Electronic Supplementary Material for CrystEngComm


Supporting Information:

# New (3, 4)-connected intrinsically chiral topology observed in a homochiral coordination polymer from achiral precursors

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**Topological analysis performed on TOPOS program**

Topology for Sc1

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Atom Sc1 links by bridge ligands and has

| Common vertex with | | | | | R(A-A) | |
|---|---|---|---|---|---|---|
| Cu 2 | -0.0093 | 0.6306 | 0.5375 | (-1 0 0) | 3.393A | 1 |
| Cu 1 | 0.0397 | 0.6958 | 0.1762 | ( 0 0 0) | 3.493A | 1 |
| Cu 2 | -0.5093 | 0.8694 | 0.4625 | (-2 1 1) | 5.075A | 1 |
| Cu 1 | 0.9603 | 0.1958 | 0.3238 | ( 1-1 0) | 5.234A | 1 |

Topology for Cu1

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Atom Cu1 links by bridge ligands and has

| Common vertex with | | | | | R(A-A) | |
|---|---|---|---|---|---|---|
| Sc 1 | 0.2298 | 0.5638 | 0.3549 | ( 0 0 0) | 3.493A | 1 |
| Cu 2 | -0.4907 | 0.3694 | 0.0375 | ( 0 1-1) | 4.911A | 1 |
| Sc 1 | 0.7702 | 1.0638 | 0.1451 | ( 1 0 0) | 5.234A | 1 |

Topology for Cu2

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Atom Cu2 links by bridge ligands and has

| Common vertex with | | | | | R(A-A) | |
|---|---|---|---|---|---|---|
| Sc 1 | 1.2298 | 0.5638 | 0.3549 | ( 1 0 0) | 3.393A | 1 |
| Cu 1 | 0.4603 | 0.3042 | 0.6762 | ( 0 1 0) | 4.911A | 1 |
| Sc 1 | 1.7298 | 0.9362 | 0.6451 | ( 1 1 1) | 5.075A | 1 |

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Structural group analysis

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Structural group No 1

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Structure consists of 3D framework with Cu2Sc

Coordination sequences

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| Sc1: | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Num | 4 | 8 | 20 | 48 | 100 | 163 | 229 | 311 | 400 | 504 |
| Cum | 5 | 13 | 33 | 81 | 181 | 344 | 573 | 884 | 1284 | 1788 |

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| Cu1: | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Num | 3 | 8 | 18 | 42 | 95 | 162 | 226 | 305 | 393 | 498 |
| Cum | 4 | 12 | 30 | 72 | 167 | 329 | 555 | 860 | 1253 | 1751 |

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| Cu2: | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Num | 3 | 8 | 18 | 42 | 97 | 159 | 219 | 308 | 393 | 496 |

Cum 4 12 30 72 169 328 547 855 1248 1744

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TD10=1761

Vertex symbols for selected sublattice

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Sc1 Schlafli symbol:{10^4;11^2}

With circuits:[10(2).10(2).10(2).11.10(2).11(5)]

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Cu1 Schlafli symbol:{10^3}

With circuits:[10.10(3).10(3)]

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Cu2 Schlafli symbol:{10^3}

With circuits:[10.10.10(3)]

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Total Schlafli symbol: {10^3}2{10^4;11^2}

3,4-c net with stoichiometry (3-c)2(4-c); 3-nodal net

New topology, please, contact the authors (66853 types in 9 databases)

**Topological analysis performed on Systre program**

Structure #1 - "wf1".

Structure of dimension 3.

Given space group is P212121.

12 nodes and 20 edges in repeat unit as given.

Given repeat unit is accurate.

Point group has 4 elements.

3 kinds of node.

Coordination sequences:

Node Sc3: 4 8 20 48 100 163 229 311 400 504

Node Cu1: 3 8 18 42 95 162 226 305 393 498

Node Cu2: 3 8 18 42 97 159 219 308 393 496

TD10 = 1761.0000

Ideal space group is P212121.

Structure is new for this run.

Relaxed cell parameters:

a = 2.02117, b = 1.02533, c = 4.67526

alpha = 90.0000, beta = 90.0000, gamma = 90.0000

Cell volume: 9.68891

Relaxed positions:

Node Sc3: 0.67121 0.42472 0.12127

Node Cu1: 0.03350 0.07186 0.08334

Node Cu2: 0.17047 0.24709 0.66904

Edges:

0.17047 0.24709 0.66904 <-> -0.17121 -0.42472 0.62127

0.03350 0.07186 0.08334 <-> -0.32879 -0.57528 0.12127

0.03350 0.07186 0.08334 <-> 0.32953 0.75291 0.16904

0.17047 0.24709 0.66904 <-> 0.17121 0.07528 0.87873

0.03350 0.07186 0.08334 <-> 0.17121 0.07528 -0.12127

Edge centers:

-0.00037 -0.08882 0.64516

-0.14765 -0.25171 0.10231

0.18151 0.41239 0.12619

0.17084 0.16118 0.77388

0.10235 0.07357 -0.01897

Edge statistics: minimum = 0.99602, maximum = 1.00395, average = 1.00000

Angle statistics: minimum = 69.97439, maximum = 176.17505, average = 118.10516

Shortest non-bonded distance = 0.79088

Degrees of freedom: 12

Finished structure #1 - "wf1".

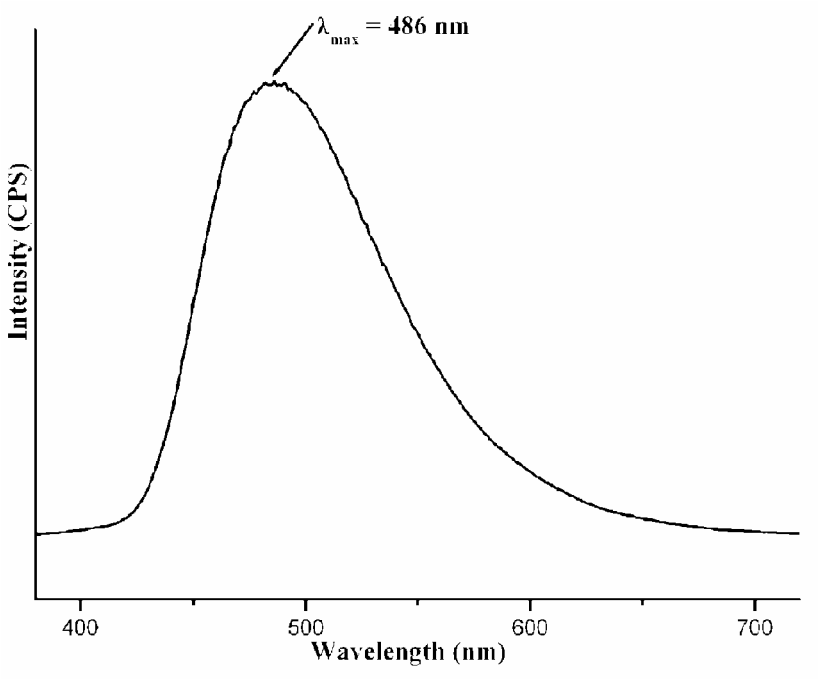


Fig. S1 Emission spectrum of compound **1** measured in the solid state at room temperature.

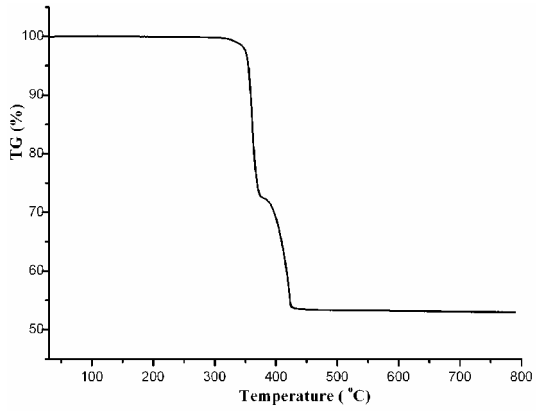


Fig. S2 Plot of TGA curves for **1** under a $N_2$ atmosphere.