```
####################
1:C52 H38 Cu2 N6 O11
####################

Structure consists of molecules (ZD1). The composition of molecule is Sc
Structure consists of molecules (ZE1). The composition of molecule is Cu
Topology for ZD1
--------------------
Atom ZD1 links by bridge ligands and has
Common vertex with                                R(A-A)        f Total SA
ZE 1    0.0000    0.2550    0.7500   ( 0 0 0)     8.125A        1  33.02
ZE 2    0.5000    0.0000    0.5000   ( 0 0 0)     8.174A        1  34.79
ZE 2    0.0000    0.5000    0.0000   ( 0 0 0)     8.806A        1  32.19
Topology for ZE1
--------------------
Atom ZE1 links by bridge ligands and has
Common vertex with                                R(A-A)        f Total SA
ZD 1    0.1668    0.2406    0.3723   ( 0 0 0)     8.125A        1  24.23
ZD 1   -0.1668    0.2406    1.1277   ( 0 0 1)     8.125A        1  24.23
ZE 1    0.5000    0.2450    1.2500   ( 0 0 0)    10.986A        1  25.77
ZE 1   -0.5000    0.2450    0.2500   (-1 0-1)    10.986A        1  25.77
Topology for ZE2
--------------------
Atom ZE2 links by bridge ligands and has
Common vertex with                                R(A-A)        f Total SA
ZD 1   -0.3332    0.2594   -0.1277   (-1 0-1)     8.174A        1  25.97
ZD 1    0.3332    0.7406    0.1277   ( 0 0 0)     8.174A        1  25.97
ZD 1   -0.1668    0.7594   -0.3723   ( 0 1 0)     8.806A        1  24.03
ZD 1    0.1668    0.2406    0.3723   ( 0 0 0)     8.806A        1  24.03
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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 ZEZD
There are 3 interpenetrating nets
FIV: Full interpenetration vectors
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[1/2,1/2,0] (14.82A)
[1/2,-1/2,0] (14.82A)
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PIC: [3/2,3/2,0][1,0,1][0,1,0] (PICVR=3)

Zt=3; Zn=1

Class Ia  Z=3

Coordination sequences
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ZD1:  1  2  3  4   5   6   7   8   9  10
Num   3  9 16 34  52  83 105 148 187 235
Cum   4 13 29 63 115 198 303 451 638 873
----------------------
ZE1:  1  2  3  4   5   6   7   8   9  10
Num   4 10 18 34  58  84 108 156 200 228
Cum   5 15 33 67 125 209 317 473 673 901
----------------------
ZE2:  1  2  3  4   5   6   7   8   9  10
Num   4  8 20 30  56  82 114 146 190 242
Cum   5 13 33 63 119 201 315 461 651 893
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TD10=885

Vertex symbols for selected sublattice
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ZD1 Point (Schlafli) symbol:{5^2;8}
Extended point symbol:[5.5.8(3)]
--------------------------------------
ZE1 Point (Schlafli) symbol:{5^4;8^2}
Extended point symbol:[5.5.5.5.8(2).8(2)]
--------------------------------------
ZE2 Point (Schlafli) symbol:{5^2;8^2;10^2}
Extended point symbol:[5.5.8.8.10(2).10(2)]
--------------------------------------
Point (Schlafli) symbol for net: {5^2;8^2;10^2}{5^2;8}2{5^4;8^2}
3,4-c net with stoichiometry (3-c)(4-c); 3-nodal net

New topology, please, contact the authors (67371 types in 9 databases)

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Non-equivalent circuits
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Circuit No 1; Type=5; Centroid: (0.367,0.200,0.749)
```

c.2

Atom	x	y	z
ZD1	0.1668	0.2406	0.3723
ZE1	0.0000	0.2550	0.7500
ZE1	0.5000	0.2450	1.2500
ZD1	0.6668	0.2594	0.8723
ZE2	0.5000	0.0000	0.5000

Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
4	ZD1	0.3332	0.2594	0.6277	ZE2	0.5000	0.0000	1.0000	8.806	5/inf 8a/inf 8a/inf 8b

Circuit No 2; Type=8a; Centroid: (0.000,0.000,0.000)

Atom	x	y	z
ZD1	0.1668	0.2406	0.3723
ZE2	0.0000	0.5000	0.0000
ZD1	-0.3332	0.2594	-0.1277
ZE2	-0.5000	0.0000	-0.5000
ZD1	-0.1668	-0.2406	-0.3723
ZE2	0.0000	-0.5000	0.0000
ZD1	0.3332	-0.2594	0.1277
ZE2	0.5000	0.0000	0.5000

Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
2	ZD1	0.1668	-0.2406	-0.1277	ZE1	0.0000	-0.2550	0.2500	8.125	5/inf 5/inf 8b/inf 8b/
2	ZD1	-0.1668	0.2406	0.1277	ZE1	0.0000	0.2550	-0.2500	8.125	5/inf 5/inf 8b/inf 8b/

Circuit No 3; Type=8b; Centroid: (0.125,0.251,0.483)

Atom	x	y	z
ZD1	0.1668	0.2406	0.3723
ZE2	0.0000	0.5000	0.0000
ZD1	-0.3332	0.2594	-0.1277
ZE1	-0.5000	0.2450	0.2500
ZE1	0.0000	0.2550	0.7500
ZE1	0.5000	0.2450	1.2500
ZD1	0.6668	0.2594	0.8723
ZE2	0.5000	0.0000	0.5000

Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
4	ZD1	0.3332	0.2594	0.6277	ZE2	0.5000	0.0000	1.0000	8.806	5/inf 8a/inf 8a/inf 8b
4	ZD1	-0.1668	0.2406	0.1277	ZE2	0.0000	0.5000	0.5000	8.806	5/inf 8a/inf 8a/inf 8b

Circuit No 4; Type=8c; Centroid: (0.250,0.250,0.000)

Atom	x	y	z
ZE1	0.0000	0.2550	-0.2500
ZD1	-0.1668	0.2406	0.1277
ZE2	0.0000	0.5000	0.5000
ZD1	0.3332	0.2594	0.6277
ZE1	0.5000	0.2450	0.2500
ZD1	0.6668	0.2594	-0.1277
ZE2	0.5000	0.0000	-0.5000
ZD1	0.1668	0.2406	-0.6277

Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
4	ZD1	0.3332	0.2594	-0.3723	ZE2	0.5000	0.0000	0.0000	8.806	5/inf 8a/inf 8a/inf 8b
4	ZD1	0.1668	0.2406	0.3723	ZE2	0.0000	0.5000	0.0000	8.806	5/inf 8a/inf 8a/inf 8b

Circuit No 5; Type=10a; Centroid: (0.300,0.476,0.525)

Atom	x	y	z
ZE2	0.0000	0.5000	0.0000
ZD1	-0.3332	0.2594	-0.1277
ZE1	-0.5000	0.2450	0.2500
ZE1	0.0000	0.2550	0.7500
ZE1	0.5000	0.2450	1.2500
ZD1	0.6668	0.2594	0.8723
ZE2	1.0000	0.5000	1.0000

c.3

ZD1 0.8332 0.7594 0.6277
ZE2 0.5000 1.0000 0.5000
ZD1 0.3332 0.7406 0.1277
Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
2	ZD1	0.6668	0.7406	0.3723	ZE1	0.5000	0.7550	0.7500	8.125	5/inf 5/inf 8b/inf 8b/
3	ZD1	0.3332	0.2594	0.6277	ZE2	0.0000	0.5000	0.5000	8.174	5/inf 8a/inf 8a/inf 8b
4	ZD1	-0.1668	0.2406	0.1277	ZE2	0.0000	0.5000	0.5000	8.806	5/inf 8a/inf 8a/inf 8b

Circuit No 6; Type=10b; Centroid: (0.450,0.526,0.225)

Atom	x	y	z
ZE2	0.0000	0.5000	0.0000
ZD1	-0.1668	0.7594	-0.3723
ZE1	0.0000	0.7450	-0.7500
ZE1	0.5000	0.7550	-0.2500
ZE1	1.0000	0.7450	0.2500
ZD1	0.8332	0.7594	0.6277
ZE2	1.0000	0.5000	1.0000
ZD1	0.6668	0.2594	0.8723
ZE2	0.5000	0.0000	0.5000
ZD1	0.1668	0.2406	0.3723

Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
2	ZD1	0.3332	0.2594	0.6277	ZE1	0.5000	0.2450	0.2500	8.125	5/inf 5/inf 8b/inf 8b/
3	ZD1	0.6668	0.7406	0.3723	ZE2	1.0000	0.5000	0.5000	8.174	5/inf 8a/inf 8a/inf 8b
4	ZD1	0.1668	0.7594	-0.1277	ZE2	0.0000	0.5000	-0.5000	8.806	5/inf 8a/inf 8a/inf 8b

Ring links

Cycle 1	Cycle 2	Chain	Cross	Link	Hopf	Mult
5	5	inf.	1	1	*	1
5	8a	inf.	1	1	*	2
5	8b	inf.	1	1	*	2
5	8c	inf.	1	1	*	1
5	10a	inf.	1	1	*	2
5	10b	inf.	1	1	*	4
8a	5	inf.	1	1	*	4
8a	8b	inf.	1	1	*	4
8a	8c	inf.	1	1	*	4
8a	10a	inf.	1	1	*	4
8a	10b	inf.	1	1	*	4
8b	5	inf.	1	1	*	2
8b	8a	inf.	1	1	*	2
8b	8a	inf.	2	0		1
8b	8b	inf.	1	1	*	2
8b	8b	inf.	2	0		1
8b	8c	inf.	1	1	*	2
8b	10a	inf.	1	1	*	2
8b	10a	inf.	2	0		1
8b	10b	inf.	1	1	*	6
8b	10b	inf.	2	0		1
8c	5	inf.	1	1	*	2
8c	8a	inf.	1	1	*	4
8c	8b	inf.	1	1	*	4
8c	8c	inf.	1	1	*	2
8c	10a	inf.	1	1	*	4
8c	10b	inf.	1	1	*	8
10a	5	inf.	1	1	*	2
10a	5	inf.	2	0		1
10a	8a	inf.	1	1	*	2
10a	8a	inf.	2	0		1
10a	8b	inf.	1	1	*	2
10a	8b	inf.	2	0		2
10a	8c	inf.	1	1	*	2
10a	8c	inf.	2	0		1
10a	10a	inf.	1	1	*	6
10a	10a	inf.	2	0		1
10a	10b	inf.	1	1	*	6
10a	10b	inf.	2	0		1
10b	5	inf.	1	1	*	4
10b	8a	inf.	1	1	*	2
10b	8a	inf.	2	0		1
10b	8b	inf.	1	1	*	6
10b	8c	inf.	1	1	*	4
10b	10a	inf.	1	1	*	6
10b	10a	inf.	2	0		1

c.4

10b	10b	inf.	1	1	*	6
10b	10b	inf.	2	0		1

Elapsed time: 17.59 sec.