Electronic Supplementary Material (ESI) for CrystEngComm


# Supporting Information

Divalent Copper *trans*-1,4-Cyclohexanedicarboxylate Coordination Polymers with Isomeric Dipyridylamide Ligands: New Pillared and Self-Penetrated Binodal Networks

Sultan H. Qiblawi, Amy L. Pochodylo and Robert L. LaDuca*

Fig. S1. Curie-Weiss Plot for **1**.

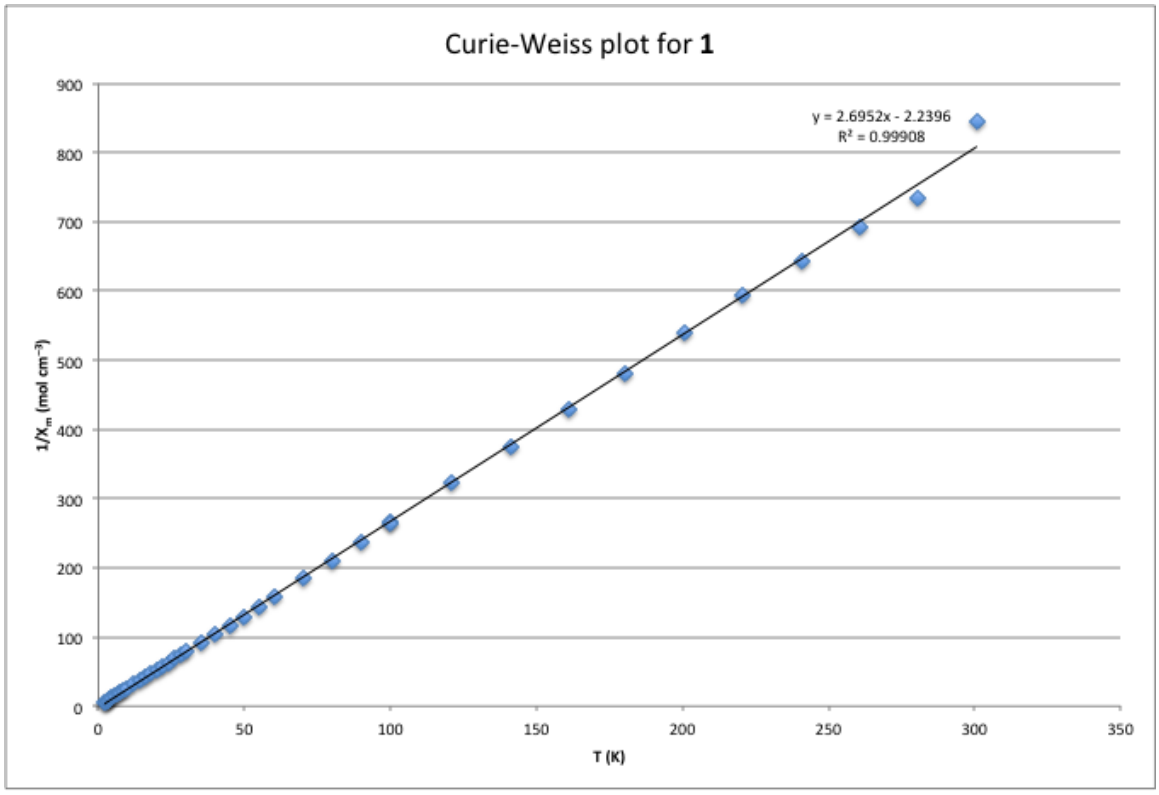


Fig. S2. Curie-Weiss Plot for **2**.

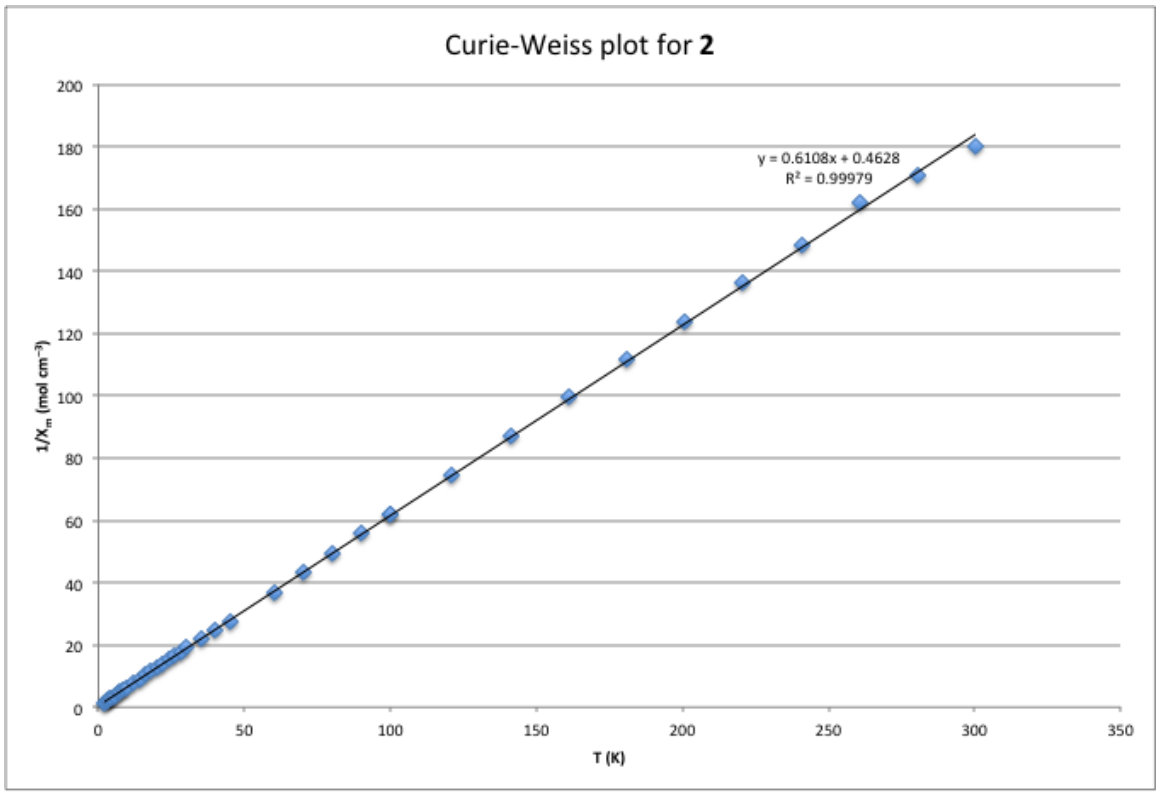


Fig. S3. Thermogravimetric analysis plot for **1**.

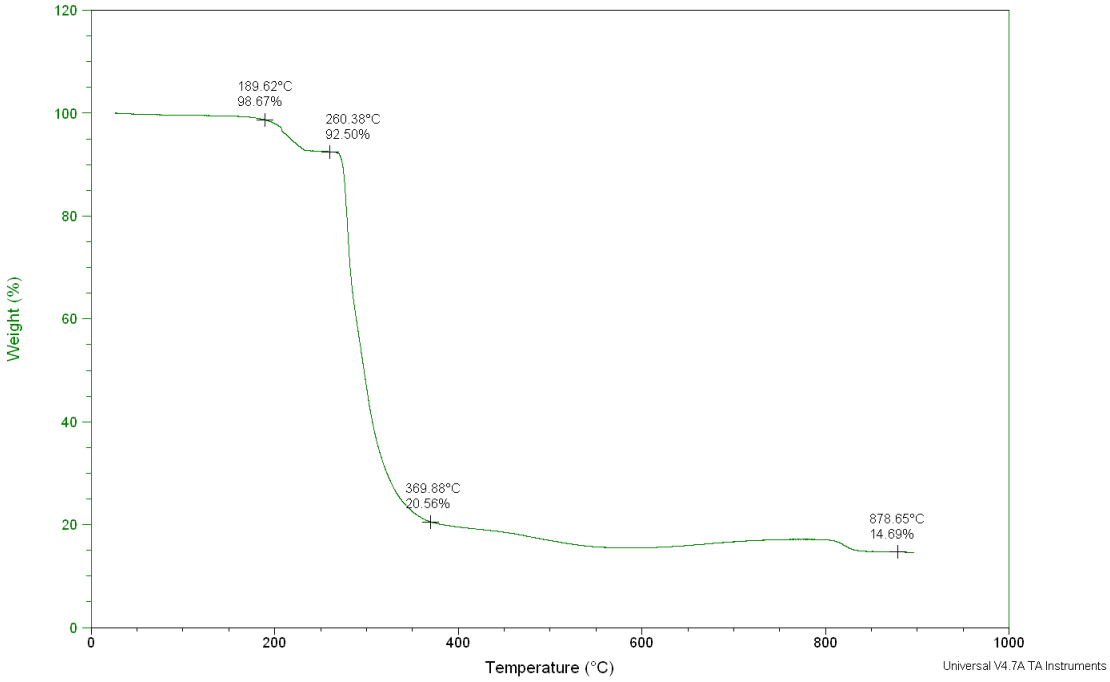
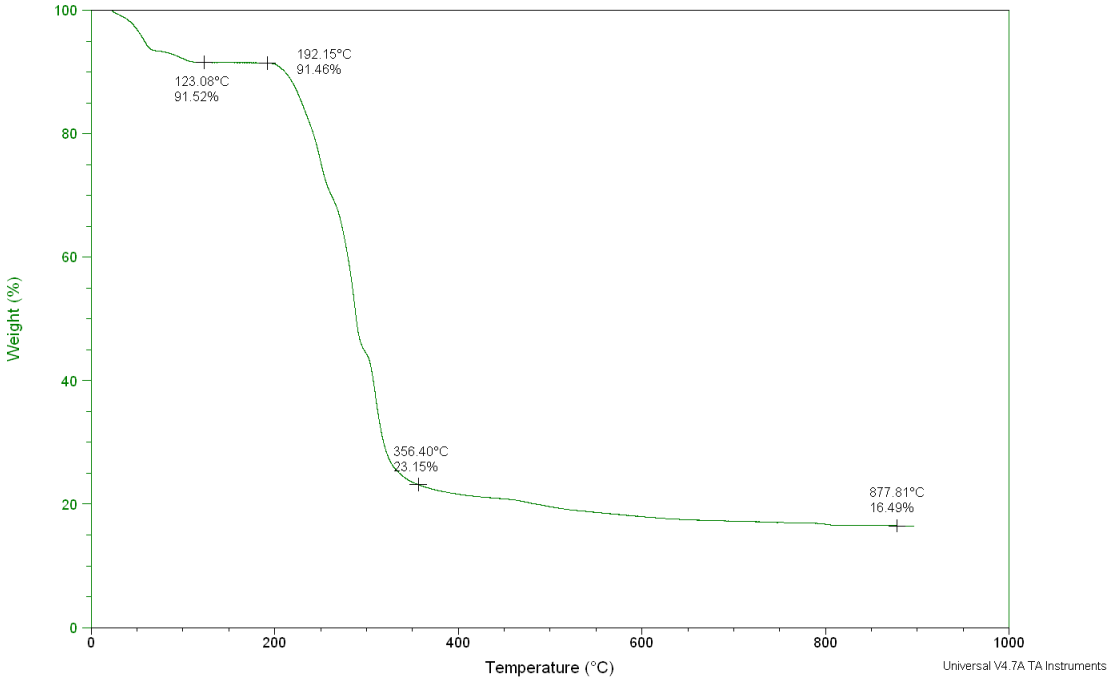



Fig. S4. Thermogravimetric analysis plot for **2**.



# Topological Analysis output for 1.

############################
229:Cu 14cyclohedicarb 3pna
############################

Topology for Cu1
---
Atom Cu1 links by bridge ligands and has
Common vertex with R(A-A)
Ag 1 0.2852 0.9859 0.0552 ( 0 0 0) 5.125A 1
Ag 1 0.2148 0.4859 0.4448 ( 0 0 0) 5.350A 1
Ag 1 0.2148 0.5141 -0.0552 ( 0 1-1) 5.389A 1
Cu 1 0.7247 0.8897 0.7015 ( 0 1 0) 11.720A 1
Cu 1 -0.2753 0.8897 -0.2985 (-1 1-1) 11.720A 1
Topology for Ag1
---
Atom Ag1 links by bridge ligands and has
Common vertex with R(A-A)
Cu 1 0.2753 0.1103 0.2985 ( 0-1 0) 5.125A 1
Cu 1 0.2247 0.6103 0.2015 ( 0 0 0) 5.350A 1
Cu 1 0.2247 0.3897 0.7015 ( 0 1 0) 5.389A 1
---
Structural group analysis
---

---
Structural group No 1
---
Structure consists of 3D framework with AgCu

Coordination sequences
---
Cu1: 1 2 3 4 5 6 7 8 9 10
Num 5 13 30 55 83 122 169 217 278 347
Cum 6 19 49 104 187 309 478 695 973 1320
Rad 7.9(3.5) 12.5(5.6) 17.0(7.1) 21.4(8.9) 26.7(10.7) 31.9(12.4) 36.9(14.3) 42.3(16.3) 47.6(18.1) 52.8(20.1)
Cmp Cu2Ag3 Cu7Ag6 Cu16Ag14 Cu27Ag28 Cu42Ag41 Cu62Ag60 Cu84Ag85 Cu109Ag108 Cu140Ag138 Cu173Ag174
---
Ag1: 1 2 3 4 5 6 7 8 9 10
Num 3 11 26 51 83 118 165 217 274 343
Cum 4 15 41 92 175 293 458 675 949 1292
Rad 5.3(0.1) 11.1(2.8) 15.3(5.6) 20.2(7.8) 25.3(9.5) 30.8(11.4) 36.0(13.4) 41.4(15.3) 46.9(17.3) 52.1(19.3)
Cmp Cu3 Cu6Ag5 Cu14Ag12 Cu28Ag23 Cu41Ag42 Cu60Ag58 Cu85Ag80 Cu108Ag109 Cu138Ag136 Cu174Ag169
---
TD10=1306

Vertex symbols for selected sublattice
---
Cu1 Point (Schlafli) symbol:{4.6^6.8^3}
Extended point symbol:[4.6.6.6(2).6(2).6(3).6(3).8(3).8(3).8(8)]
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Ag1 Point (Schlafli) symbol:{4.6.8}
Extended point symbol:[4.6(2).8(9)]
---
Point (Schlafli) symbol for net: {4.6.8}{4.6^6.8^3}
3,5-c net with stoichiometry (3-c)(5-c); 2-nodal net

New topology, please, contact the authors (23682 types in 6 databases)
---
Minimum circuits for independent edges (bonds)

| No | Atom | x | y | z | Atom | x | y | z | Dist. | N |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Cu1 | 0.2247 | 0.6103 | 0.2015 | Ag1 | 0.2852 | 0.9859 | 0.0552 | 5.125 | 4 |
| 2 | Cu1 | 0.2247 | 0.6103 | 0.2015 | Ag1 | 0.2148 | 0.4859 | 0.4448 | 5.350 | 6 |
| 3 | Cu1 | 0.2247 | 0.6103 | 0.2015 | Ag1 | 0.2148 | 0.5141 | -0.0552 | 5.389 | 4 |
| 4 | Cu1 | 1.2247 | 0.6103 | 1.2015 | Cu1 | 0.7247 | 0.8897 | 0.7015 | 11.720 | 6 |

---
Non-equivalent circuits
---
Circuit No 1; Type=4; Centroid: (0.250,0.750,0.000)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Ag1 | 0.2148 | 0.5141 | -0.0552 |
| Cu1 | 0.2753 | 0.8897 | -0.2015 |
| Ag1 | 0.2852 | 0.9859 | 0.0552 |

Circuit No 2; Type=6a; Centroid: (0.500,0.000,0.500)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | -0.3897 | 0.2015 |
| Ag1 | 0.2852 | -0.0141 | 0.0552 |
| Cu1 | 0.2753 | 0.1103 | 0.2985 |
| Cu1 | 0.7753 | 0.3897 | 0.7985 |
| Ag1 | 0.7148 | 0.0141 | 0.9448 |
| Cu1 | 0.7247 | -0.1103 | 0.7015 |

Circuit No 3; Type=6b; Centroid: (0.500,0.829,0.250)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Ag1 | 0.2852 | 0.9859 | 0.0552 |
| Cu1 | 0.2753 | 0.8897 | -0.2015 |
| Cu1 | 0.7753 | 0.6103 | 0.2985 |
| Ag1 | 0.7148 | 0.9859 | 0.4448 |
| Cu1 | 0.7247 | 0.8897 | 0.7015 |

Circuit No 4; Type=6c; Centroid: (0.512,0.750,0.268)

| Atom | x | y | z |
|---|---|---|---|

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| | | | |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Ag1 | 0.2852 | 0.9859 | 0.0552 |
| Cu1 | 0.2753 | 0.8897 | -0.2015 |
| Cu1 | 0.7753 | 0.6103 | 0.2985 |
| Ag1 | 0.7852 | 0.5141 | 0.5552 |
| Cu1 | 0.7247 | 0.8897 | 0.7015 |

Circuit No 5; Type=6d; Centroid: (0.000,0.000,0.000)

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| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | -0.3897 | 0.2015 |
| Ag1 | 0.2852 | -0.0141 | 0.0552 |
| Cu1 | 0.2753 | 0.1103 | 0.2985 |
| Cu1 | -0.2247 | 0.3897 | -0.2015 |
| Ag1 | -0.2852 | 0.0141 | -0.0552 |
| Cu1 | -0.2753 | -0.1103 | -0.2985 |

Circuit No 6; Type=6e; Centroid: (0.000,0.829,0.750)

---

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 1.2015 |
| Ag1 | 0.2852 | 0.9859 | 1.0552 |
| Cu1 | 0.2753 | 0.8897 | 0.7985 |
| Cu1 | -0.2247 | 0.6103 | 0.2985 |
| Ag1 | -0.2852 | 0.9859 | 0.4448 |
| Cu1 | -0.2753 | 0.8897 | 0.7015 |

Circuit No 7; Type=8a; Centroid: (0.250,0.750,0.500)

---

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Ag1 | 0.2148 | 0.4859 | 0.4448 |
| Cu1 | 0.2247 | 0.3897 | 0.7015 |
| Ag1 | 0.2148 | 0.5141 | 0.9448 |
| Cu1 | 0.2753 | 0.8897 | 0.7985 |
| Ag1 | 0.2852 | 1.0141 | 0.5552 |
| Cu1 | 0.2753 | 1.1103 | 0.2985 |
| Ag1 | 0.2852 | 0.9859 | 0.0552 |

Circuit No 8; Type=8b; Centroid: (0.451,0.575,0.306)

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| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Ag1 | 0.2148 | 0.4859 | 0.4448 |
| Cu1 | 0.2753 | 0.1103 | 0.2985 |
| Cu1 | 0.7753 | 0.3897 | 0.7985 |
| Ag1 | 0.7852 | 0.5141 | 0.5552 |
| Cu1 | 0.7753 | 0.6103 | 0.2985 |
| Cu1 | 0.2753 | 0.8897 | -0.2015 |
| Ag1 | 0.2852 | 0.9859 | 0.0552 |

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| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 1.2015 |
| Ag1 | 0.2148 | 0.4859 | 1.4448 |
| Cu1 | 0.2753 | 0.1103 | 1.2985 |
| Cu1 | -0.2247 | 0.3897 | 0.7985 |
| Ag1 | -0.2148 | 0.5141 | 0.5552 |
| Cu1 | -0.2247 | 0.6103 | 0.2985 |
| Cu1 | 0.2753 | 0.8897 | 0.7985 |
| Ag1 | 0.2852 | 0.9859 | 1.0552 |

Circuit No 10; Type=8d; Centroid: (0.443,0.516,0.293)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Ag1 | 0.2148 | 0.5141 | -0.0552 |
| Cu1 | 0.2753 | 0.8897 | -0.2015 |
| Cu1 | 0.7753 | 0.6103 | 0.2985 |
| Ag1 | 0.7852 | 0.5141 | 0.5552 |
| Cu1 | 0.7753 | 0.3897 | 0.7985 |
| Cu1 | 0.2753 | 0.1103 | 0.2985 |
| Ag1 | 0.2148 | 0.4859 | 0.4448 |

Circuit No 11; Type=8e; Centroid: (0.068,0.516,0.918)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 1.2015 |
| Ag1 | 0.2148 | 0.5141 | 0.9448 |
| Cu1 | 0.2753 | 0.8897 | 0.7985 |
| Cu1 | -0.2247 | 0.6103 | 0.2985 |
| Ag1 | -0.2148 | 0.5141 | 0.5552 |
| Cu1 | -0.2247 | 0.3897 | 0.7985 |
| Cu1 | 0.2753 | 0.1103 | 1.2985 |
| Ag1 | 0.2148 | 0.4859 | 1.4448 |

Circuit No 12; Type=8f; Centroid: (0.259,0.538,0.201)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Cu1 | -0.2753 | 0.8897 | -0.2985 |
| Ag1 | -0.2148 | 0.5141 | -0.4448 |
| Cu1 | -0.2247 | 0.3897 | -0.2015 |
| Cu1 | 0.2753 | 0.1103 | 0.2985 |
| Cu1 | 0.7753 | 0.3897 | 0.7985 |
| Ag1 | 0.7852 | 0.5141 | 0.5552 |
| Cu1 | 0.7247 | 0.8897 | 0.7015 |

Circuit No 13; Type=8g; Centroid: (0.222,0.004,0.450)

| Atom | x | y | z |
|---|---|---|---|

| | | | |
|---|---|---|---|
| Cu1 | 0.2247 | -0.3897 | 0.2015 |
| Cu1 | -0.2753 | -0.1103 | -0.2985 |
| Ag1 | -0.2852 | 0.0141 | -0.0552 |
| Cu1 | -0.2753 | 0.1103 | 0.2015 |
| Cu1 | 0.2247 | 0.3897 | 0.7015 |
| Cu1 | 0.7247 | 0.1103 | 1.2015 |
| Ag1 | 0.7148 | 0.0141 | 0.9448 |
| Cu1 | 0.7247 | -0.1103 | 0.7015 |

Crossed with bonds

| No | Atom | x | y | z | Atom | x | y | z | Dist. | N Cycles |
|---|---|---|---|---|---|---|---|---|---|---|
| * 3 | Cu1 | 0.2753 | 0.1103 | 0.2985 | Ag1 | 0.2852 | 0.0141 | 0.5552 | 5.389 | 8g/1 8g/1 |

Circuit No 14; Type=8h; Centroid: (0.241,0.809,0.986)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 1.2015 |
| Cu1 | -0.2753 | 0.8897 | 0.7015 |
| Ag1 | -0.2852 | 0.9859 | 0.4448 |
| Cu1 | -0.2247 | 0.6103 | 0.2985 |
| Cu1 | 0.2753 | 0.8897 | 0.7985 |
| Cu1 | 0.7753 | 0.6103 | 1.2985 |
| Ag1 | 0.7148 | 0.9859 | 1.4448 |
| Cu1 | 0.7247 | 0.8897 | 1.7015 |

Circuit No 15; Type=8i; Centroid: (0.250,0.750,0.000)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Cu1 | -0.2753 | 0.8897 | -0.2985 |
| Ag1 | -0.2148 | 0.5141 | -0.4448 |
| Cu1 | -0.2247 | 0.6103 | -0.7015 |
| Cu1 | 0.2753 | 0.8897 | -0.2015 |
| Cu1 | 0.7753 | 0.6103 | 0.2985 |
| Ag1 | 0.7148 | 0.9859 | 0.4448 |
| Cu1 | 0.7247 | 0.8897 | 0.7015 |

Circuit No 16; Type=8j; Centroid: (0.250,0.750,0.000)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.2247 | 0.6103 | 0.2015 |
| Cu1 | -0.2753 | 0.8897 | -0.2985 |
| Ag1 | -0.2852 | 0.9859 | -0.5552 |
| Cu1 | -0.2247 | 0.6103 | -0.7015 |
| Cu1 | 0.2753 | 0.8897 | -0.2015 |
| Cu1 | 0.7753 | 0.6103 | 0.2985 |
| Ag1 | 0.7852 | 0.5141 | 0.5552 |
| Cu1 | 0.7247 | 0.8897 | 0.7015 |

Circuit No 17; Type=8k; Centroid: (0.439,0.425,0.532)

| Atom | x | y | z |
|---|---|---|---|
| Ag1 | 0.2148 | 0.4859 | 0.4448 |
| Cu1 | 0.2247 | 0.3897 | 0.7015 |
| Ag1 | 0.2852 | 0.0141 | 0.5552 |
| Cu1 | 0.2753 | 0.1103 | 0.2985 |
| Cu1 | 0.7753 | 0.3897 | 0.7985 |
| Ag1 | 0.7852 | 0.5141 | 0.5552 |
| Cu1 | 0.7247 | 0.8897 | 0.7015 |
| Cu1 | 0.2247 | 0.6103 | 0.2015 |

Circuit No 18; Type=8l; Centroid: (0.064,0.425,0.157)

| Atom | x | y | z |
|---|---|---|---|
| Ag1 | 0.2148 | 0.4859 | 0.4448 |
| Cu1 | 0.2247 | 0.3897 | 0.7015 |
| Ag1 | 0.2852 | 0.0141 | 0.5552 |
| Cu1 | 0.2753 | 0.1103 | 0.2985 |
| Cu1 | -0.2247 | 0.3897 | -0.2015 |
| Ag1 | -0.2148 | 0.5141 | -0.4448 |
| Cu1 | -0.2753 | 0.8897 | -0.2985 |
| Cu1 | 0.2247 | 0.6103 | 0.2015 |

Ring links

| Cycle 1 | Cycle 2 | Chain | Cross | Link | Hopf | Mult |
|---|---|---|---|---|---|---|
| 8g | 8g | 1 | 1 | 1 | * | 2 |

# Topological Analysis output for **2**.

```
##############################
228:Cu 14cyclohexdicarb 3pina
##############################

Topology for Cu1
---------------------
Common vertex with                          R(A-A)
Cu 1    1.9395    0.3639    0.4101   ( 1 0 0)    10.350A       1
Cu 1   -0.0605    0.3639    0.4101   (-1 0 0)    10.350A       1
Au 1    1.5000    1.0000    0.0000   ( 1 1 0)    11.749A       1
Au 1    0.5000    0.0000    1.0000   ( 0 0 1)    12.476A       1
Topology for Au1
---------------------
Atom Au1 links by bridge ligands and has
Common vertex with                          R(A-A)
Au 1    0.5000    1.0000    0.0000   ( 0 1 0)    10.834A       1
Au 1    0.5000   -1.0000    0.0000   ( 0-1 0)    10.834A       1
Cu 1   -0.0605   -0.6361    0.4101   (-1-1 0)    11.749A       1
Cu 1    1.0605    0.6361   -0.4101   ( 2 1 0)    11.749A       1
Cu 1    0.9395    0.3639   -0.5899   ( 0 0-1)    12.476A       1
Cu 1    0.0605   -0.3639    0.5899   ( 1 0 1)    12.476A       1
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Structural group analysis
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Structural group No 1
-------------------------
Structure consists of 3D framework with AuCu2

Coordination sequences
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Cu1:  1  2  3   4   5   6   7    8    9   10
Num   4 15 42  84 138 204 282  372  474  588
Cum   5 20 62 146 284 488 770 1142 1616 2204
Rad 11.2(1.1) 17.9(5.8) 22.8(7.3) 29.1(8.9) 36.5(9.8) 44.2(10.8) 51.9(11.9) 59.6(13.1) 67.3(14.4)
75.0(15.8)
Cmp Cu2Au2 Cu7Au8 Cu24Au18 Cu52Au32 Cu88Au50 Cu132Au72 Cu184Au98 Cu244Au128
Cu312Au162 Cu388Au200
----------------------
Au1:  1  2  3   4   5   6   7    8    9   10
Num   6 20 48  90 144 210 288  378  480  594
Cum   7 27 75 165 309 519 807 1185 1665 2259
Rad 11.7(0.7) 17.1(4.5) 23.2(7.0) 30.1(8.0) 37.6(9.1) 45.1(10.3) 52.8(11.6) 60.4(13.0) 68.1(14.4)
75.7(15.8)
Cmp Cu4Au2 Cu16Au4 Cu36Au12 Cu64Au26 Cu100Au44 Cu144Au66 Cu196Au92 Cu256Au122
Cu324Au156 Cu400Au194
----------------------
TD10=2222

Vertex symbols for selected sublattice
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Cu1 Point (Schlafli) symbol:{4.6^4.8}
```

Extended point symbol:[4.8(8).6(4).6(4).6(4).6(4)]

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Au1 Point (Schlafli) symbol:{4^2.6^12.8}
Extended point symbol:[4.4.6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).6(2).8(8)]

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Point (Schlafli) symbol for net: {4.6^4.8}2{4^2.6^12.8}
4,6-c net with stoichiometry (4-c)2(6-c); 2-nodal net

New topology, please, contact the authors (23682 types in 6 databases)

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Minimum circuits for independent edges (bonds)

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| No | Atom | x | y | z | Atom | x | y | z | Dist. | N |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Cu1 | 0.9395 | 0.3639 | 0.4101 | Cu1 | -0.0605 | 0.3639 | 0.4101 | 10.350 | 6 |
| 2 | Cu1 | -0.0605 | 0.3639 | 0.4101 | Au1 | 0.5000 | 1.0000 | 0.0000 | 11.749 | 4 |
| 3 | Cu1 | 0.9395 | 0.3639 | 0.4101 | Au1 | 0.5000 | 0.0000 | 1.0000 | 12.476 | 4 |
| 4 | Au1 | 0.5000 | 1.0000 | 0.0000 | Au1 | 0.5000 | 0.0000 | 0.0000 | 10.834 | 6 |

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Non-equivalent circuits

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Circuit No 1; Type=4; Centroid: (0.000,0.500,0.500)

---

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | 0.3639 | 0.4101 |
| Au1 | -0.5000 | -0.0000 | 1.0000 |
| Cu1 | 0.0605 | 0.6361 | 0.5899 |
| Au1 | 0.5000 | 1.0000 | -0.0000 |

Circuit No 2; Type=6a; Centroid: (0.500,0.500,0.500)

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| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | 0.3639 | 0.4101 |
| Cu1 | 0.9395 | 0.3639 | 0.4101 |
| Au1 | 0.5000 | 0.0000 | 1.0000 |
| Cu1 | 1.0605 | 0.6361 | 0.5899 |
| Cu1 | 0.0605 | 0.6361 | 0.5899 |
| Au1 | 0.5000 | 1.0000 | -0.0000 |

Circuit No 3; Type=6b; Centroid: (0.667,0.667,0.333)

---

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | 0.3639 | 0.4101 |
| Cu1 | 0.9395 | 0.3639 | 0.4101 |
| Au1 | 1.5000 | 1.0000 | 0.0000 |
| Cu1 | 1.0605 | 0.6361 | 0.5899 |
| Cu1 | 0.0605 | 0.6361 | 0.5899 |
| Au1 | 0.5000 | 1.0000 | -0.0000 |

Circuit No 4; Type=6c; Centroid: (0.960,0.909,0.940)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | 0.3639 | 1.4101 |
| Cu1 | 0.9395 | 0.3639 | 1.4101 |
| Au1 | 1.5000 | 1.0000 | 1.0000 |
| Cu1 | 1.9395 | 1.3639 | 0.4101 |
| Cu1 | 0.9395 | 1.3639 | 0.4101 |
| Au1 | 0.5000 | 1.0000 | 1.0000 |

Circuit No 5; Type=6d; Centroid: (0.000,0.000,0.000)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -1.0605 | -0.6361 | 0.4101 |
| Cu1 | -0.0605 | -0.6361 | 0.4101 |
| Au1 | 0.5000 | 0.0000 | 0.0000 |
| Cu1 | 1.0605 | 0.6361 | -0.4101 |
| Cu1 | 0.0605 | 0.6361 | -0.4101 |
| Au1 | -0.5000 | -0.0000 | -0.0000 |

Circuit No 6; Type=6e; Centroid: (0.000,0.000,0.000)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | 0.3639 | -0.5899 |
| Cu1 | 0.9395 | 0.3639 | -0.5899 |
| Au1 | 0.5000 | 0.0000 | 0.0000 |
| Cu1 | 0.0605 | -0.3639 | 0.5899 |
| Cu1 | -0.9395 | -0.3639 | 0.5899 |
| Au1 | -0.5000 | -0.0000 | -0.0000 |

Circuit No 7; Type=6f; Centroid: (0.500,0.500,0.500)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | 0.3639 | 0.4101 |
| Cu1 | 0.9395 | 0.3639 | 0.4101 |
| Au1 | 1.5000 | 1.0000 | 0.0000 |
| Cu1 | 1.0605 | 0.6361 | 0.5899 |
| Cu1 | 0.0605 | 0.6361 | 0.5899 |
| Au1 | -0.5000 | -0.0000 | 1.0000 |

Circuit No 8; Type=6g; Centroid: (0.000,0.000,0.500)

| Atom | x | y | z |
|---|---|---|---|
| Au1 | 0.5000 | 0.0000 | 0.0000 |
| Au1 | 0.5000 | 1.0000 | -0.0000 |
| Cu1 | 0.0605 | 0.6361 | 0.5899 |
| Au1 | -0.5000 | -0.0000 | 1.0000 |
| Au1 | -0.5000 | -1.0000 | 1.0000 |
| Cu1 | -0.0605 | -0.6361 | 0.4101 |

Crossed with bonds

---

| No | Atom | x | y | z | Atom | x | y | z | Dist. | N Cycles |
|---|---|---|---|---|---|---|---|---|---|---|
| * 1 | Cu1 | -0.9395 | -0.3639 | 0.5899 | Cu1 | 0.0605 | -0.3639 | 0.5899 | 10.350 | 8a/1 8a/1 8b/1 8c/1 |
| * 1 | Cu1 | 0.9395 | 0.3639 | 0.4101 | Cu1 | -0.0605 | 0.3639 | 0.4101 | 10.350 | 8a/1 8a/1 8b/1 8c/1 |

---

Circuit No 9; Type=6h; Centroid: (0.980,0.955,0.470)

| Atom | x | y | z |
|---|---|---|---|
| Au1 | 1.5000 | 1.0000 | 0.0000 |
| Au1 | 1.5000 | 2.0000 | 0.0000 |
| Cu1 | 0.9395 | 1.3639 | 0.4101 |
| Au1 | 0.5000 | 1.0000 | 1.0000 |
| Au1 | 0.5000 | 0.0000 | 1.0000 |
| Cu1 | 0.9395 | 0.3639 | 0.4101 |

Crossed with bonds

| No | Atom | x | y | z | Atom | x | y | z | Dist. | N Cycles |
|---|---|---|---|---|---|---|---|---|---|---|
| * 1 | Cu1 | 0.0605 | 0.6361 | 0.5899 | Cu1 | 1.0605 | 0.6361 | 0.5899 | 10.350 | 8a/1 8a/1 8b/1 8c/1 |

---

Circuit No 10; Type=6i; Centroid: (0.000,0.000,0.500)

| Atom | x | y | z |
|---|---|---|---|
| Au1 | -0.5000 | -1.0000 | 1.0000 |
| Au1 | -0.5000 | -0.0000 | 1.0000 |
| Cu1 | -0.0605 | 0.3639 | 0.4101 |
| Au1 | 0.5000 | 1.0000 | -0.0000 |
| Au1 | 0.5000 | 0.0000 | 0.0000 |
| Cu1 | 0.0605 | -0.3639 | 0.5899 |

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | 0.3639 | 1.4101 |
| Cu1 | -1.0605 | 0.3639 | 1.4101 |
| Au1 | -0.5000 | 1.0000 | 1.0000 |
| Cu1 | -0.0605 | 1.3639 | 0.4101 |
| Cu1 | 0.9395 | 1.3639 | 0.4101 |
| Cu1 | 1.9395 | 1.3639 | 0.4101 |
| Au1 | 1.5000 | 1.0000 | 1.0000 |
| Cu1 | 0.9395 | 0.3639 | 1.4101 |

Crossed with bonds

| No | Atom | x | y | z | Atom | x | y | z | Dist. | N Cycles |
|---|---|---|---|---|---|---|---|---|---|---|
| * 4 | Au1 | 0.5000 | 1.0000 | 1.0000 | Au1 | 0.5000 | 0.0000 | 1.0000 | 10.834 | 6g/1 6g/1 6h/1 6h/1 8g/1 8g/1 8g/1 8g/1 8g/1 8h/1 8h/1 8i/1 8i/1 8i/1 8i/1 |

---

Circuit No 12; Type=8b; Centroid: (0.500,0.000,0.000)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | -0.0605 | -0.6361 | 0.4101 |
| Cu1 | -1.0605 | -0.6361 | 0.4101 |
| Au1 | -0.5000 | -0.0000 | -0.0000 |
| Cu1 | 0.0605 | 0.6361 | -0.4101 |
| Cu1 | 1.0605 | 0.6361 | -0.4101 |
| Cu1 | 2.0605 | 0.6361 | -0.4101 |
| Au1 | 1.5000 | 0.0000 | 0.0000 |
| Cu1 | 0.9395 | -0.6361 | 0.4101 |

Crossed with bonds

| No | Atom | x | y | z | Atom | x | y | z | Dist. | N Cycles |
|---|---|---|---|---|---|---|---|---|---|---|
| * 3 | Cu1 | 0.0605 | -0.3639 | 0.5899 | Au1 | 0.5000 | 0.0000 | 0.0000 | 12.476 | 6g/1 6h/1 6h/1 6i/1 8c/1 8c/1 8g/1 8g/1 8h/1 8i/1 |
| * 3 | Cu1 | 0.9395 | 0.3639 | -0.5899 | Au1 | 0.5000 | 0.0000 | 0.0000 | 12.476 | 6g/1 6h/1 6h/1 6i/1 8c/1 8c/1 8g/1 8g/1 8h/1 8i/1 |
| * 4 | Au1 | 0.5000 | 0.0000 | 0.0000 | Au1 | 0.5000 | -1.0000 | 0.0000 | 10.834 | 6g/1 6h/1 6h/1 6i/1 8g/1 8g/1 8g/1 8g/1 8g/1 8g/1 8h/1 8h/1 8h/1 8i/1 8i/1 8i/1 |
| * 4 | Au1 | 0.5000 | 1.0000 | 0.0000 | Au1 | 0.5000 | 0.0000 | 0.0000 | 10.834 | 6g/1 6h/1 6h/1 6i/1 8g/1 8g/1 8g/1 8g/1 8g/1 8g/1 8h/1 8h/1 8h/1 8i/1 8i/1 8i/1 |

Circuit No 13; Type=8c; Centroid: (0.500,0.000,0.000)

| Atom | x | y | z |
|---|---|---|---|
| Cu1 | 0.9395 | 0.3639 | -0.5899 |
| Cu1 | -0.0605 | 0.3639 | -0.5899 |
| Au1 | -0.5000 | -0.0000 | -0.0000 |
| Cu1 | -0.9395 | -0.3639 | 0.5899 |
| Cu1 | 0.0605 | -0.3639 | 0.5899 |
| Cu1 | 1.0605 | -0.3639 | 0.5899 |
| Au1 | 1.5000 | 0.0000 | 0.0000 |
| Cu1 | 1.9395 | 0.3639 | -0.5899 |

Crossed with bonds

| No | Atom | x | y | z | Atom | x | y | z | Dist. | N Cycles |
|---|---|---|---|---|---|---|---|---|---|---|
| * 2 | Cu1 | 1.0605 | 0.6361 | -0.4101 | Au1 | 0.5000 | 0.0000 | 0.0000 | 11.749 | 6g/1 6h/1 6h/1 6i/1 8b/1 8b/1 8g/1 8g/1 8h/1 8i/1 |
| * 2 | Cu1 | -0.0605 | -0.6361 | 0.4101 | Au1 | 0.5000 | 0.0000 | 0.0000 | 11.749 | 6g/1 6h/1 6h/1 6i/1 8b/1 8b/1 8g/1 8g/1 8h/1 8i/1 |
| * 4 | Au1 | 0.5000 | 0.0000 | 0.0000 | Au1 | 0.5000 | -1.0000 | 0.0000 | 10.834 | 6g/1 6h/1 6h/1 6i/1 8g/1 8g/1 8g/1 8g/1 8g/1 8g/1 8h/1 8h/1 8h/1 8i/1 8i/1 8i/1 |
| * 4 | Au1 | 0.5000 | 1.0000 | 0.0000 | Au1 | 0.5000 | 0.0000 | 0.0000 | 10.834 | 6g/1 6h/1 6h/1 6i/1 8g/1 8g/1 8g/1 8g/1 8g/1 8g/1 8h/1 8h/1 8h/1 8i/1 8i/1 8i/1 |

Circuit No 14; Type=8d; Centroid: (0.875,0.375,0.625)

| Atom | x | y | z |
|---|---|---|---|

---
Cu1 0.9395 0.3639 0.4101
Cu1 -0.0605 0.3639 0.4101
Au1 -0.5000 -0.0000 1.0000
Cu1 0.0605 0.6361 0.5899
Cu1 1.0605 0.6361 0.5899
Cu1 2.0605 0.6361 0.5899
Au1 1.5000 0.0000 1.0000
Cu1 1.9395 0.3639 0.4101

Circuit No 15; Type=8e; Centroid: (0.000,0.500,0.500)
---
Atom x y z
---
Cu1 -0.0605 0.3639 0.4101
Cu1 -1.0605 0.3639 0.4101
Au1 -0.5000 1.0000 -0.0000
Cu1 -0.9395 0.6361 0.5899
Cu1 0.0605 0.6361 0.5899
Cu1 1.0605 0.6361 0.5899
Au1 0.5000 0.0000 1.0000
Cu1 0.9395 0.3639 0.4101

Circuit No 16; Type=8f; Centroid: (0.000,0.500,0.500)
---
Atom x y z
---
Cu1 -0.0605 0.3639 0.4101
Cu1 -1.0605 0.3639 0.4101
Au1 -1.5000 -0.0000 1.0000
Cu1 -0.9395 0.6361 0.5899
Cu1 0.0605 0.6361 0.5899
Cu1 1.0605 0.6361 0.5899
Au1 1.5000 1.0000 0.0000
Cu1 0.9395 0.3639 0.4101

Circuit No 17; Type=8g; Centroid: (0.985,0.466,0.478)
---
Atom x y z
---
Au1 0.5000 0.0000 1.0000
Au1 0.5000 -1.0000 1.0000
Cu1 0.9395 -0.6361 0.4101
Au1 1.5000 0.0000 0.0000
Au1 1.5000 1.0000 0.0000
Au1 1.5000 2.0000 0.0000
Cu1 0.9395 1.3639 0.4101
Au1 0.5000 1.0000 1.0000
Crossed with bonds
---
No | Atom x y z | Atom x y z | Dist. | N Cycles
---
* 1 | Cu1 0.0605 -0.3639 0.5899 | Cu1 1.0605 -0.3639 0.5899 | 10.350 | 8a/1 8a/1 8b/1 8c/1
* 1 | Cu1 0.0605 0.6361 0.5899 | Cu1 1.0605 0.6361 0.5899 | 10.350 | 8a/1 8a/1 8b/1 8c/1 8d/1 8d/1 8e/1 8f/1

* 1 | Cu1 1.9395 0.3639 0.4101 | Cu1 0.9395 0.3639 0.4101 | 10.350 | 8a/1 8a/1 8b/1 8c/1 8d/1 8d/1 8e/1 8f/1

---

Circuit No 18; Type=8h; Centroid: (0.000,0.500,0.500)

---

Atom x y z

---

Au1 -0.5000 -0.0000 1.0000
Au1 -0.5000 -1.0000 1.0000
Cu1 0.0605 -0.3639 0.5899
Au1 0.5000 0.0000 0.0000
Au1 0.5000 1.0000 -0.0000
Au1 0.5000 2.0000 0.0000
Cu1 -0.0605 1.3639 0.4101
Au1 -0.5000 1.0000 1.0000

Crossed with bonds

---

No | Atom x y z | Atom x y z | Dist. | N Cycles

---

* 1 | Cu1 -0.9395 0.6361 0.5899 | Cu1 0.0605 0.6361 0.5899 | 10.350 | 8a/1 8a/1 8b/1 8c/1 8d/1 8d/1 8e/1 8f/1
* 1 | Cu1 0.9395 0.3639 0.4101 | Cu1 -0.0605 0.3639 0.4101 | 10.350 | 8a/1 8a/1 8b/1 8c/1 8d/1 8d/1 8e/1 8f/1

---

Circuit No 19; Type=8i; Centroid: (0.000,0.500,0.500)

---

Atom x y z

---

Au1 -0.5000 -0.0000 1.0000
Au1 -0.5000 -1.0000 1.0000
Cu1 -0.0605 -0.6361 0.4101
Au1 0.5000 0.0000 0.0000
Au1 0.5000 1.0000 -0.0000
Au1 0.5000 2.0000 0.0000
Cu1 0.0605 1.6361 0.5899
Au1 -0.5000 1.0000 1.0000

Crossed with bonds

---

No | Atom x y z | Atom x y z | Dist. | N Cycles

---

* 1 | Cu1 -0.9395 -0.3639 0.5899 | Cu1 0.0605 -0.3639 0.5899 | 10.350 | 8a/1 8a/1 8b/1 8c/1
* 1 | Cu1 -0.9395 0.6361 0.5899 | Cu1 0.0605 0.6361 0.5899 | 10.350 | 8a/1 8a/1 8b/1 8c/1 8d/1 8d/1 8e/1 8f/1
* 1 | Cu1 0.9395 0.3639 0.4101 | Cu1 -0.0605 0.3639 0.4101 | 10.350 | 8a/1 8a/1 8b/1 8c/1 8d/1 8d/1 8e/1 8f/1
* 1 | Cu1 0.9395 1.3639 0.4101 | Cu1 -0.0605 1.3639 0.4101 | 10.350 | 8a/1 8a/1 8b/1 8c/1

---

Ring links

---

Cycle 1 | Cycle 2 | Chain | Cross | Link | Hopf | Mult

---

6g | 8a | 1 | 1 | 1 | * | 4
6g | 8b | 1 | 1 | 1 | * | 2

| | | | | | | |
|---|---|---|---|---|---|---|
| 6g | 8c | 1 | 1 | 1 | * | 2 |
| 6h | 8a | 1 | 1 | 1 | * | 2 |
| 6h | 8b | 1 | 1 | 1 | * | 1 |
| 6h | 8c | 1 | 1 | 1 | * | 1 |
| 8a | 6g | 1 | 1 | 1 | * | 2 |
| 8a | 6h | 1 | 1 | 1 | * | 2 |
| 8a | 8g | 1 | 1 | 1 | * | 6 |
| 8a | 8h | 1 | 1 | 1 | * | 2 |
| 8a | 8i | 1 | 1 | 1 | * | 4 |
| 8b | 6g | 1 | 1 | 1 | * | 2 |
| 8b | 6h | 1 | 1 | 1 | * | 2 |
| 8b | 8c | 1 | 1 | 1 | * | 2 |
| 8b | 8g | 1 | 1 | 1 | * | 6 |
| 8b | 8h | 1 | 1 | 1 | * | 2 |
| 8b | 8i | 1 | 1 | 1 | * | 4 |
| 8c | 6g | 1 | 1 | 1 | * | 2 |
| 8c | 6h | 1 | 1 | 1 | * | 2 |
| 8c | 8b | 1 | 1 | 1 | * | 2 |
| 8c | 8g | 1 | 1 | 1 | * | 6 |
| 8c | 8h | 1 | 1 | 1 | * | 2 |
| 8c | 8i | 1 | 1 | 1 | * | 4 |
| 8g | 8a | 1 | 1 | 1 | * | 6 |
| 8g | 8b | 1 | 1 | 1 | * | 3 |
| 8g | 8c | 1 | 1 | 1 | * | 3 |
| 8g | 8d | 1 | 2 | 0 | | 2 |
| 8g | 8e | 1 | 2 | 0 | | 1 |
| 8g | 8f | 1 | 2 | 0 | | 1 |
| 8h | 8a | 1 | 1 | 1 | * | 4 |
| 8h | 8b | 1 | 1 | 1 | * | 2 |
| 8h | 8c | 1 | 1 | 1 | * | 2 |
| 8h | 8d | 1 | 2 | 0 | | 2 |
| 8h | 8e | 1 | 2 | 0 | | 1 |
| 8h | 8f | 1 | 2 | 0 | | 1 |
| 8i | 8a | 1 | 1 | 1 | * | 8 |
| 8i | 8b | 1 | 1 | 1 | * | 4 |
| 8i | 8c | 1 | 1 | 1 | * | 4 |
| 8i | 8d | 1 | 2 | 0 | | 2 |
| 8i | 8e | 1 | 2 | 0 | | 1 |
| 8i | 8f | 1 | 2 | 0 | | 1 |

---