Open MOFs with the unique hexatopic zinc-5,15-bis(4'-carboxyphenyl)-10,20-bis(3',5'-dicarboxyphenyl)porphyrin linker

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Section-1

Table S1. Reaction Conditions

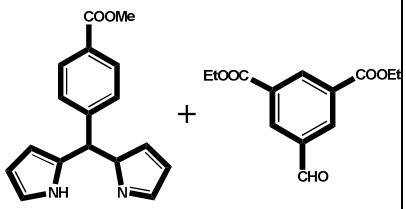
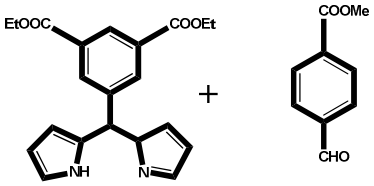
Reactants	Propionic acid	$BF_3.ET_2O$ /DDQ	Stiochiometric TFA/DDQ	Excess TFA/DDQ
	No Yield	1 % Yield	8 % Yield without any scrambling products	18-20 % Yield without any scrambling products
	No Yield	1 % Yield	8 % Yield without any scrambling products	18-20 % Yield without any scrambling products

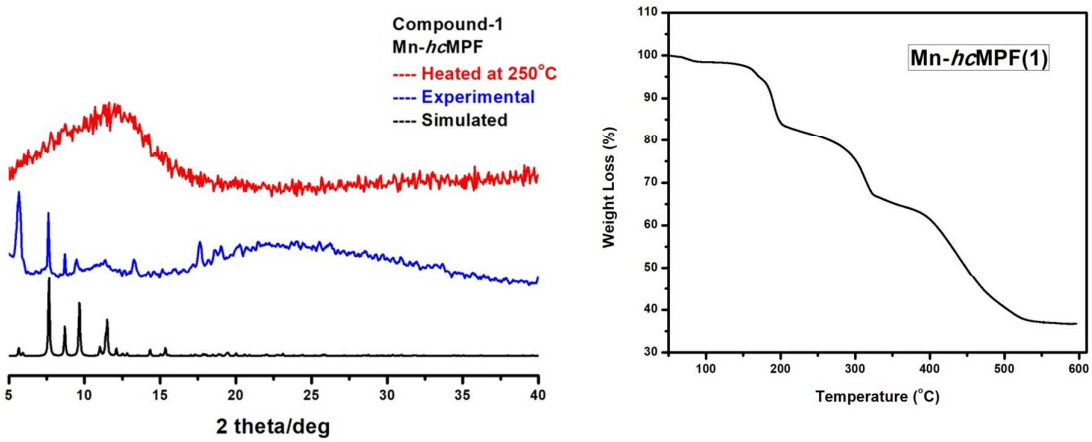
Table S2. Summary of structural parameters features in *hc*MPFs

C. Name	Topology	Twisting of benzoate arms				Ruffling angle C_α–N···N–C_α
		4-C	**4-C**	**3,5-C**	**3,5-C**	
Mn-*hc*MPF	6-c uninodal	65.18	65.18	80.24	80.24	-5.44 (8)
Co-*hc*MPF	6,6-binodal, *nia*	69.44	69.44	76.85	76.85	-3.35(8)
Zn-hcMPF	6-c uninodal	63.93	63.93	77.51	77.51	-0.87 (3)
In-*hc*MPF	5,6-binodal, *tcj/hc*	62.04	65.03	88.13	88.34	-7.19(10)
Pb-*hc*MPF	6-c uninodal, *pcu alpha-Po*	71.68	62.26	56.94	62.98	-6.53(10)
Ln-*hc*MPF (Ln=Pr,Gd)	6,7-c, *tcj/hc*	65.65	65.65	61.40	61.40	-10.96(8)
Yb-*hc*MPF	6-c uninodal, *pcu alpha-Po*	65.61	65.61	61.64	61.64	-1.13(6)

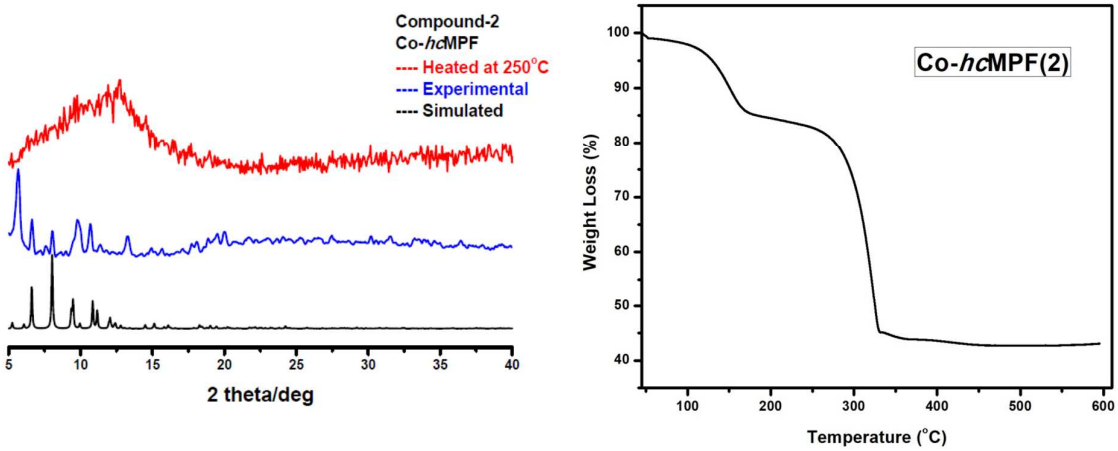
Table S3: Calculation of solvent molecules based on squeezed electrons and TGA

Compound	Squeezed electrons	Z	Squeezed electrons per Molecular formula	% Wt Loss from TGA till 350°C	Estimated DMF	Estimated H_2O	Plausible Molecular formula
Mn-*hc*MPF	1096	4	1096/2=548	38	13	3	$\{Mn_2[Zn(H_2O)\text{-}H_2HCPP]\}_n\cdot 13DMF\cdot 3H_2O$
Co-*hc*MPF	1201	8	1201/4=300.25	48.5	7	2	$\{[Co_3(H_2O)_3](Zn(H_2O)\text{-}HCPP)\}\cdot 7DMF\cdot 2H_2O$
In-*hc*MPF	1102	4	1102/4=275.5	24	6	3	$\{InNa_2(H_2O)_3(Zn\text{-}HHCPP)\}\cdot 6DMF\cdot 3H_2O$
Pb-*hc*MPF	524	4	524/4=131	17	3	1	$\{Pb_2[Zn(H_2O)\text{-}H_2HCPP]\}\cdot 3DMF\cdot H_2O$
Gd-*hc*MPF	1289	4	1289/4=322	28	7	4	$\{GdNa_2(H_2O)_2(\mu_2\text{-}H_2O)_2(Zn\text{-}HHCPP)\}\cdot 7DMF\cdot 4H_2O$

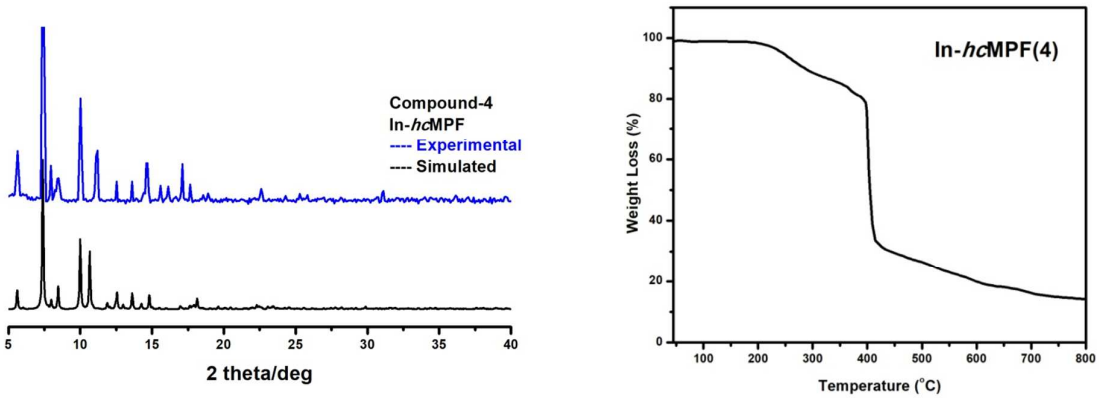
Section-2



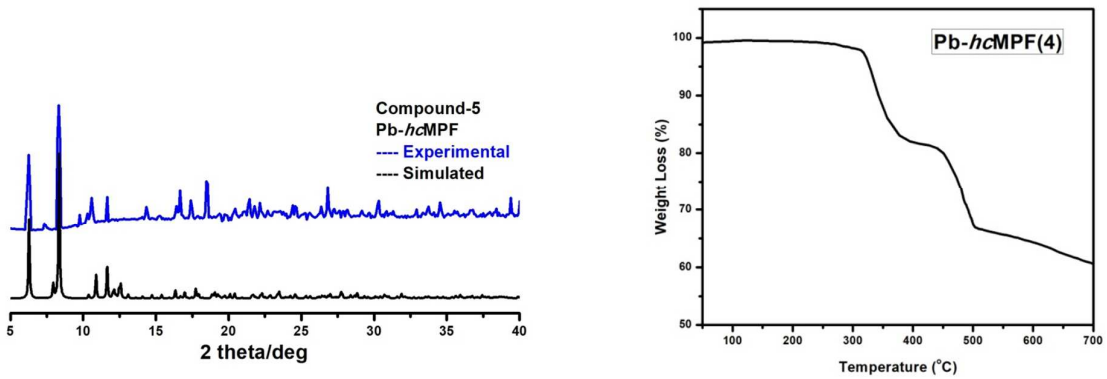
Spectra S1: TGA and PXRD curves of compound Mn-*hc*MPF



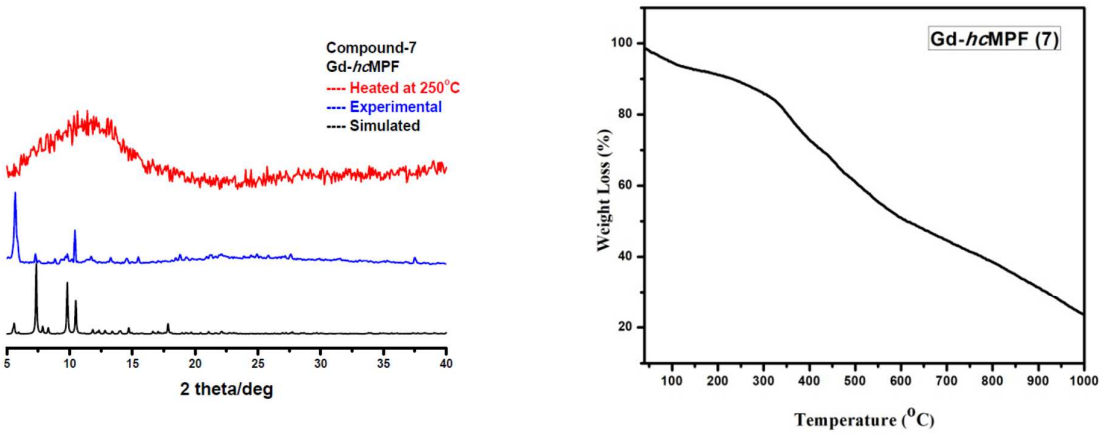
Spectra S2: TGA and PXRD curves of compound Co-*hc*MPF



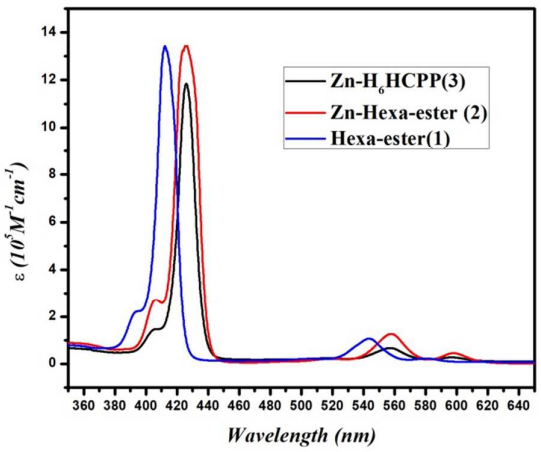
Spectra S3: TGA and PXRD curves of compound In-*hc*MPF



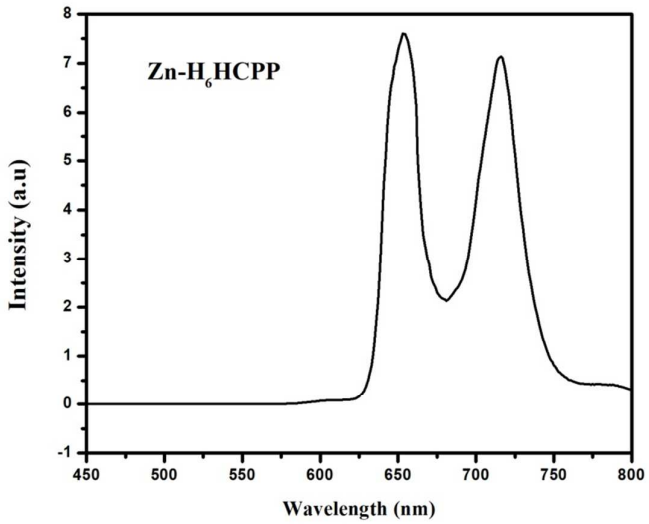
Spectra S4: TGA and PXRD curves of compound Pb-*hc*MPF



Spectra S5: TGA and PXRD curves of compound Gd-*hc*MPF



Spectra S6: UV-VIS spectra of the Zn-H_6HCPP linkers and its precursors



Spectra S7: Emission spectra of the Zn-H_6HCPP when excited at 420 nm

Section-3

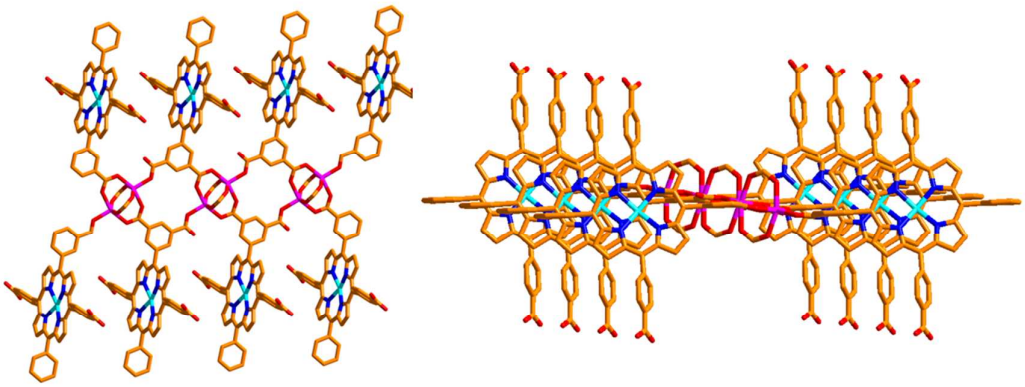
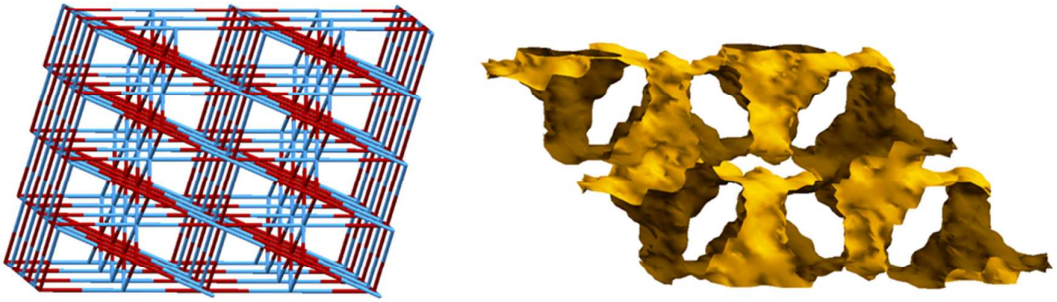
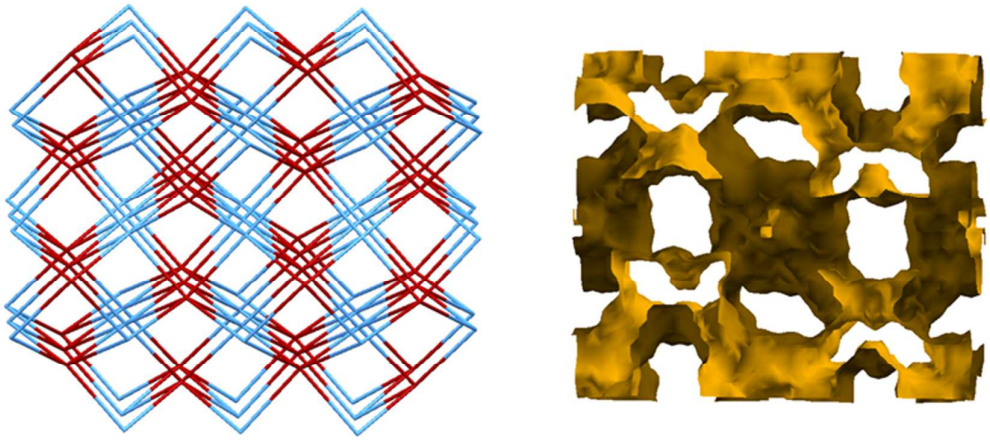


Figure S1. Two dimensional layers formed in the Mn-*hc*MPF projecting the (4-c) arms above and below the layers (along b- axis and c-axis)

Mn-*hc*MPF



Co-*hc*MPF



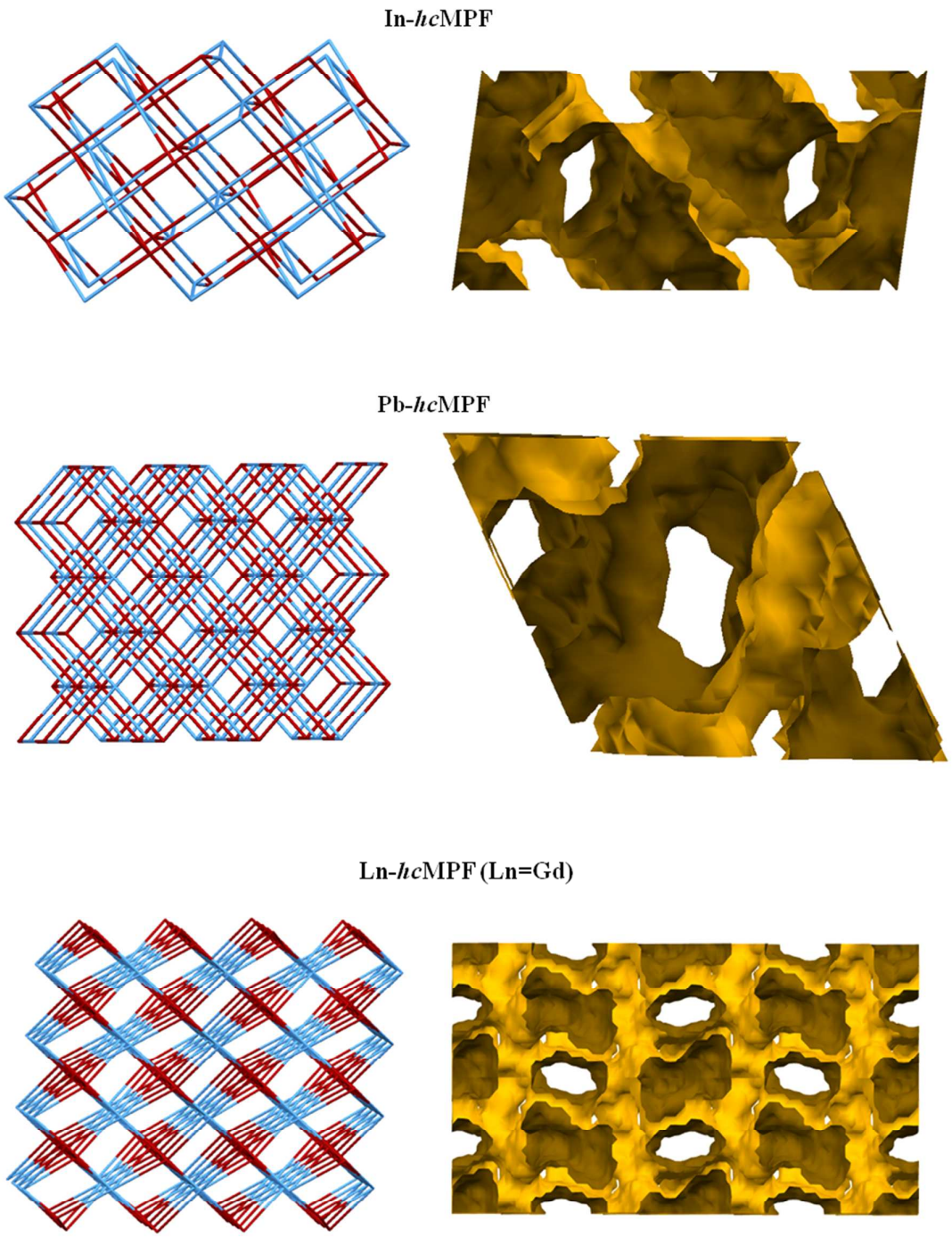


Figure S2. Topological diagrams and void diagrams of all the *hc*MPFs reported in the article.

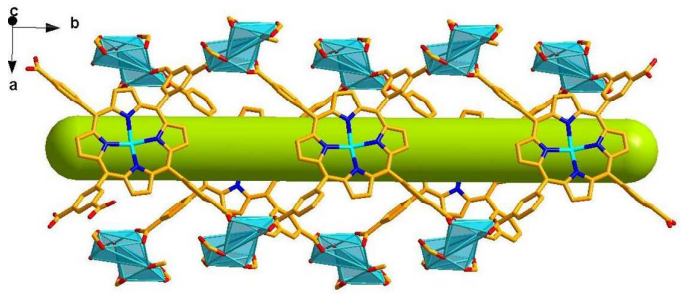


Figure S3. 1D channels running through b-axis in Pb-*hc*MPF

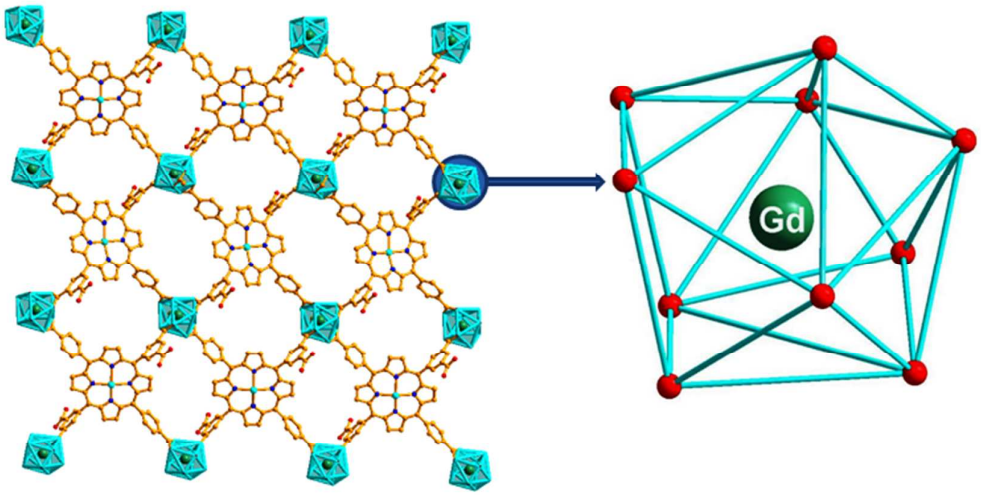


Figure S4. Two dimensional layers formed during the framework formation of Ln-*hc*MPF (Ln=Gd) and the coordination sphere of Gd(III).

Section-4

Summary of SHAPE analysis of metal coordination spheres in *hc*MPFs.

Mn-*hc*MPF

Code	*Entry*	*Symmetry*	*Geometry*
PP-5	1	D5h	Pentagon
vOC-5	2	C4v	Vacant octahedron
TBPY-5	3	D3h	Trigonal bipyramid
SPY-5	**4**	**C4v**	**Spherical square pyramid**
JTBPY-5	5	D3h	Johnson trigonal bipyramid J12

Structure [ML5]	PP-5	vOC-5	TBPY-5	**SPY-5**	JTBPY-5
Mn1,	30.186,	1.248,	5.717,	**0.281**,	8.059

Co-*hc*MPF

Code	*Entry*	*Symmetry*	*Geometry*
HP-6	1	D6h	Hexagon
PPY-6	2	C5v	Pentagonal pyramid
OC-6	**3**	**Oh**	**Octahedron**
TPR-6	4	D3h	Trigonal prism
JPPY-6	5	C5v	Johnson pentagonal pyramid J2

Structure [ML6]	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-6
Co1,	30.117,	27.092,	**0.192,**	15.550,	30.542
Co2,	31.763,	22.682,	**3.443,**	11.870,	25.975

In-*hc*MPF

Structure [ML6]	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-6
In1,	32.252,	21.184,	**3.899**,	13.159,	24.976
Na1,	27.938,	26.224,	1.089,	14.993,	29.393

Pb-*hc*MPF

Pb1

Code	*Entry*	*Symmetry*	*Geometry*
HP-6	1	D6h	Hexagon
PPY-6	2	C5v	Pentagonal pyramid
OC-6	3	Oh	Octahedron
TPR-6	4	D3h	Trigonal prism
JPPY-6	**5**	**C5v**	**Johnson pentagonal pyramid J2**

Structure [ML6]	HP-6	PPY-6	OC-6	TPR-6	**JPPY-6**
Pb1,	22.567,	14.637,	20.952,	20.167,	**13.594**

Pb2

Code	*Entry*	*Symmetry*	*Geometry*
HP-7	1	D7h	Heptagon
HPY-7	2	C6v	Hexagonal pyramid
PBPY-7	3	D5h	Pentagonal bipyramid
COC-7	4	C3v	Capped octahedron
CTPR-7	**5**	**C2v**	**Capped trigonal prism**
JPBPY-7	6	D5h	Johnson pentagonal bipyramid J13

JETPY-7 7 C3v Johnson elongated triangular pyramid J7

Structure [ML7] HP-7 HPY-7 PBPY-7 COC-7 **CTPR-7** JPBPY-7 JETPY-7

Pb2, 18.622, 15.391, 13.359, 12.394, **10.338**, 17.030, 21.521

Gd-*hc*MPF

Gd1

Code	*Entry*	*Symmetry*	*Geometry*
DP-10	1	D10h	Decagon
EPY-10	2	C9v	Enneagonal pyramid
OBPY-10	3	D8h	Octagonal bipyramid
PPR-10	4	D5h	Pentagonal prism
PAPR-10	5	D5d	Pentagonal antiprism
JBCCU-10	6	D4h	Bicapped cube J15
JBCSAPR-10	7	D4d	Bicapped square antiprism J17
JMBIC-10	8	C2v	Metabidiminished icosahedron J62
JATDI-10	9	C3v	Augmented tridiminished icosahedron J64
JSPC-10	10	C2v	Sphenocorona J87
SDD-10	11	D2	Staggered Dodecahedron (2:6:2)
TD-10	**12**	**C2v**	**Tetradecahedron (2:6:2)**
HD-10	13	D4h	Hexadecahedron (2:6:2) or (1:4:4:1)

Structure [ML10] DP-10 EPY-10 OBPY-10 PPR-10 PAPR-10 JBCCU-10 JBCSAPR-10 JMBIC-10 JATDI-10 JSPC-10 SDD-10 **TD-10** HD-10

Gd1, 36.144, 24.060, 16.538, 10.885, 10.441, 9.741, 6.210, 7.179, 18.286, 3.179, 2.488, **1.557**, 6.395

Code	*Entry*	*Symmetry*	*Geometry*
PP-5	1	D5h	Pentagon
vOC-5	2	C4v	Vacant octahedron
TBPY-5	3	D3h	Trigonal bipyramid
SPY-5	**4**	**C4v**	**Spherical square pyramid**
JTBPY-5	5	D3h	Johnson trigonal bipyramid J12

Structure [ML6] HP-6 PPY-6 **OC-6** TPR-6 JPPY-6

Na1, 27.938, 26.224, **1.089**, 14.993, 29.393

Yb-*hc*MPF

Code	*Entry*	*Symmetry*	*Geometry*
HP-7	1	D7h	Heptagon
HPY-7	2	C6v	Hexagonal pyramid
PBPY-7	3	D5h	Pentagonal bipyramid
COC-7	4	C3v	Capped octahedron
CTPR-7	5	C2v	Capped trigonal prism
JPBPY-7	6	D5h	Johnson pentagonal bipyramid J13
JETPY-7	7	C3v	Johnson elongated triangular pyramid J7

Structure [ML7] HP-7 HPY-7 PBPY-7 COC-7 **CTPR-7** JPBPY-7 JETPY-7

Yb1, 25.698, 14.367, 8.573, 9.072, **7.008**, 10.384, 12.251

<u>Topological analyses</u>

1. Mn-*hc*MPF

```
#####################################################################
1:C50 H26 Mn2 N4 O13 Zn/intercluster bonds and atoms for rings>6
#####################################################################

Topology for ZA1
--------------------
Atom ZA1 links by bridge ligands and has
Common vertex with                    R(A-A)
ZB 1   0.5000   0.0000   0.5000  ( 0 0 0)   10.444A      1
ZB 1   1.0000   0.5000   0.5000  ( 1 0 1)   10.444A      1
ZB 1   1.0000   0.5000   1.0000  ( 0 0 0)   11.800A      1
ZB 1   0.5000   0.0000   0.0000  ( 1 0 0)   11.800A      1
ZB 1   1.0000  -0.5000   0.5000  ( 1-1 1)   12.455A      1
ZB 1   0.5000   1.0000   0.5000  ( 0 1 0)   12.455A      1
Topology for ZB1
--------------------
Atom ZB1 links by bridge ligands and has
Common vertex with                    R(A-A)
ZA 1   0.7500   0.2500   0.5000  ( 0 0 0)   10.444A      1
ZA 1   0.2500  -0.2500   0.5000  ( 1 0 1)   10.444A      1
ZA 1   0.2500   0.2500   0.0000  ( 1 0 0)   11.800A      1
ZA 1   0.7500  -0.2500   1.0000  ( 0 0 0)   11.800A      1
ZA 1   0.7500  -0.7500   0.5000  ( 0-1 0)   12.455A      1
```

ZA 1 0.2500 0.7500 0.5000 (1 1 1) 12.455A 1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZBZA

Coordination sequences

ZA1: 1 2 3 4 5 6 7 8 9 10
Num 6 20 48 90 150 222 310 410 526 654
Cum 7 27 75 165 315 537 847 1257 1783 2437

ZB1: 1 2 3 4 5 6 7 8 9 10
Num 6 20 48 90 150 222 310 410 526 654
Cum 7 27 75 165 315 537 847 1257 1783 2437

TD10=2437

Vertex symbols for selected sublattice

ZA1 Point symbol:{4^10.6^5}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.6(2).6(2).6(8).6(8).6(8)]

ZB1 Point symbol:{4^10.6^5}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.6(2).6(2).6(8).6(8).6(8)]

Point symbol for net: {4^10.6^5}
6-c net; uninodal net

Topological type: wxy1 (personal.ttd) {4^10.6^5} - VS
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Elapsed time: 8.60 sec.

2. Co-*hc*MPF

##
#
1:C50 H26 Co3 N4 O15 Zn, H2 O/intercluster bonds and atoms for rings>6
##
#

Topology for ZA1

Atom ZA1 links by bridge ligands and has
Common vertex with R(A-A)
ZB 1 0.6916 0.7500 0.2173 (0 0 0) 10.462A 1

ZB 1 0.3084 0.2500 0.7827 (1-1 1) 10.462A 1
ZB 1 0.6916 0.7500 1.2173 (0 0 1) 12.310A 1
ZB 1 0.3084 0.2500 -0.2173 (1-1 0) 12.310A 1
ZB 1 0.1916 0.7500 0.2827 (-1 1 0) 12.483A 1
ZB 1 0.8084 0.2500 0.7173 (1 1 0) 12.483A 1
Topology for ZB1

Atom ZB1 links by bridge ligands and has
Common vertex with R(A-A)
ZA 1 0.5000 0.5000 0.5000 (0 0 0) 10.462A 1
ZA 1 0.5000 1.0000 0.5000 (1 0 1) 10.462A 1
ZA 1 0.5000 0.5000 -0.5000 (0 0-1) 12.310A 1
ZA 1 0.5000 1.0000 -0.5000 (1 0 0) 12.310A 1
ZA 1 1.0000 0.5000 0.0000 (1 1-1) 12.483A 1
ZA 1 1.0000 1.0000 0.0000 (0 1 0) 12.483A 1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZBZA

Coordination sequences

ZA1: 1 2 3 4 5 6 7 8 9 10
Num 6 20 42 74 114 164 222 290 366 452
Cum 7 27 69 143 257 421 643 933 1299 1751

ZB1: 1 2 3 4 5 6 7 8 9 10
Num 6 18 42 74 114 162 222 290 366 450
Cum 7 25 67 141 255 417 639 929 1295 1745

TD10=1748

Vertex symbols for selected sublattice

ZA1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]

ZB1 Point symbol:{4^9.6^6}
Extended point symbol:[4.4.4.4.4.4.4(2).4(2).4(2).6(8).6(8).6(8).6(8).6(8).6(8)]

Point symbol for net: {4^12.6^3}{4^9.6^6}
6,6-c net with stoichiometry (6-c)(6-c); 2-nodal net

Topological type: nia (topos&RCSR.ttd) {4^12.6^3}{4^9.6^6} - VS
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(17477 types in 3 databases)

Elapsed time: 9.14 sec.

3. In-*hc*MPF

```
#######################################################################
####
1:C50 H30 In N4 Na0.50 O12 Zn0.50/intercluster bonds and atoms at rings>6
#######################################################################
####

Topology for Sc1
--------------------
Atom Sc1 links by bridge ligands and has
Common vertex with                          R(A-A)
Sc 1    0.4157   -0.2553    0.4592   ( 1 0 1)    9.148A        1
Ti 1    1.0758    0.2250    0.7888   ( 2-1 1)   10.329A        1
Ti 1    0.9242    0.7250    0.7112   ( 0 0 0)   10.548A        1
Ti 1    0.0758    0.2750    0.2888   ( 1 1 1)   10.578A        1
Ti 1    1.0758    0.2750    0.2888   ( 2 1 1)   11.905A        1
Ti 1    0.0758    0.2250    0.7888   ( 1-1 1)   12.020A        1
Topology for Ti1
--------------------
Atom Ti1 links by bridge ligands and has
Common vertex with                          R(A-A)
Sc 1    1.4157    0.7553    0.9592   ( 2 0 1)   10.329A        1
Sc 1    0.5843    0.2553    0.5408   ( 0 0 0)   10.548A        1
Sc 1    0.4157    0.7447    0.4592   ( 1 1 1)   10.578A        1
Sc 1    1.4157    0.7447    0.4592   ( 2 1 1)   11.905A        1
Sc 1    0.4157    0.7553    0.9592   ( 1 0 1)   12.020A        1
--------------------------
Structural group analysis
--------------------------


--------------------------
Structural group No 1
--------------------------
Structure consists of 3D framework with TiSc

Coordination sequences
----------------------
Sc1:  1  2  3   4   5   6   7    8    9   10
Num   6 19 45  83 123 184 245  320  412  500
Cum   7 26 71 154 277 461 706 1026 1438 1938
----------------------
Ti1:  1  2  3   4   5   6   7    8    9   10
Num   5 19 44  78 131 175 246  325  402  508
Cum   6 25 69 147 278 453 699 1024 1426 1934
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TD10=1936
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Vertex symbols for selected sublattice

Sc1 Point symbol:{4^6.5^6.6^2.7}
Extended point symbol:[4.4.4.4.4.4.5.5.5.5(2).5(2).5(2).6(2).6(2).7(3)]

Ti1 Point symbol:{4^6.5^3.6}
Extended point symbol:[4.4.4.4.4.4.5.5.5(2).6(2)]

Point symbol for net: {4^6.5^3.6}{4^6.5^6.6^2.7}
5,6-c net with stoichiometry (5-c)(6-c); 2-nodal net

ATTENTION! If the name below is written in a long notation s/... or s-d-G-n, this net is a subnet of the net s (see Manual for details)
Topological type: tcj/hc;P 63/m m c->P 21/c (-a-b,a-b,c; 0,1/2,0);Bond sets: 4,6,7,8,9,14:tcj (binodal.ttd) {4^6.5^3.6}{4^6.5^6.6^2.7} - VS [4.4.4.4.4.4.5.5.5(2).*] [4.4.4.4.4.4.5.5.5.5(2).5(2).5(2).*.*.*] (76179 types in 11 databases)
Elapsed time: 11.24 sec.

4. Pb-hcMPF

##
1:C50 H30 N4 O12 Pb Zn/intercluster bonds and atoms at rings>6
##

Topology for Sc1

Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
Ti 1	0.9903	0.4813	1.2442	(1-1 2)	8.489A	1
Ti 1	-0.0097	0.4813	0.2442	(0-1 1)	8.490A	1
Ti 1	0.0097	0.9813	0.7558	(0 0 0)	11.542A	1
Ti 1	1.0097	0.9813	0.7558	(1 0 0)	11.547A	1
Ti 1	0.0097	-0.0187	0.7558	(0-1 0)	11.568A	1
Ti 1	1.0097	-0.0187	0.7558	(1-1 0)	11.573A	1

Topology for Ti1

Atom Ti1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc 1	0.4997	0.9824	1.2643	(1 0 2)	8.489A	1
Sc 1	-0.5003	0.9824	0.2643	(0 0 1)	8.490A	1
Sc 1	0.5003	0.4824	0.7357	(0 0 0)	11.542A	1
Sc 1	-0.4997	0.4824	0.7357	(-1 0 0)	11.547A	1
Sc 1	0.5003	1.4824	0.7357	(0 1 0)	11.568A	1
Sc 1	-0.4997	1.4824	0.7357	(-1 1 0)	11.573A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with TiSc

Coordination sequences

Sc1: 1 2 3 4 5 6 7 8 9 10
Num 6 18 38 66 102 146 198 258 326 402
Cum 7 25 63 129 231 377 575 833 1159 1561

Ti1: 1 2 3 4 5 6 7 8 9 10
Num 6 18 38 66 102 146 198 258 326 402
Cum 7 25 63 129 231 377 575 833 1159 1561

TD10=1561

Vertex symbols for selected sublattice

Sc1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]

Ti1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]

Point symbol for net: {4^12.6^3}
6-c net; uninodal net

Topological type: pcu alpha-Po primitive cubic; 6/4/c1; sqc1 (topos&RCSR.ttd)
{4^12.6^3} - VS [4.4.4.4.4.4.4.4.4.4.4.*.*.*] (76179 types in 11 databases)
Elapsed time: 11.49 sec.

7. Gd-*hc*MPF

##
1:C100 H60 Gd2 N8 Na2 O24 Zn2/intercluster bonds and atoms at rings>6
##

Topology for Sc1

Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc 1	0.6134	0.7441	0.5447	(1 1 1)	9.313A	1
Ti 1	-0.0948	0.2793	0.2105	(0-1 0)	10.353A	1
Ti 1	0.0948	-0.2207	0.2895	(0-1 0)	10.430A	1
Ti 1	0.9052	0.2207	0.7105	(1 1 1)	10.983A	1
Ti 1	-0.0948	0.2207	0.7105	(0 1 1)	11.948A	1
Ti 1	0.9052	0.2793	0.2105	(1-1 0)	12.148A	1

Topology for Ti1

Atom Ti1 links by bridge ligands and has

Common vertex with					R(A-A)	
Ti 1	-0.0948	0.2793	0.2105	(0-1 0)	9.214A	1
Ti 1	-0.0948	1.2793	0.2105	(0 0 0)	9.214A	1
Sc 1	-0.3866	0.7559	0.0447	(0 0 0)	10.353A	1
Sc 1	0.3866	1.2559	0.4553	(0 1 0)	10.430A	1
Sc 1	0.6134	0.7441	0.5447	(1 1 1)	10.983A	1
Sc 1	-0.3866	0.7441	0.5447	(0 1 1)	11.948A	1
Sc 1	0.6134	0.7559	0.0447	(1 0 0)	12.148A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with TiSc

Coordination sequences

Sc1: 1 2 3 4 5 6 7 8 9 10
Num 6 23 53 93 146 209 283 372 469 577
Cum 7 30 83 176 322 531 814 1186 1655 2232

Ti1: 1 2 3 4 5 6 7 8 9 10
Num 7 23 53 94 146 210 284 368 469 581
Cum 8 31 84 178 324 534 818 1186 1655 2236

TD10=2234

Vertex symbols for selected sublattice

Sc1 Point symbol:{3.4^10.5^3.6}
Extended point symbol:[3.4.4.4.4.4.4.4.4.4.4.5.5.5(4).6(4)]

Ti1 Point symbol:{3^2.4^10.5^7.6^2}
Extended point symbol:[3.3.4.4.4.4.4.4.4.4.4.4.5.5.5.5.5(3).5(3).5(4).6(2).6(3)]

Point symbol for net: {3.4^10.5^3.6}{3^2.4^10.5^7.6^2}
6,7-c net with stoichiometry (6-c)(7-c); 2-nodal net

ATTENTION! If the name below is written in a long notation s/... or s-d-G-n, this net is a subnet of the net s (see Manual for details)
Topological type: tcj/hc;P 63/m m c->P 21/c (-a-b,a-b,c; 0,1/2,0);Bond sets: 3,4,6,7,8,9,14:tcj (binodal.ttd) {3.4^10.5^3.6}{3^2.4^10.5^7.6^2} - VS [3.3.4.4.4.4.4.4.4.4.4.4.5(2).5(2).5(3).*.*.*.*.*.*] [3.4.4.4.4.4.4.4.4.4.4.5(3).*.*.*]
(76154 types in 11 databases)
Elapsed time: 14.81 sec.

8. Yb-*hc*MPF

```
##############################################################
####
1:C50 H28 N4 O16 Yb2 Zn/intercluster bonds and atoms at rings>6
##############################################################
####

Topology for Sc1
--------------------
Atom Sc1 links by bridge ligands and has
Common vertex with                          R(A-A)
Ti 1    1.0000    0.3260    0.7500   ( 0 0 0)    10.594A        1
Ti 1    0.5000    1.1740    0.2500   ( 0 1 0)    10.594A        1
Ti 1    1.0000    0.6740    1.2500   ( 1 0 1)    12.418A        1
Ti 1    0.5000    0.8260   -0.2500   ( 1 1 0)    12.418A        1
Ti 1    1.0000    1.3260    0.7500   ( 0 1 0)    12.596A        1
Ti 1    0.5000    0.1740    0.2500   ( 0 0 0)    12.596A        1
Topology for Ti1
--------------------
Atom Ti1 links by bridge ligands and has
Common vertex with                          R(A-A)
Sc 1    0.2500   -0.2500    0.0000   ( 1-1 0)    10.594A        1
Sc 1    0.7500   -0.2500    0.5000   ( 0-1 0)    10.594A        1
Sc 1    0.2500    0.2500   -0.5000   ( 1 1 0)    12.418A        1
Sc 1    0.7500    0.2500    1.0000   ( 0 1 0)    12.418A        1
Sc 1    0.2500    0.7500    0.0000   ( 1 0 0)    12.596A        1
Sc 1    0.7500    0.7500    0.5000   ( 0 0 0)    12.596A        1
--------------------------
Structural group analysis
--------------------------

--------------------------
Structural group No 1
--------------------------
Structure consists of 3D framework with TiSc

Coordination sequences
----------------------
Sc1:  1  2  3   4   5   6   7   8    9   10
Num   6 18 38  66 102 146 198 258  326  402
```

Cum 7 25 63 129 231 377 575 833 1159 1561

Ti1: 1 2 3 4 5 6 7 8 9 10
Num 6 18 38 66 102 146 198 258 326 402
Cum 7 25 63 129 231 377 575 833 1159 1561

TD10=1561

Vertex symbols for selected sublattice

Sc1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]

Ti1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]

Point symbol for net: {4^12.6^3}
6-c net; uninodal net

Topological type: pcu alpha-Po primitive cubic; 6/4/c1; sqc1
(topos&RCSR.ttd) {4^12.6^3} - VS [4.4.4.4.4.4.4.4.4.4.4.4.*.*.*] (76154 types in 11 databases)
Elapsed time: 12.15 sec.