     Please Do !
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        65 Do !
          N2  -MN1 -N1  -C1      5.00  0.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        70 Do !
          N2  -MN1 -N1  -C1     13.00  0.00   1.555   1.555   1.555   2.655
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        77 Do !
          N1  -MN1 -N2  -C8      9.00  0.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        82 Do !
          N1  -MN1 -N2  -C8      9.00  0.00   1.555   1.555   1.555   2.655
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       113 Do !
          O3  -MN1 -O3  -C30   132.60  0.40   2.655   1.555   1.555   1.555
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        2 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .     1.13 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        4 Note
PLAT899_ALERT_4_G SHELXL97    is Deprecated and Succeeded by SHELXL    2014 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still        77 %
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.
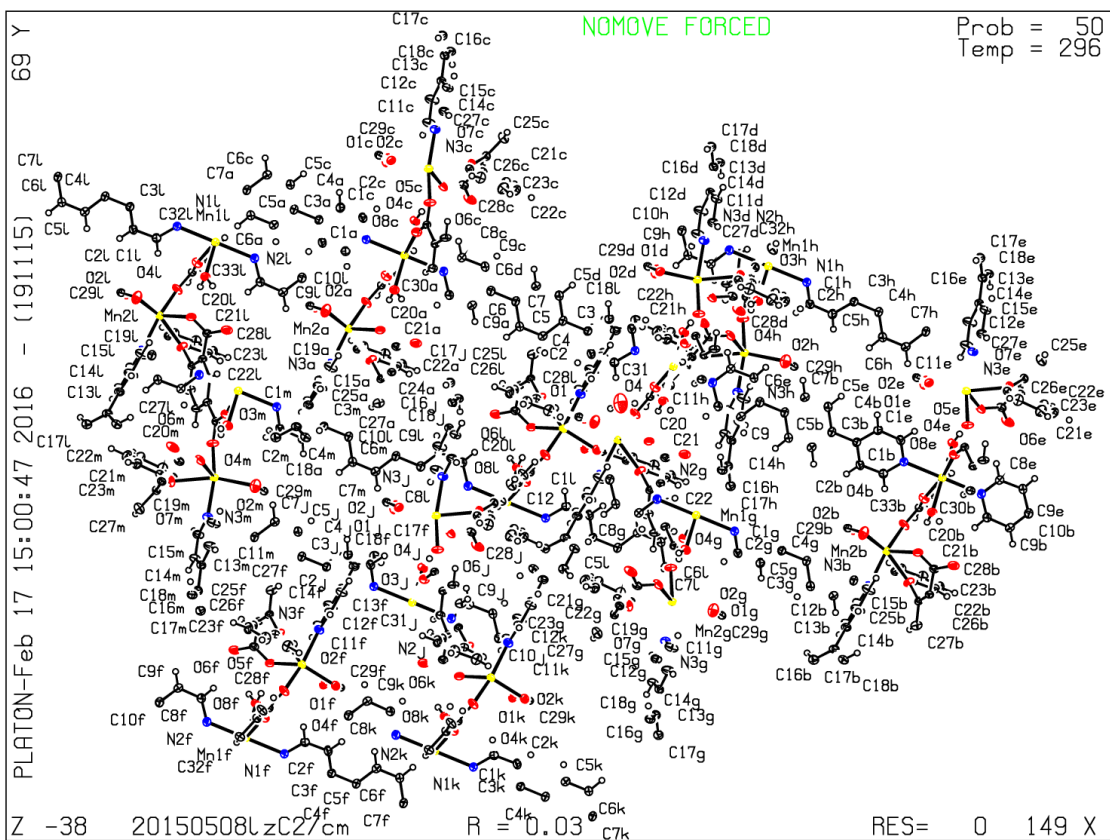
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20151130lz_0m

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: 20151130lz_0m

```
Bond precision:   C-C = 0.0042 A            Wavelength=0.71073

Cell:          a=8.7046(10)       b=10.9913(13)     c=12.5931(13)
               alpha=113.076(3)   beta=104.784(3)   gamma=96.875(4)
Temperature:   296 K

                  Calculated                  Reported
Volume         1038.5(2)                   1038.5(2)
Space group    P -1                        P -1
Hall group     -P 1                        -P 1
Moiety formula C44 H28 N4 O14 Zn3          ?
Sum formula    C44 H28 N4 O14 Zn3          C44 H28 N4 O14 Zn3
Mr             1032.87                     1032.81
Dx,g cm-3      1.652                       1.651
Z              1                           1
Mu (mm-1)      1.795                       1.795
F000           522.0                       522.0
F000'          523.08
h,k,lmax       10,13,14                    10,13,14
Nref           3667                        3623
Tmin,Tmax      0.611,0.674
Tmin'          0.599

Correction method= Not given

Data completeness= 0.988          Theta(max)= 25.025

R(reflections)= 0.0265( 3296)     wR2(reflections)= 0.0699( 3623)

S = 1.048                Npar= 296
```

The following ALERTS were generated. Each ALERT has the format
      test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.
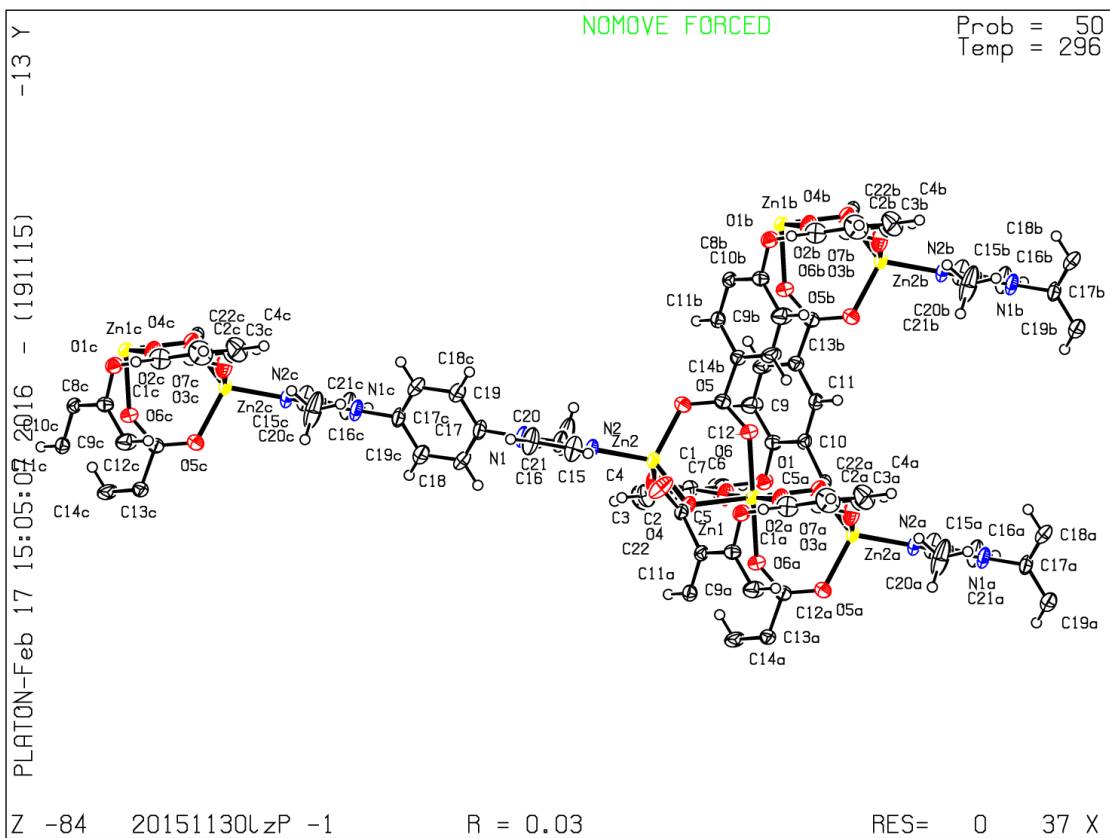
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Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: 20160306lz_0m_a

```
Bond precision:   C-C = 0.0054 A            Wavelength=0.71073

Cell:          a=8.726(4)           b=11.468(6)        c=12.458(6)
               alpha=113.856(8)  beta=100.893(8)  gamma=97.113(9)
Temperature:   296 K

                 Calculated                Reported
Volume         1091.4(9)                 1091.5(9)
Space group    P -1                      P-1
Hall group     -P 1                      ?
Moiety formula C46 H32 N4 O14 Zn3        ?
Sum formula    C46 H32 N4 O14 Zn3        C46 H32 N4 O14 Zn3
Mr             1060.93                   1060.87
Dx,g cm-3      1.614                     1.614
Z              1                         1
Mu (mm-1)      1.710                     1.710
F000           538.0                     538.0
F000'          539.08
h,k,lmax       10,13,14                  10,13,14
Nref           3858                      3814
Tmin,Tmax      0.637,0.814               0.655,0.821
Tmin'          0.624

Correction method= # Reported T Limits: Tmin=0.655 Tmax=0.821
AbsCorr = MULTI-SCAN

Data completeness= 0.989          Theta(max)= 25.010

R(reflections)= 0.0367( 3428)     wR2(reflections)= 0.1186( 3814)

S = 1.112                    Npar= 305
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The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
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  ● Alert level C
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range       3.1 Ratio
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        77 Ang3


  ● Alert level G
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF    Please Do !
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as     mixed Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        74 Do !
           C9  -O2  -ZN1 -O2     48.00 21.00   1.555   1.555   1.555  2.777
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.11 Ratio
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2014 Note


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