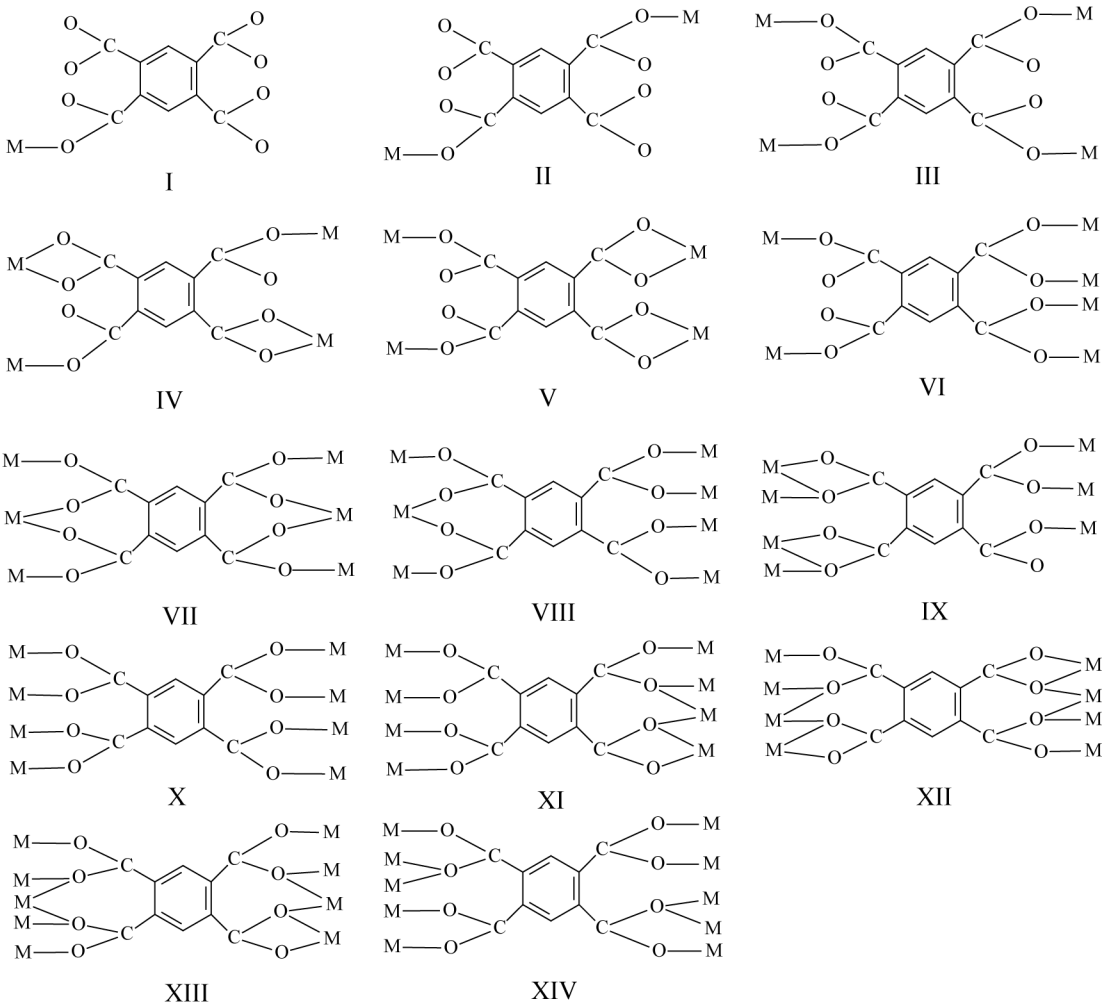
Supporting Information

A High-connected Cobalt(II) Pyromellitate MOF Displaying An Uncommon Decadentate Coordination Mode

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Scheme S1. The versatile coordination modes of the pm^{4-} ligand.

Table S1. Crystallographic data and structure refinement parameters for **1**

Formula	$C_{32}H_{24}Co_4N_4O_{17}$
Fw	972.27
Crystal system	Orthorhombic
Space group	*Pbcn*
a /Å	14.008(12)
b /Å	15.864(13)
c /Å	14.558(14)
α (°)	90
β (°)	90
γ (°)	90
V /Å^3	3235(5)
Z	4
d_{cal} /g cm^{-3}	1.996
F(000)	1952
θ range (°)	1.94−27.10
Reflections collected/unique	17579/3573
R (int)	0.0460
GOF on F^2	0.996
$\Delta\rho_{max}$ /$\Delta\rho_{min}$ (e Å^{-3})	0.422 / −0.361
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0331 and wR_2 = 0.0816
R indices (all data)	R_1 = 0.0488, wR_2 = 0.0895

$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $^b wR_2 = \{\Sigma\,[w\,F_o^2 - F_c^2\,^2]/\Sigma\,[w\,F_o^2\,^2]\}^{1/2}$

Table S2. Selected bond lengths (Å) and angles (°) for the complex **1**

Co(1)-O(8)A	1.982(2)	O(4)C-Co(1)-O(2)	104.63(10)
Co(1)-O(5)B	1.993(2)	O(1)-Co(1)-O(2)	59.60(8)
Co(1)-O(4)C	2.019(2)	O(8)A-Co(1)-O(9)	75.17(13)
Co(1)-O(1)	2.185(2)	O(5)B-Co(1)-O(9)	92.30(12)
Co(1)-O(2)	2.194(2)	O(4)C-Co(1)-O(9)	101.58(13)
Co(1)-O(9)	2.289(4)	O(1)-Co(1)-O(9)	93.79(12)
Co(2)-O(1)	2.039(2)	O(2)-Co(1)-O(9)	153.15(12)
Co(2)-O(3)	2.051(2)	O(1)-Co(2)-O(3)	87.22(11)
Co(2)-O(6)D	2.055(2)	O(1)-Co(2)-O(6)D	89.45(10)
Co(2)-O(7)D	2.084(2)	O(3)-Co(2)-O(6)D	167.71(8)
Co(2)-N(1)	2.102(5)	O(1)-Co(2)-O(7)D	164.15(8)
Co(2)-O(7)A	2.364(3)	O(3)-Co(2)-O(7)D	95.71(10)
O(8)A-Co(1)-O(5)B	165.26(9)	O(6)D-Co(2)-O(7)D	84.41(10)
O(8)A-Co(1)-O(4)C	91.29(10)	O(1)-Co(2)-N(1)	102.45(14)
O(5)B-Co(1)-O(4)C	98.94(10)	O(3)-Co(2)-N(1)	88.34(14)
O(8)A-Co(1)-O(1)	87.34(11)	O(6)D-Co(2)-N(1)	103.99(14)
O(5)B-Co(1)-O(1)	85.76(10)	O(7)D-Co(2)-N(1)	93.22(14)
O(4)C-Co(1)-O(1)	163.69(8)	O(3)-Co(2)-O(7)A	83.99(8)
O(8)A-Co(1)-O(2)	98.35(11)	O(6)D-Co(2)-O(7)A	83.93(7)
O(5)B-Co(1)-O(2)	89.35(9)	O(7)D-Co(2)-O(7)A	80.06(8)
O(1)-Co(2)-O(7)A	84.75(7)	N(1)-Co(2)-O(7)A	169.22(15)

*Symmetry mode for the complex: A: -*x*+1/2, *y*-1/2, *z*; B: -x+1/2, -*y*+1/2, *z*-1/2; C: *x*, -*y*, *z*-1/2; D: *x*-1/2, -*y*+1/2, -*z*+1.

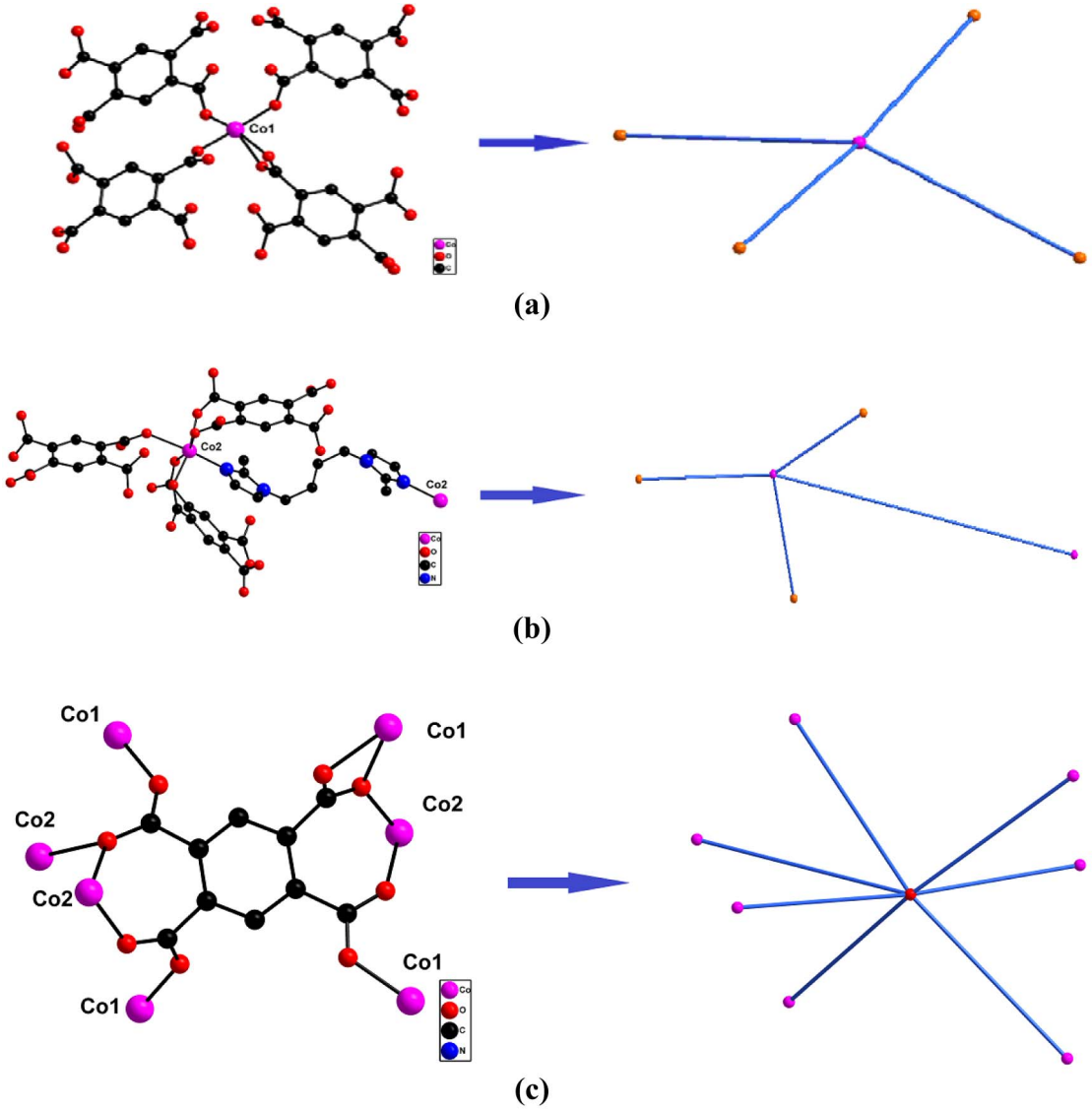


Figure S1. (a) 4-connected node for Co1; (b) 4-connected node for Co2; (c) 7-connected node for pm^{4-}.

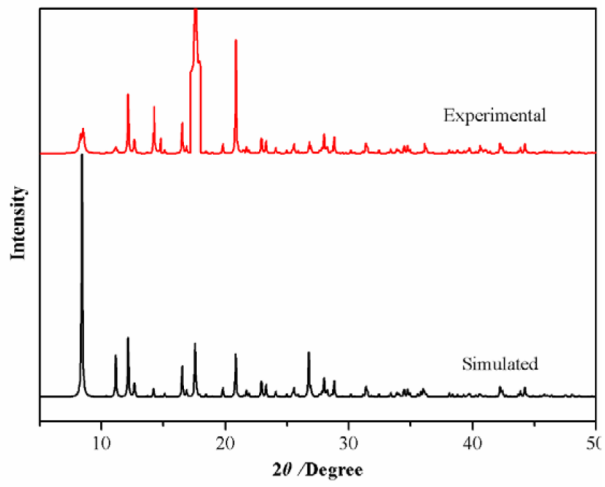


Figure S2. X-ray powder diffraction patterns of the complex **1**.

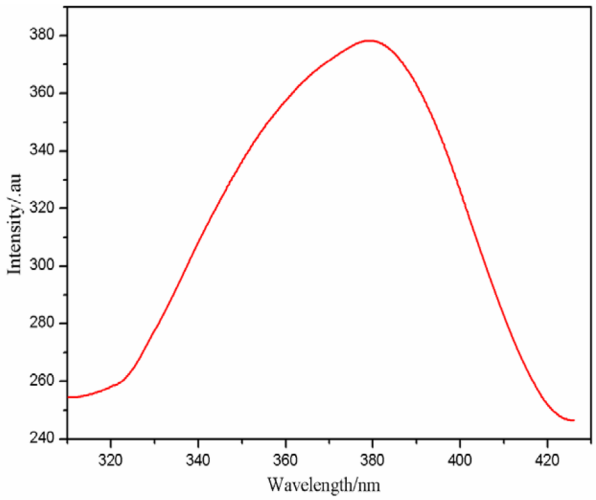


Figure S4. Solid-state fluorescence emission spectrum for the complex **1**.

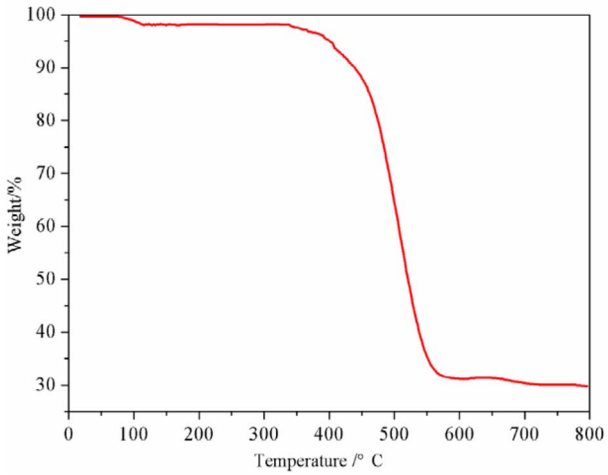


Figure S3. The TG curve for compound **1**.

The result checked by TOPOS 4.0 program for the complex

$[Co_2(pm)(bib)_{0.5}(H_2O)_{0.5}]_n$ (1)

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1:C32 H22 Co4 N4 O17

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Topology for Ti1

Atom Ti1 links by bridge ligands and has

Common vertex with					R(A-A)	
Co 2	0.0605	0.0899	0.4730	(0 0 0)	4.297A	1
Co 2	0.5605	0.4101	0.5270	(0 0 1)	4.398A	1
Co 1	0.2001	0.0030	0.2664	(0 0 0)	5.425A	1
Co 1	0.2999	0.5030	0.2664	(0 0 0)	5.452A	1
Co 1	0.2999	0.4970	0.7664	(0 0 0)	5.501A	1
Co 1	0.2001	-0.0030	0.7664	(0 0 0)	5.610A	1
Co 2	0.4395	0.5899	0.4730	(0 0 0)	5.826A	1

Topology for Co1

Atom Co1 links by bridge ligands and has

Common vertex with					R(A-A)	
Ti 1	0.3111	0.2423	0.5103	(0 0 0)	5.425A	1
Ti 1	0.1889	-0.2577	0.5103	(0-1 0)	5.452A	1
Ti 1	0.1889	0.2577	0.0103	(0 0-1)	5.501A	1
Ti 1	0.3111	-0.2423	0.0103	(0 0-1)	5.610A	1

Topology for Co2

Atom Co2 links by bridge ligands and has

Common vertex with					R(A-A)	
Ti 1	0.3111	0.2423	0.5103	(0 0 0)	4.297A	1
Ti 1	-0.1889	0.2577	0.4897	(-1 0 1)	4.398A	1
Ti 1	0.1889	-0.2577	0.5103	(0-1 0)	5.826A	1
Co 2	-0.0605	0.9101	0.5270	(0 1 1)	13.144A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Co2Ti

Coordination sequences

Ti1:	1	2	3	4	5	6	7	8	9	10

Num 7 14 49 65 138 169 257 302 439 459
Cum 8 22 71 136 274 443 700 1002 1441 1900

Co1: 1 2 3 4 5 6 7 8 9 10
Num 4 18 28 86 102 200 226 334 374 552
Cum 5 23 51 137 239 439 665 999 1373 1925

Co2: 1 2 3 4 5 6 7 8 9 10
Num 4 18 32 83 103 195 228 341 371 554
Cum 5 23 55 138 241 436 664 1005 1376 1930

TD10=1918
Vertex symbols for selected sublattice

Ti1 Point symbol:{4^9.5^6.6^6}
Extended point symbol:[4.4.4.4.4.4.4.4.4.5.5.5.5.5.5.6.6.6.6.6(2).6(2)]

Co1 Point symbol:{4^4.6^2}
Extended point symbol:[4.4.4(2).4(2).6(4).6(4)]

Co2 Point symbol:{4^2.5^2.6.7}
Extended point symbol:[4.5(3).4(2).5(3).6(2).7(11)]

Point symbol for net: {4^2.5^2.6.7}{4^4.6^2}{4^9.5^6.6^6}
4,4,7-c net with stoichiometry (4-c)(4-c)(7-c); 3-nodal net

New topology, please, contact the authors (76154 types in 11 databases)