Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information

Two-dimensional metal-organic frameworks with blue luminescence

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Table S1. Comparison of selected bond lengths [Å] and angles [°] for Zn(**1**), Co(**2**), and Ni(**3**) compounds.

	Zn (**1**)	Co (**2**)	Ni (**3**)
M(1)-N(1)$^{\#1}$	2.137(3)	2.107(3)	2.055(3)
M(1)-N(2)$^{\#1}$	2.109(3)	2.106(3)	2.052(3)
M(1)-O(1)$^{\#2}$	2.105(2)	2.163(2)	2.125(3)
M(1)-O(2)$^{\#2}$	2.425(3)	2.225(2)	2.169(3)
M(1)-O(3)$^{\#3}$	2.005(3)	2.036(2)	2.033(3)
M(1)-O(5)(water)	2.076(3)	2.074(3)	2.038(3)
O(1)-C(1)	1.260(5)	1.273(4)	1.274(5)
O(2)-C(1)	1.253(5)	1.250(4)	1.257(4)
O(3)-C(12)	1.279(4)	1.270(4)	1.272(5)
O(4)-C(12)	1.224(4)	1.236(4)	1.246(5)
C(1)-O(1)-M(1)$^{\#4}$	96.5(2)	90.4(2)	89.2(2)
C(1)-O(2)-M(1)$^{\#4}$	82.2(2)	88.2(2)	87.6(2)
C(12)-O(3)-M(1)$^{\#5}$	136.4(2)	135.9(2)	136.0(3)
O(2)-C(1)-O(1)	123.2(3)	121.2(3)	121.2(4)
O(2)-C(1)-C(2)	118.2(3)	120.0(3)	120.2(4)
O(4)-C(12)-O(3)	127.4(3)	127.4(3)	127.3(4)

$^{\#1}$ Symmetry operators for the generated atoms: $-x+3/2, y-1/2, -z+1/2$ for **3**.

$^{\#2}$ Symmetry operators for the generated atoms: $-x+1/2, y-1/2, -z+1/2$ for **2**.

$^{\#3}$ Symmetry operators for the generated atoms: $-x+3/2, y+1/2, -z+1/2$ for **2**; $x+1, y-1, z$ for **3**.

$^{\#4}$ Symmetry operators for the generated atoms: $x+1/2, -y+3/2, z-1/2$ for **2**.

$^{\#5}$ Symmetry operators for the generated atoms: $-x+3/2, y-1/2, -z+1/2$ for **2**; $x-1, y+1, z$. for **3**.

Table S2. Hydrogen-bond geometry (Å, °)

	Zn (**1**)		Co (**2**)		Ni (**3**)	
D—H···*A*	*D*···*A*	*D*—H···*A*	*D*···*A*	*D*—H···*A*	*D*···*A*	*D*—H···*A*
O(5)—H(5A)···O(4)[#1]	2.668(4)	174(4)	2.649(3)	178(3)	2.646(4)	174
O(5)—H(5B)···O(1)[#2]	2.743(4)	148(4)	2.712(4)	158(4)	2.719(4)	159
O(1S)—H(1S1)···O(2)[#3]	2.925(5)	148(5)	2.951(4)	180	2.956(5)	143
O(1S)—H(1S2)···O(3)	2.952(5)	168(7)	2.930(4)	180	2.955(5)	152

[#1] Symmetry operators for the generated atoms: −*x*+1, −*y*, −*z*+1 for **1**; *x*−1/2, −*y*+1/2, *z*−1/2 for **2**; −*x*+1, −*y*+1, −*z* for **3**.

[#2] Symmetry operators for the generated atoms: −*x*+1, −*y*, −*z*+1 for **1**; *x*+1/2, −*y*+3/2, *z*−1/2 for **2**; −*x*+2, −*y*, −*z* for **3**.

[#3] Symmetry operators for the generated atoms: *x*, *y*+1, *z* for **1**; *x*+1, *y*, *z*. for **2**; *x*−1, *y*, *z*. for **3**

Table S3. TOPOS analysis for **1** by Topos 4.0 Pro (http://www.topos.ssu.samara.ru).

```
##################
1:C12 H10 N2 O6 Zn
##################

Topology for Zn1
--------------------
Atom Zn1 links by bridge ligands and has
Common vertex with                                  R(A-A)          f
Zn 1      0.0159      0.5764      0.1938    ( 0 0 0)      6.940A          1
Zn 1      0.0159     -0.4236      0.1938    ( 0-1 0)      6.940A          1
Zn 1      1.0159      0.5764      0.1938    ( 1 0 0)      7.907A          1
Zn 1      1.0159     -0.4236      0.1938    ( 1-1 0)      7.907A          1
Zn 1     -0.5159      1.0764      0.3062    (-1 1 0)     14.563A          1
Zn 1      1.4841     -0.9236      0.3062    ( 1-1 0)     14.563A          1

Coordination sequences
----------------------
Zn1:   1   2   3    4    5    6    7    8    9   10
Num    6  20  36   52   68   84  100  116  132  148
Cum    7  27  63  115  183  267  367  483  615  763
Rad 9.8(3.7) 17.2(5.9) 27.8(6.8) 39.2(8.0) 50.7(9.5) 62.3(11.1) 73.9(12.8) 85.6(14.5) 97.3(16.2)
109.0(18.0)
Cmp Zn6 Zn20 Zn36 Zn52 Zn68 Zn84 Zn100 Zn116 Zn132 Zn148
----------------------
TD10=763

Vertex symbols for selected sublattice
--------------------------------------
Zn1 Point (Schlafli) symbol:{3^3.4^4.5^5.6^2.7}
Extended point symbol:[3.3.3.4.4.4.4.5(2).5(2).5(2).5(2).5(2).6(4).6(4).7(8)]
--------------------------------------
Point (Schlafli) symbol for net: {3^3.4^4.5^5.6^2.7}
6-c net; uninodal net
New topology, please, contact the authors (66909 types in 9 databases)
```

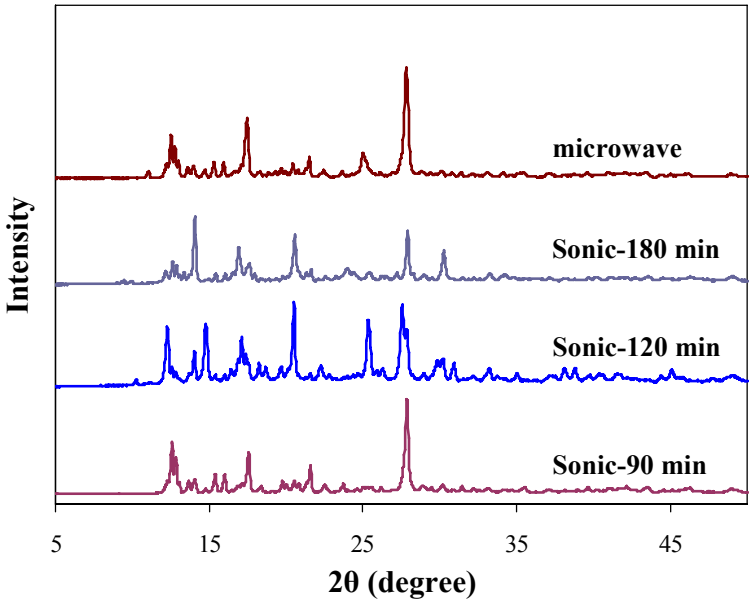

Figure S1. PXRD patterns of **1** synthesized by ultrasonification and microwave irradiation. Ultrasonic wave was irradiated for 90, 120, 180 min. Microwave was applied for 9 min without an addition of LiOH.

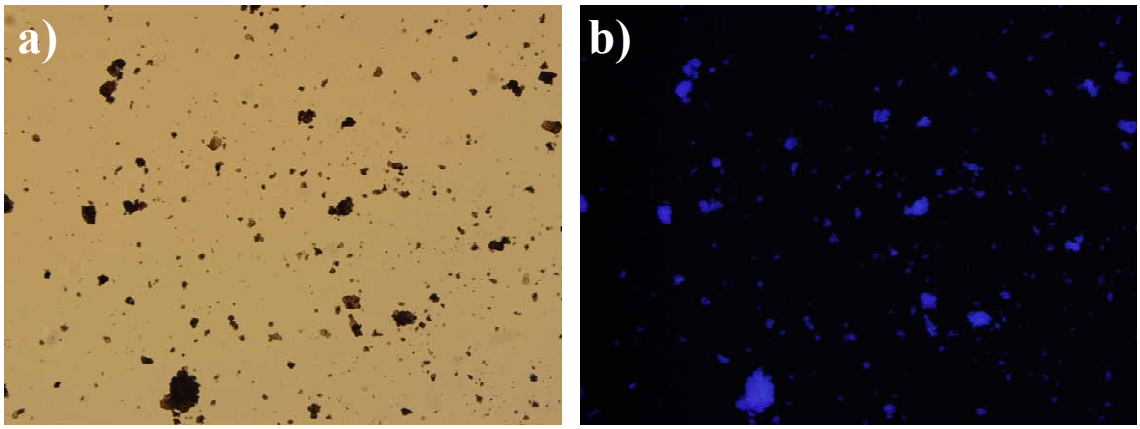

Figure S2. Microscopic images of **1** synthesized by microwave irradiation. a) An optical microscopic image. b) A fluorescence microscopic image of the same region.