Supporting Information

A Crystal Engineering Rationale in Designing A Cd^{II} Coordination Polymer Based Metallogel Derived from a C3 Symmetric Tris-amide-tris-carboxylate Ligand

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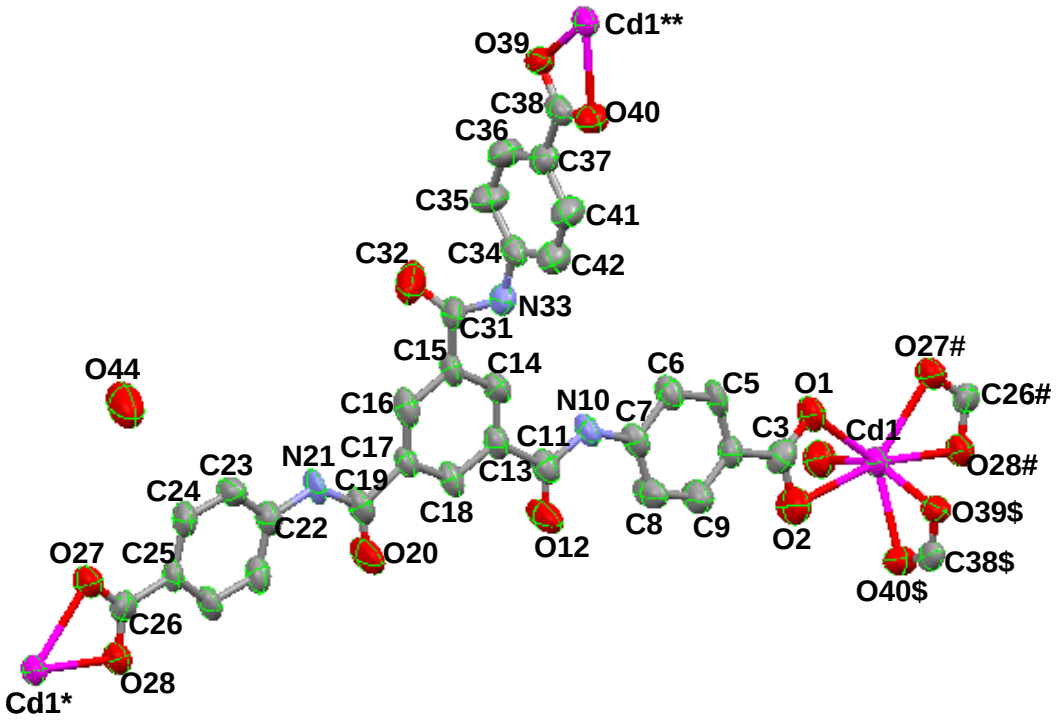
Contents **Page No**

Molecular plot and Hydrogen Bonding Parameters for CP1 (Figure S1)

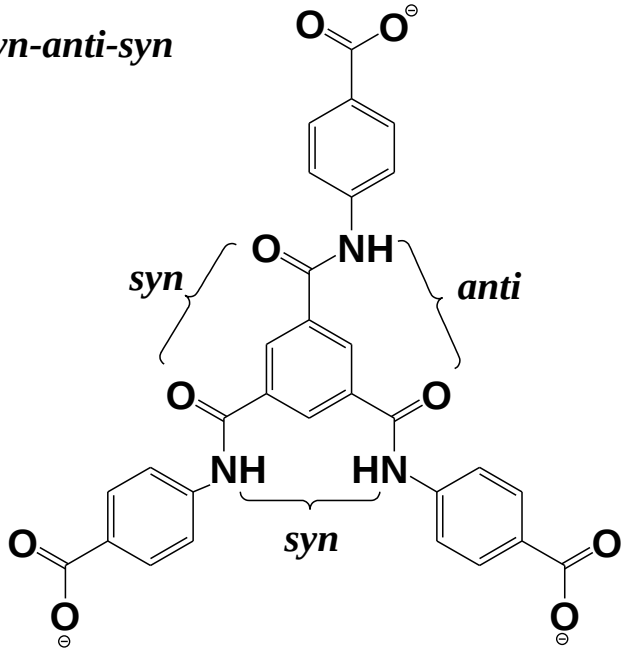


* 1+x, y, 2+z; ** -x, -1/2+y, 1/2-z ; # -1+x, y, -2+z ; $ -x, 1/2+y, 1/2-z

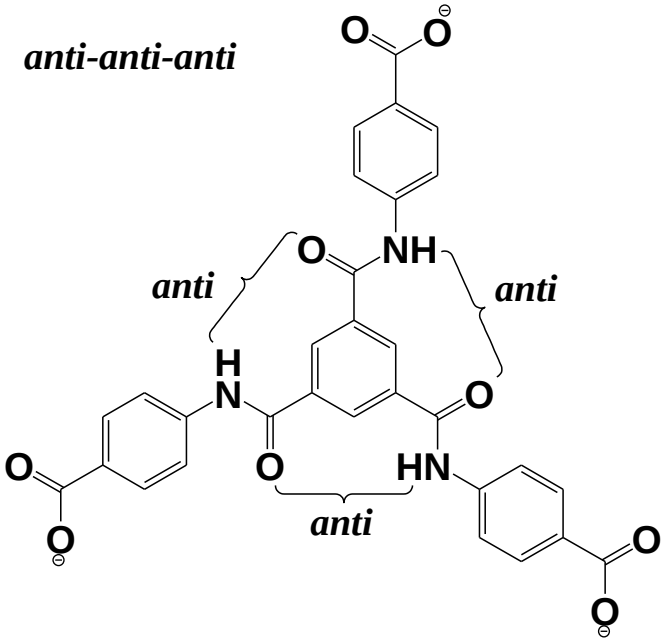
Hydrogen bonding parameters of **CP1**					
D–H•••A	D–H (Å)	H•••A (Å)	D•••A (Å)	D–H•••A (^{0})	Symmetry operation for A
N(10)–H(10)•••O(39)	0.86	2.13	2.929(6)	154.1	x, -y+3/2, z-1/2
N(33)–H(33)•••O(28)	0.86	2.07	2.881(6)	157.1	-x+1, -y+2, -z+2
O(44)•••O(43)			2.745(7)		
O(44)•••O(27)			2.744(7)		
O(43)•••O(1)			2.618		

Various conformations of L1

syn-anti-syn



anti-anti-anti



Scheme S1

TGA of CP1

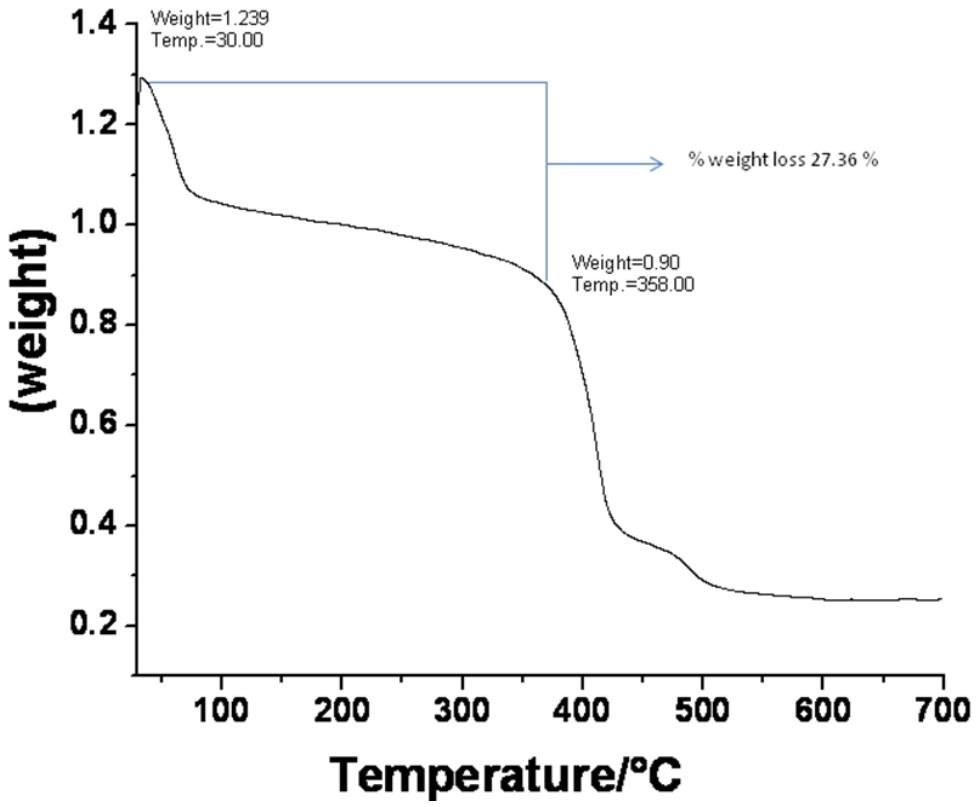


Figure. S2

Unit cell contents = 4 Ligand(L1) + 4 Cd^{2+} + 4 H_2O (occluded) + 4 H_2O (coordinated)+ 48 disorderd H_2O (488 electrons from SQUEEZE results approximately attributed to 12 H_2O molecule)

Monoclinic, $P2_1/c$ space group, Z = 4

Therefore FW = Unitcell contents/4

= 1Ligand(L1) + 1 Cd^{2+} + 1 H_2O (coordinated)+1(occluded) + 12 H_2O (occluded)
= 1 X 564.11 + 113.9 + 18.01+18.01 +12X 18.01= 929.11

Weight loss for $13H_2O$ = 14 X 18.01/929.11

= 252/912.11
= 27.12 % (experimental 27.36 %)

PXRD comparison between bulk and xerogel state of G2,G3, G4

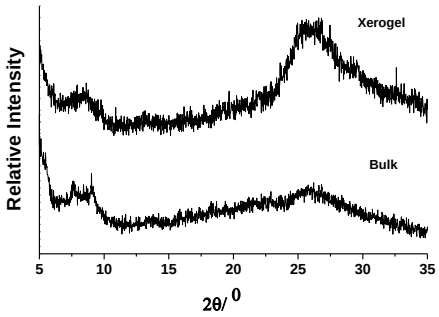


Figure **S3** : PXRD comparison between bulk (**CP2**) and xerogel of G2

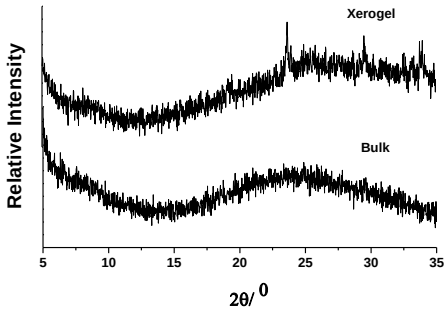


Figure **S4** : PXRD comparison between bulk (**CP3**) and xerogel of G3

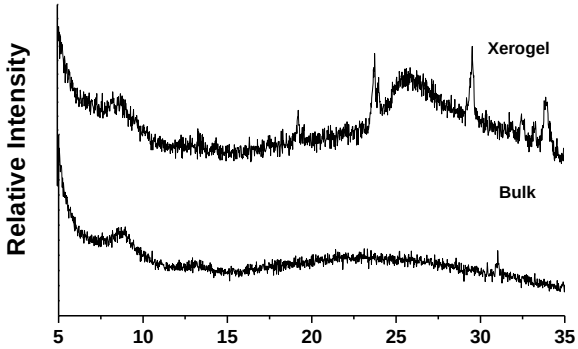


Figure **S5** : PXRD comparison between bulk (**CP4**) and xerogel of G4

S4

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: pdann

Bond precision: C-C = 0.0096 A Wavelength=0.71073

Cell: a=17.9224(13) b=26.390(2) c=9.0841(7)
alpha=90 beta=99.700(2) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	4235.1(6)	4235.1(6)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C30 H18 Cd N3 O10, O	?
Sum formula	C30 H18 Cd N3 O11	C30 H46 Cd N3 O23
Mr	708.88	929.10
Dx,g cm-3	1.112	1.457
Z	4	4
Mu (mm-1)	0.562	0.601
F000	1420.0	1916.0
F000'	1417.52	
h,k,lmax	17,25,8	16,25,8
Nref	3819	3803
Tmin,Tmax	0.829,0.919	0.831,0.921
Tmin'	0.825	

Correction method= MULTI-SCAN

Data completeness= 0.996 Theta(max)= 19.750

R(reflections)= 0.0437(3109) wR2(reflections)= 0.1023(3803)

S = 1.107 Npar= 406

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 A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 4

```
From the CIF: _chemical_formula_weight          929.10
TEST: Calculate formula weight from _atom_site_*
atom     mass     num     sum
C        12.01   30.00  360.33
H         1.01   18.00   18.14
N        14.01    3.00   42.02
O        16.00   11.00  175.99
Cd      112.41    1.00  112.41
Calculated formula weight             708.89
```

Author Response: We have used SQUEEZE to remove the contributions of disordered solvent molecules (which we could not be modeled) within the crystal lattice. Therefore, the contribution of disordered solvent molecules removed by the SQUEEZE process are included in the overall formula, formula weight, density, F(000) *etc*. The output of the *PLATON* (generated as. sqf file) is also appended to the bottom of the CIF.

```
THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.4755
```

Author Response: The crystal was poorly diffracting at higher Bragg angles. The situation did not improve even after repeating crystallization and fresh data collection.

```
PLAT043_ALERT_1_A Check Reported Molecular Weight .................     929.10
```

Author Response: We have used SQUEEZE to remove the contributions of disordered solvent molecules (which we could not be modeled) within the crystal lattice. Therefore, the contribution of disordered solvent molecules removed by the SQUEEZE process are included in the overall formula, formula weight, density, F(000) etc. The output of the PLATON (generated as \ .sqf file) is also appended to the bottom of the CIF.

```
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......        O44
```

Author Response: The hydrogen atoms of the lattice included water molecules could not be located from differnce Fourier map.

Alert level B

```
PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       6.45 Perc.
```

Author Response: We have used SQUEEZE to remove the contributions of disordered solvent molecules (which we could not be modeled) within the crystal lattice. Therefore, the contribution of disordered solvent molecules removed by the SQUEEZE process are included in the overall formula, formula weight, density, F(000) *etc*. The output of the *PLATON* (generated as. sqf file) is also appended to the bottom of the CIF.

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O27    ..  O44     ..       2.74 Ang.
```

Author Response: The short contact is due to the hydrogen bonding between the lattice included water and carboxylate. Since the hydrogen atom associated with the lattice included water could not located in the differnece fourier map, it shows as short contact alert.

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O43    ..  O44     ..       2.75 Ang.
```

Author Response: The short contact is due to the hydrogen bonding between the lattice included water and carboxylate. Since the hydrogen atom associated with the lattice included water could not located in the differnece fourier map, it shows as short contact alert.

Alert level C

```
REFNR01_ALERT_3_C  Ratio of reflections to parameters is < 10 for a
           centrosymmetric structure
           sine(theta)/lambda               0.4755
           Proportion of unique data used   1.0000
           Ratio reflections to parameters  9.3670
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT088_ALERT_3_C Poor Data / Parameter Ratio .....................       9.37
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O1     --  C3      ..        5.3 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C4     --  C5      ..        5.5 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C16    --  C17     ..        5.2 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         O2
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C35
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         Cd1
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C34    -C42          1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0096 Ang
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C11    -   C13    ...       1.53 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H10    ..  H14     ..       1.96 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H16    ..  H21     ..       1.93 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N21    -   H21    ...          ?
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C30 H46 Cd1 N3 O23
           Atom count from the _atom_site data:  C30 H18 Cd1 N3 O11
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C30 H46 Cd N3 O23
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        120.00    120.00    0.00
          H        184.00     72.00  112.00
          Cd         4.00      4.00    0.00
          N         12.00     12.00    0.00
```

```
          O         92.00     44.00   48.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms ............          3
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT804_ALERT_5_G ARU-Pack Problem in PLATON Analysis ............          6 Times
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

```
   4 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  17 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

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   4 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*, 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 19/04/2012; check.def file version of 14/04/2012

Datablock pdann - ellipsoid plot