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Supporting information for article:

A three-dimensional gadolinium organic framework based on a pyridinedicarboxylic acid organic linker with a paddle-wheel-type network structure

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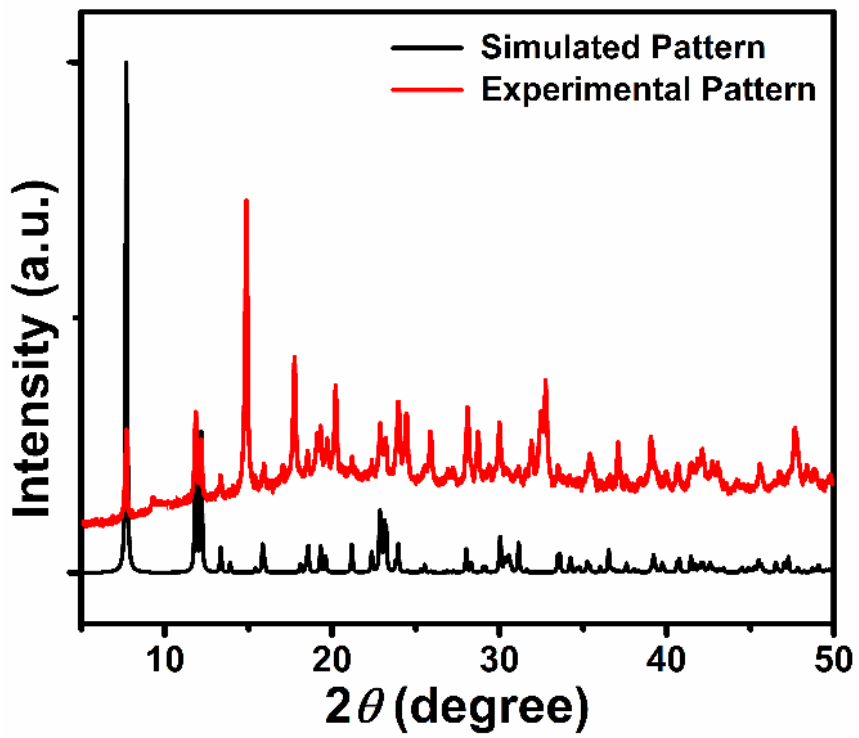

Figure S1. PXRD pattern of CP-**1**.

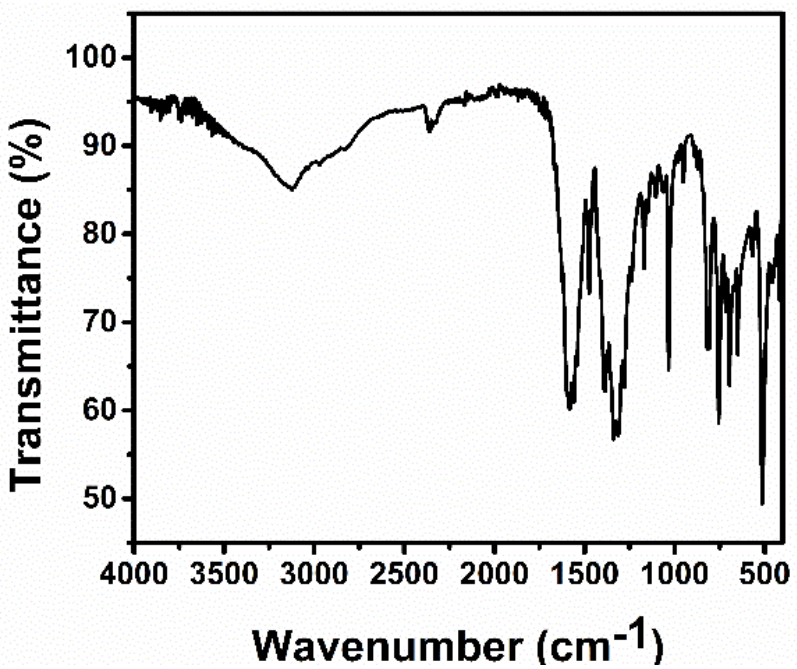

Figure S2. FTIR spectra of CP-**1**.

Bond valence sum calculation

The bond valence sum (BVS) calculation of CP-**1** was calculated from the formula as given below

$S = \exp[(Ro-R)/B]$

And

$V = \Sigma S$

Where V is the oxidation state of cation and S is bond valence

Where B = 0.37, Ro for Gd-O = 2.031 Å and Gd-N = 2.146 Å and R is Gd-O and Gd-N bond length

S1= exp[(2.031 - 2.3704)/0.37] = 0.3996

S2= exp[(2.031 - 2.3704)/0.37] = 0.3996

S3= exp[(2.031 - 2.3229)/0.37] = 0.45434

S4= exp[(2.031 - 2.3229)/0.37] = 0.45434

S5= exp[(2.031 - 2.3916)/0.37] = 0.37734

S6= exp[(2.031 - 2.3916)/0.37] = 0.37734

S7= exp[(2.146 - 2.5702)/0.37] = 0.22253

S8= exp[(2.146 - 2.5702)/0.37] = 0.22253

And $V = \Sigma S$

V = S1+S2+S3+S4+S5+S6+S7+S8 = 2.907

(1) I. D. Brown, Chem. Rev., 2009, 109, 6858-6919.

Table S1. Hydrogen bonding table for CP-**1**[#]

D—H···A	Symmetry of A	D—H **1**	H···A	D—A	∠D—H···A
N2—H2A···O1	-1/4+x,1/4+y,1/2-z	0.86	2.27	3.0043(1)	144
N2—H2A···O2	-1/4+x,1/4+y,1/2-z	0.86	2.10	2.8399(1)	144
C2—H2···O2	1-x,-y,-z	0.93	2.60	3.3088(1)	134
C5—H5···O4	1/2-x,1/2-y,-z	0.91	2.36	2.9606(1)	124

[#]Where ‘D’ is donor and ‘A’ is acceptor, the bond lengths are in (Å) and angles are in (°).

Table S2. Complete list of bond lengths [Å] and bond angles [◦] for CP-**1**[#]

1					
Gd1-O1^{b}	2.3704(18)	Gd1-N1^{c}	2.5702(19)	N2-C8	1.424(6)
Gd1-O1^{c}	2.3704(18)	O1-C6	1.264(4)	C1-C2	1.368(4)
Gd1-O3	2.3229(18)	O2-C6	1.223(4)	C1-C6	1.518(4)
Gd1-O3^{a}	2.3229(18)	O3-C7	1.236(3)	C2-C3	1.366(5)
Gd1-O4^{d}	2.3916(18)	O4-C7	1.237(3)	C3-C4	1.363(4)
Gd1-O4^{e}	2.3916(18)	N1-C1	1.312(3)	C4-C5	1.369(4)
Gd1-N1^{b}	2.5702(19)	N1-C5	1.342(3)	C4-C7	1.499(3)
O3^{a}-Gd1-O3	117.08(11)	O1^{b}-Gd1-N1^{c}	71.81(7)	N1-C1-C2	121.9(3)
O3^{a}-Gd1-O1^{b}	79.48(8)	O1^{c}-Gd1-N1^{c}	64.25(6)	N1-C1-C6	114.4(2)
O3-Gd1-O1^{b}	150.98(8)	O4^{d}-Gd1-N1^{c}	143.54(7)	C2-C1-C6	123.7(3)
O3^{a}-Gd1-O1^{c}	150.98(8)	O4^{e}-Gd1-N1^{c}	73.39(7)	C3-C2-C1	120.4(3)
O3-Gd1-O1^{c}	79.48(8)	O3^{a}-Gd1-N1^{b}	80.94(7)	C4-C3-C2	118.8(3)
O1^{b}-Gd1-O1^{c}	96.98(10)	O3-Gd1-N1^{b}	138.20(7)	C3-C4-C5	117.3(3)
O3^{a}-Gd1-O4^{d}	77.79(9)	O1^{b}-Gd1-N1^{b}	64.25(6)	C3-C4-C7	122.8(2)
O3-Gd1-O4^{d}	74.40(8)	O1^{c}-Gd1-N1^{b}	71.81(7)	C5-C4-C7	119.9(2)
O1^{b}-Gd1-O4^{d}	134.34(7)	O4^{d}-Gd1-N1^{b}	73.39(7)	N1-C5-C4	124.4(2)
O1^{c}-Gd1-O4^{d}	84.90(7)	O4^{e}-Gd1-N1^{b}	143.54(7)	O2-C6-O1	124.8(3)
O3^{a}-Gd1-O4^{e}	74.40(8)	N1^{c}-Gd1-N1^{b}	111.44(9)	O2-C6-C1	118.6(3)
O3-Gd1-O4^{e}	77.79(9)	C1-N1-C5	117.2(2)	O1-C6-C1	116.6(2)
O1^{b}-Gd1-O4^{e}	84.90(7)	C1-N1-Gd1^{g}	118.00(17)	O3-C7-O4	126.1(2)
O1^{c}-Gd1-O4^{e}	134.34(7)	C5-N1-Gd1^{g}	124.32(16)	O3-C7-C4	116.4(2)
O4^{d}-Gd1-O4^{e}	125.20(10)	C8-N2-C8^{f}	116.2(6)	O4-C7-C4	117.5(2)
O3^{a}-Gd1-N1^{c}	138.20(7)	C6-O1-Gd1^{g}	126.09(17)	C7-O4-Gd1^{e}	140.38(17)
O3-Gd1-N1^{c}	80.94(7)	C7-O3-Gd1	151.57(19)		

[#]Symmetry transformations used to generate equivalent atoms:

a) x,-y+7/4,-z+3/4; b) x+1/4,-y+3/2,z-1/4; c) x+1/4,y+1/4,-z+1; d) -x+3/4,y,-z+3/4;

e) -x+3/4,-y+7/4,z; f) -x+3/4,-y+3/4,z; g) x-1/4,y-1/4,-z+1

Table S3. Filtering fingerprint by element type. Surface area included (as percentage of the total surface area) for close contacts between atoms inside and outside the surface for CP-**1**.

Inside Atom	**Outside Atom**					
	1					
Atom	Gd	O	N	H	C	All
C	.	0.8 17.5 5.9	.	9.7	0.8	11.3
Gd	.	2.1 6.0	2.6	13.6	5.0	38.6
H	.	32.3	.	13.5	0.9	20.3
N	0.9		.	0.9	.	3.9
O	2.4		1.9	15.2	0.4	25.9
All	3.2		4.5	52.9	7.0	

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å \times 10^3$) for CP-**1** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	X	y	Z	U(eq)		x	Y	Z	U(eq)
				1					
Gd1	5009(1)	8750	3750	20(1)	C2	4358(3)	5906(3)	5008(2)	108(2)
O1	3386(1)	5284(1)	6131(1)	42(1)	C3	4353(2)	6504(2)	4692(2)	87(2)
O2	4222(2)	4675(2)	5684(1)	138(2)	C4	3803(1)	7018(2)	4746(1)	35(1)
O3	4333(1)	7967(1)	4273(1)	53(1)	C5	3304(1)	6916(1)	5130(1)	33(1)
O4	3105(1)	7897(1)	4301(1)	50(1)	C6	3820(2)	5211(2)	5759(1)	62(1)
N1	3317(1)	6344(1)	5452(1)	30(1)	C7	3740(1)	7684(1)	4412(1)	30(1)
N2	3750	3750	6489(2)	98(2)	C8	4412(3)	3880(3)	6772(2)	109(2)
C1	3839(2)	5844(2)	5383(1)	54(1)					

Table S5. Anisotropic displacement parameters (Å2×103) for CP-1. The anisotropic displacement factor exponent takes the form: -2 π2 [h2 a*2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12		U11	U22	U33	U23	U13	U12
						1							
Gd1	22(1)	18(1)	18(1)	-3(1)	0	0	C2	125(4)	99(3)	99(3)	67(3)	82(3)	86(3)
O1	51(1)	37(1)	39(1)	12(1)	9(1)	19(1)	C3	92(3)	91(3)	79(3)	54(2)	60(2)	57(2)
O2	204(4)	96(2)	114(3)	71(2)	107(3)	114(3)	C4	37(1)	36(1)	31(1)	10(1)	5(1)	6(1)
O3	45(1)	56(1)	58(1)	23(1)	11(1)	-11(1)	C5	34(1)	33(1)	34(1)	11(1)	4(1)	7(1)
O4	43(1)	55(1)	51(1)	30(1)	4(1)	14(1)	C6	85(2)	46(2)	54(2)	24(2)	31(2)	36(2)
N1	32(1)	32(1)	26(1)	6(1)	4(1)	6(1)	C7	38(1)	29(1)	23(1)	9(1)	4(1)	1(1)
N2	197(7)	53(3)	44(3)	0	0	-26(3)	C8	130(5)	96(4)	100(4)	24(3)	-6(4)	34(3)
C1	68(2)	46(2)	48(2)	20(1)	24(2)	30(2)							