Supporting Information:

Topological Derivation from Centrosymmetry to Noncentrosymmetry in a Three-dimensional Polar Framework Materia

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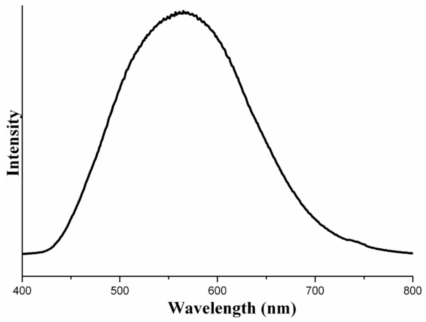
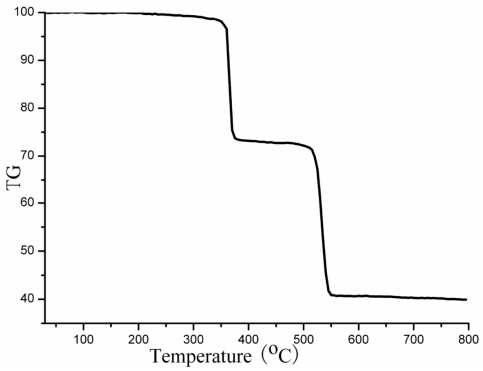


Fig. s1 Emission spectrum of compound **1** measured in the solid state at room temperature.



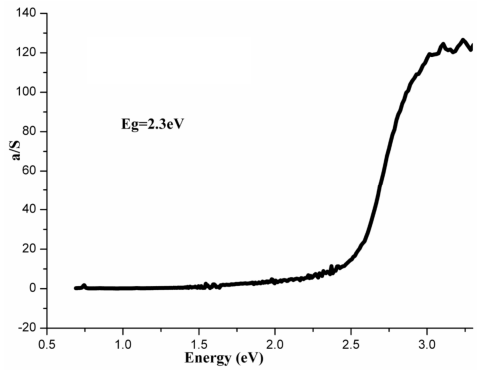


Fig. s2 The TG Plot for **1** under N_2 atmosphere. Fig. s3 The Diffuse reflectance spectrum of **1**.

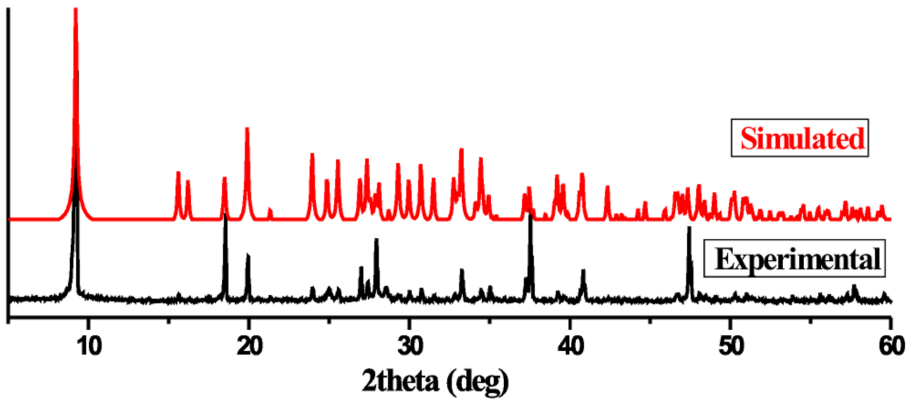


Fig. s4 The powder X-ray diffraction patterns of **1**.

Topological analysis performed on TOPOS program

Topology for ZD1

Atom ZD1 links by bridge ligands and has

Common vertex with					R(A-A)	f	Total SA
ZE 1	0.7631	0.5047	0.8187	(0 0 0)	2.536A	1	35.81
ZE 1	0.7631	-0.4953	0.8187	(0-1 0)	2.589A	1	33.21
ZE 2	0.8585	-0.3595	0.6382	(0 0 0)	2.611A	1	30.98

Topology for ZE1

Atom ZE1 links by bridge ligands and has

Common vertex with					R(A-A)	f	Total SA
ZD 1	0.8513	0.0142	0.8232	(0 0 0)	2.536A	1	21.17
ZD 1	0.8513	1.0142	0.8232	(0 1 0)	2.589A	1	19.63
ZF 1	0.6089	0.3189	0.5823	(0 1 0)	3.674A	1	27.58
ZF 1	0.6089	0.6811	1.0823	(0 0 1)	4.839A	1	31.61

Topology for ZE2

Atom ZE2 links by bridge ligands and has

Common vertex with					R(A-A)	f	Total SA
ZD 1	0.8513	-0.0142	0.3232	(0 0-1)	2.611A	1	23.06
ZF 1	0.6089	0.6811	0.0823	(0 0 0)	4.965A	1	40.67
ZF 1	1.1089	0.1811	0.0823	(0-1 0)	5.168A	1	36.27

Topology for ZF1

Atom ZF1 links by bridge ligands and has

Common vertex with					R(A-A)	f	Total SA
ZE 1	0.7631	0.4953	0.3187	(0 1-1)	3.674A	1	22.93
ZE 1	0.7631	0.5047	-0.1813	(0 0-1)	4.839A	1	26.28
ZE 2	0.8585	0.3595	0.1382	(0 0 0)	4.965A	1	26.84
ZE 2	0.3585	0.8595	0.1382	(-1 0 0)	5.168A	1	23.94

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZFZE2ZD

Coordination sequences

ZD1:	1	2	3	4	5	6	7	8	9	10
Num	3	7	17	34	55	82	118	160	210	265
Cum	4	11	28	62	117	199	317	477	687	952

ZE1:	1	2	3	4	5	6	7	8	9	10
Num	4	9	19	36	58	87	125	166	219	273
Cum	5	14	33	69	127	214	339	505	724	997

ZE2:	1	2	3	4	5	6	7	8	9	10
Num	3	7	17	34	58	85	122	164	214	269
Cum	4	11	28	62	120	205	327	491	705	974

ZF1:	1	2	3	4	5	6	7	8	9	10
Num	4	9	19	38	61	92	129	172	223	279
Cum	5	14	33	71	132	224	353	525	748	1027

TD10=987

Vertex symbols for selected sublattice

ZD1 Schlafli symbol:{4;8^2}

With circuits:[4.8(2).8(3)]

ZE1 Schlafli symbol:{4;8^4;10}

With circuits:[4.8(3).8.10(5).8(2).8(2)]

ZE2 Schlafli symbol:{4;8^2}

With circuits:[4.8.8]

ZF1 Schlafli symbol:{4;8^4;10}

With circuits:[4.8.8.8(2).8(3).10(3)]

Total Schlafli symbol: {4;8^2}{4;8^4;10}

3,4-c net with stoichiometry (3-c)(4-c); 4-nodal net

New topology, please, contact the authors (23744 types in 6 databases).

Topological analysis performed on Systre program

Structure #1 - "wf1".

Structure of dimension 3.

Given space group is Cc.

8 nodes and 14 edges in repeat unit as given.

Given repeat unit is accurate.

Point group has 2 elements.

4 kinds of node.

Coordination sequences:

Node Br1: 3 7 17 34 55 82 118 160 210 265

Node Sc1: 4 9 19 38 61 92 129 172 223 279

Node Cu2: 4 9 19 36 58 87 125 166 219 273

Node Cu1: 3 7 17 34 58 85 122 164 214 269

TD10 = 987.5000

Ideal space group is C1c1.

Structure is new for this run.

Relaxed cell parameters:

a = 3.46782, b = 1.96814, c = 3.97203

alpha = 90.0000, beta = 95.0272, gamma = 90.0000

Cell volume: 27.00541

Relaxed positions:

Node Br1: 0.04256 0.02957 0.33002

Node Sc1: 0.48281 0.02456 0.04138

Node Cu2: 0.50976 0.02946 0.29426

Node Cu1: 0.22229 0.19919 0.52140

Edges:

0.04256 0.02957 0.33002 <-> 0.00976 -0.47054 0.29426

0.04256 0.02957 0.33002 <-> 0.22229 0.19919 0.52140

0.48281 0.02456 0.04138 <-> 0.22229 -0.19919 0.02140

0.48281 0.02456 0.04138 <-> 0.72229 0.30081 0.02140

0.48281 0.02456 0.04138 <-> 0.50976 0.02946 0.29426

0.48281 0.02456 0.04138 <-> 0.50976 -0.02946 -0.20574

0.04256 0.02957 0.33002 <-> 0.00976 0.52946 0.29426

Edge centers:

0.02616 -0.22049 0.31214

0.13243 0.11438 0.42571

0.35255 -0.08731 0.03139

0.60255 0.16269 0.03139

0.49628 0.02701 0.16782

0.49628 -0.00245 -0.08218

0.02616 0.27951 0.31214

Edge statistics: minimum = 0.99739, maximum = 1.00191, average = 1.00000

Angle statistics: minimum = 76.99411, maximum = 168.66428, average = 117.09819

Shortest non-bonded distance = 1.24431

Degrees of freedom: 14

Finished structure #1 - "wf1".