Supplementary Material for

Topological studies of three related MOFs of Gd(III) and 5-nitroisophthalate

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Synopsis: Three gadolinium/5-nitroisophthalate MOFs prepared under controlled but similar conditions were found to be related topologically through a simple C-C bond rotation.

Compound I:

Thermogravimetric (TG) and Differential Scanning Calorimetry (DSC)traces

PXRD: experimental versus the single crystal calculated pattern, vapour diffusion experiments, and variable temperature experiments.

Topological analysis: SYSTRE and OLEX output

Compound II:

TG and DSC traces.

PXRD: experimental versus single crystal calculated pattern.

Topological analysis: SYSTRE and OLEX output

Compound III:

TG and DSC traces.

Topological analysis: SYSTRE, OLEX and TOPOS output

Compound I

Fig S1. TG (blue) and DSC (red) traces for **I**.

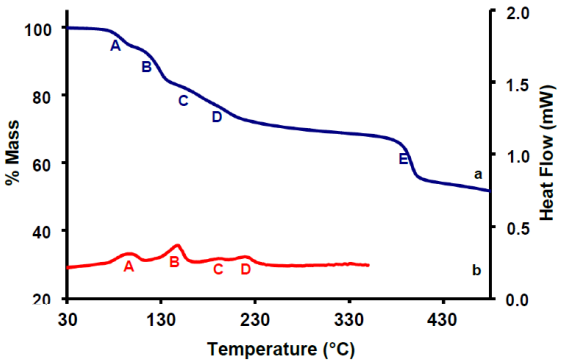


Fig S2. Calculated (blue) vs experimental (red) powder X-ray diffraction patterns of **I**.

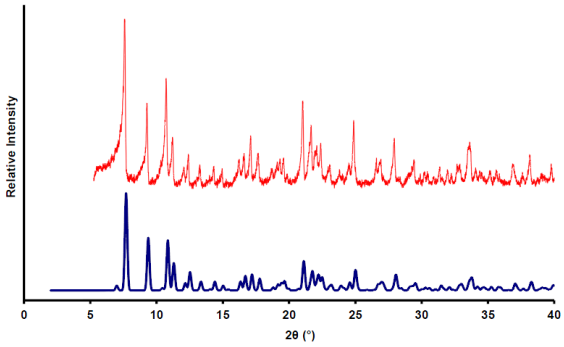


Fig S3. Variable temperature PXRD of **I**.

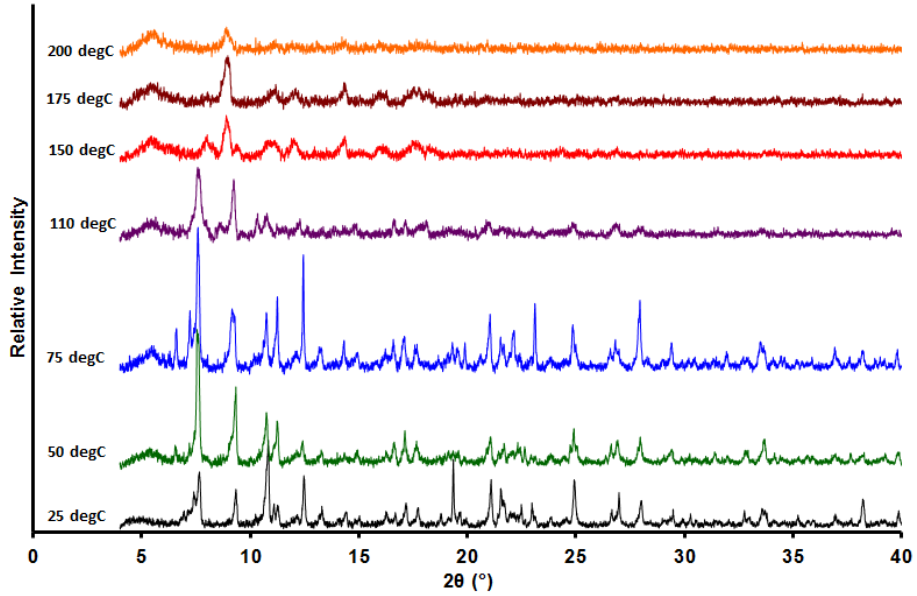
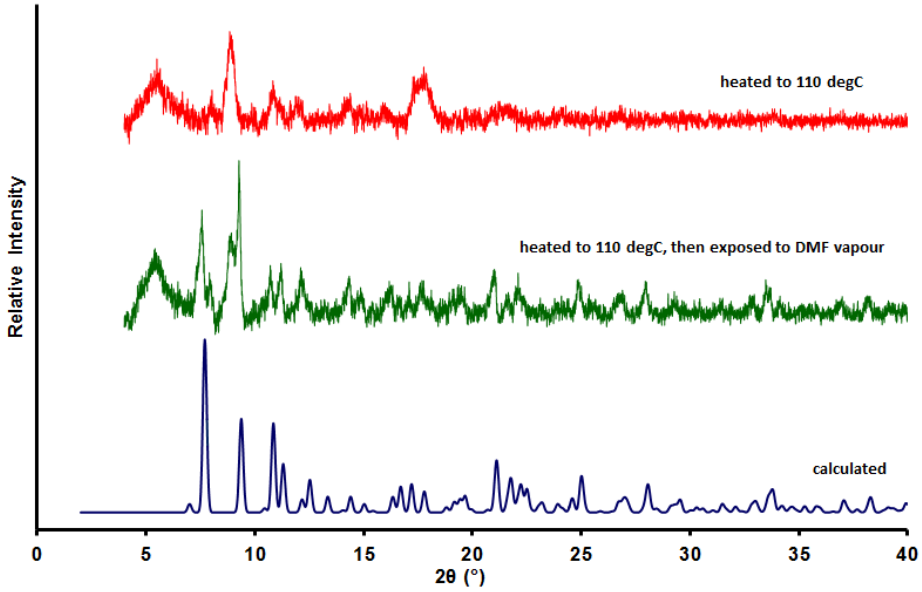


Fig S4. PXRD of **I** on heating and subsequent exposure to DMF vapour.



SYSTRE Output for **I**:

Structure #1 - "1".

Structure of dimension 3.
Given space group is P21.
2 nodes and 6 edges in repeat unit as given.

Ideal repeat unit smaller than given (3 vs 6 edges).
Point group has 48 elements.
1 kind of node.

Coordination sequences:
Node 1: 6 18 38 66 102 146 198 258 326 402

TD10 = 1561.0000

Ideal space group is Pm-3m.
Ideal group differs from given (Pm-3m vs P1211).

Structure was found in builtin archive:
Name: pcu

Relaxed cell parameters:
a = 1.00000, b = 1.00000, c = 1.00000
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 1.00000
Relaxed positions:
Node 1: 0.00000 0.00000 0.00000
Edges:
0.00000 0.00000 0.00000 <-> 0.00000 0.00000 1.00000
Edge centers:
0.00000 0.00000 0.50000

Edge statistics: minimum = 1.00000, maximum = 1.00000, average = 1.00000
Angle statistics: minimum = 90.00000, maximum = 180.00000, average = 108.00000
Shortest non-bonded distance = 1.41421

Degrees of freedom: 1

Finished structure #1 - "1".

OLEX output for **I**:

Topological analysis for: Compound 1 IN C2/C

Topological Terms for:	short	long
LC23 (mixed atoms, count: 200)	4(12).6(3)	4.4.4.4.4.4.4.4.4.4.4.4

Compound II

Fig S5. TG (blue) and DSC (red) traces for **II**.

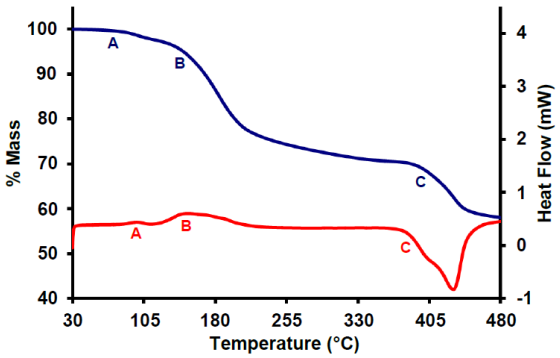
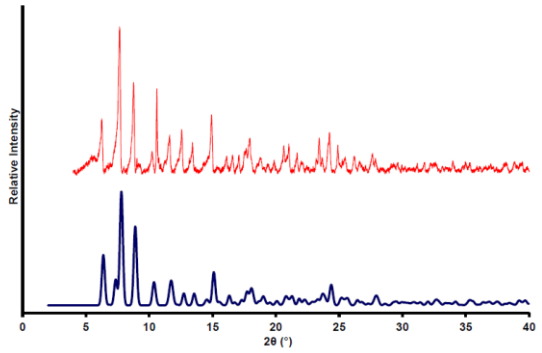


Fig S6. Calculated (blue) vs experimental (red) powder X-ray diffraction patterns of **II**.



SYSTRE Output for **II**:

Structure #1 – "2".

Structure of dimension 3.
Given space group is C2/c.
4 nodes and 8 edges in repeat unit as given.

Given repeat unit is accurate.
Point group has 16 elements.
2 kinds of node.

Coordination sequences:
Node 1: 4 10 24 42 64 92 124 162 204 252
Node 2: 4 10 24 42 64 90 124 162 204 250

TD10 = 977.0000

Ideal space group is P42/mmc.
Ideal group differs from given (P42/mmc vs C12/c1).

Structure was found in builtin archive:
Name: pts

Relaxed cell parameters:
a = 1.63299, b = 1.63299, c = 2.30940
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 6.15840
Relaxed positions:

Node 1: 0.50000 0.00000 0.00000
Node 2: 0.00000 0.00000 0.25000
Edges:
0.00000 0.00000 0.25000 <-> 0.50000 0.00000 0.00000
Edge centers:
0.25000 0.00000 0.12500

Edge statistics: minimum = 1.00000, maximum = 1.00000, average = 1.00000
Angle statistics: minimum = 70.52878, maximum = 180.00000, average = 114.73561
Shortest non-bonded distance = 1.15470

Degrees of freedom: 2

Finished structure #1 - "2".

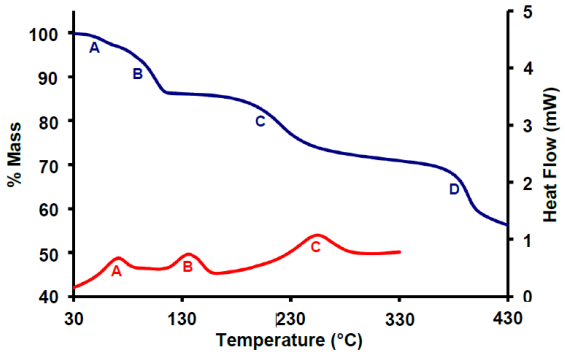
OLEX output for **II**:

Topological analysis for: Compound 2 IN C2/C

Topological Terms for:	short	long
LC39 (mixed atoms, count: 121)	4(2).8(4)	4.4.8(2).8(2).8(8).8(8)
LC40 (mixed atoms, count: 144)	4(2).8(4)	4.4.8(7).8(7).8(7).8(7)

Compound III

Fig S7. TG (blue) and DSC (red) traces for **III**.



SYSTRE Output for **III:**

Structure #1 - "3".

Structure of dimension 3.
Given space group is P-1.
4 nodes and 10 edges in repeat unit as given.

Given repeat unit is accurate.
Point group has 4 elements.
3 kinds of node.

Coordination sequences:
Node 2: 5 15 33 58 89 127 173 226 285 351
Node 1: 4 12 34 56 86 126 176 224 280 350
Node 3: 6 16 32 58 92 128 170 226 290 352

TD10 = 1361.5000

Ideal space group is C12/m1.
Ideal group differs from given (C12/m1 vs P-1).

Structure is new for this run.

Relaxed cell parameters:
a = 2.98322, b = 1.33276, c = 2.66656
alpha = 90.0000, beta = 116.5464, gamma = 90.0000
Cell volume: 9.48431
Relaxed positions:
Node 2: 0.12469 0.50000 0.31235
Node 1: 0.00000 0.00000 0.00000
Node 3: 0.00000 0.00000 0.50000
Edges:
0.00000 0.00000 0.00000 <-> 0.12469 0.50000 0.31235
0.00000 0.00000 0.50000 <-> 0.12469 0.50000 0.31235
0.00000 0.00000 0.50000 <-> 0.37531 0.00000 0.68765
Edge centers:
0.06234 0.25000 0.15617
0.06234 0.25000 0.40617
0.18766 0.00000 0.59383

Edge statistics: minimum = 0.99960, maximum = 1.00159, average = 1.00000
Angle statistics: minimum = 70.55564, maximum = 180.00000, average = 108.51464
Shortest non-bonded distance = 1.15577

Degrees of freedom: 6

Finished structure #1 - "3".

OLEX output for **III**:

Topological analysis for: Compound 3

Topological Terms for:	short	long
LC79 (mixed atoms, count: 36)	4(8).6(6).8	4.4.4.4.4.4.4.4.6(2).6(2).6(2).6(2)
LC78 (mixed atoms, count: 54)	4(6).6(4)	4.4.4.4.4.4.6(2).6(2).7.7
LC80 (mixed atoms, count: 36)	4(4).6(2)	4.4.4.4.7(2).8(4)

TOPOS output for **3**:

```
###########
1:eu2 Pr Sm
###########
Atoms       Dist.     SA    rs-rs   rs-Rsd   Rsd-rs   Rsd-Rsd  Ovr.
--------------------------------------------------------------------------
Pr1 vEu1     3.083    19.81   1.0448   1.7412   1.7412   2.6530    4
   vEu1      3.083    19.81   1.0448   1.7412   1.7412   2.6530    4
   vEu1      3.795    13.31    No      0.2672   0.2672   1.5496    3
   vEu1      3.795    13.31    No      0.2672   0.2672   1.5496    3
   vEu1      3.805    13.38    No      0.2727   0.2727   1.6276    3
   vEu1      3.805    13.38    No      0.2727   0.2727   1.6276    3
    Pr1      4.775     0.82    No      No       No       0.3191    1
    Pr1      4.775     0.82    No      No       No       0.3191    1
    Pr1      5.106     1.33    No      No       No       0.1402    1
    Pr1      5.106     1.33    No      No       No       0.1402    1
    Eu1      5.603     0.58    No      No       No       0.0057    1
    Eu1      5.603     0.58    No      No       No       0.0057    1
--------------------------------------------------------------------------
Sm1 vEu1     3.196    19.59   0.7050   1.5761   1.5761   2.8680    4
   vEu1      3.196    19.62   0.7050   1.5862   1.5862   2.8968    4
   vEu1      3.578    15.78   0.0428   0.6501   0.6501   2.0929    4
   vEu1      3.578    15.78   0.0428   0.6501   0.6501   2.0929    4
   wEu1      4.301     9.84    No      No       No       1.0255    1
   wEu1      4.301     9.84    No      No       No       1.0255    1
    Sm1      4.775     0.18    No      No       No       0.5374    1
    Sm1      4.775     0.18    No      No       No       0.5374    1
   wSm1      5.106     2.82    No      No       No       0.3845    1
   wSm1      5.106     2.73    No      No       No       0.3231    1
    Sm1      5.201     0.96    No      No       No       0.2846    1
    Sm1      5.201     0.94    No      No       No       0.2539    1
    Eu1      5.902     0.17    No      No       No       0.0015    1
--------------------------------------------------------------------------
Eu1 vPr1     3.083    19.81   1.0448   1.7412   1.7412   2.6530    4
   vSm1      3.196    19.59   0.7050   1.5761   1.5761   2.8680    4
   vSm1      3.578    15.78   0.0428   0.6501   0.6501   2.0929    4
   vPr1      3.795    13.31    No      0.2672   0.2672   1.5496    3
   vPr1      3.805    13.38    No      0.2727   0.2727   1.6276    3
   wSm1      4.301     9.84    No      No       No       1.0255    1
   wEu1      4.573     2.44    No      No       No       0.4452    1
    Eu1      4.775     0.58    No      No       No       0.4540    1
    Eu1      4.775     0.58    No      No       No       0.4540    1
   wEu1      5.106     1.97    No      No       No       0.2239    1
   wEu1      5.106     1.97    No      No       No       0.2239    1
    Pr1      5.603     0.58    No      No       No       0.0057    1
    Sm1      5.902     0.17    No      No       No       0.0015    1
--------------------------------------------------------------------------

Coordination numbers for eu2 Pr Sm
--------------------------------------------------------------------------
Atom   CN  Sp  vdW   Hb    Composition          0  1  2  3  4
--------------------------------------------------------------------------
Pr1     6   0    0    0     Eu6                  4  6  0  4  2
Sm1     4   0    4    0     Eu4                  4  9  0  0  4
Eu1     5   0    4    0     Pr3Sm2               0  8  0  2  3
--------------------------------------------------------------------------

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```

Pr - Node 1
Sm - Node 2
Eu - Node 3