

1:C17 H17 Mn N O7
#####

Structure consists of molecules (ZD1). The composition of molecule is Sc
Structure consists of molecules (ZD2). The composition of molecule is Sc
Structure consists of molecules (ZE1). The composition of molecule is Mn
Structure consists of molecules (ZE2). The composition of molecule is Mn
Topology for ZD1

Atom ZD1 links by bridge ligands and has
Common vertex with

					R(A-A)	f	Total SA
ZE 1	1.0000	0.5000	0.5000	(1 0 0)	6.413A	1	16.74
ZE 1	0.0000	0.5000	0.5000	(0 0 0)	6.413A	1	16.74
ZE 2	1.0000	0.5938	0.7500	(1 1 1)	7.283A	1	17.17
ZE 2	0.0000	0.4062	0.2500	(0 0 0)	7.283A	1	17.17
ZE 1	1.0000	0.5000	1.0000	(1 0 1)	7.843A	1	16.09
ZE 1	0.0000	0.5000	0.0000	(0 0 0)	7.843A	1	16.09

Topology for ZD2

Atom ZD2 links by bridge ligands and has
Common vertex with

					R(A-A)	f	Total SA
ZE 2	1.0000	0.5938	0.7500	(1 1 1)	5.991A	1	24.53
ZE 2	0.5000	0.9062	0.2500	(0 0 0)	5.991A	1	24.53
ZE 1	1.0000	0.5000	0.5000	(1 0 0)	7.927A	1	25.47
ZE 1	0.5000	1.0000	0.5000	(0 1 1)	7.927A	1	25.47

Topology for ZE1

Atom ZE1 links by bridge ligands and has
Common vertex with

					R(A-A)	f	Total SA
ZD 1	0.5000	0.5000	0.5000	(0 0 0)	6.413A	1	16.43
ZD 1	-0.5000	0.5000	0.5000	(-1 0 0)	6.413A	1	16.43
ZD 1	-0.5000	0.5000	0.0000	(0 0 0)	7.843A	1	15.79
ZD 1	0.5000	0.5000	1.0000	(1 0 1)	7.843A	1	15.79
ZD 2	-0.2500	0.7500	0.5000	(-1 0 0)	7.927A	1	17.78
ZD 2	0.2500	0.2500	0.5000	(1 1 1)	7.927A	1	17.78

Topology for ZE2

Atom ZE2 links by bridge ligands and has
Common vertex with

					R(A-A)	f	Total SA
ZD 2	-0.2500	0.2500	0.0000	(-1 1-1)	5.991A	1	25.20
ZD 2	0.2500	0.2500	0.5000	(1 1 1)	5.991A	1	25.20
ZD 1	-0.5000	0.5000	0.0000	(0 0 0)	7.283A	1	24.80
ZD 1	0.5000	0.5000	0.5000	(0 0 0)	7.283A	1	24.80

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZE2D

Coordination sequences

ZD1: 1 2 3 4 5 6 7 8 9 10
Num 6 16 36 70 114 172 240 318 414 518
Cum 7 23 59 129 243 415 655 973 1387 1905

ZD2: 1 2 3 4 5 6 7 8 9 10
Num 4 12 30 58 100 152 216 294 384 486
Cum 5 17 47 105 205 357 573 867 1251 1737

ZE1: 1 2 3 4 5 6 7 8 9 10
Num 6 18 38 70 114 170 240 322 416 522
Cum 7 25 63 133 247 417 657 979 1395 1917

ZE2: 1 2 3 4 5 6 7 8 9 10
Num 4 12 28 56 100 150 216 292 382 480
Cum 5 17 45 101 201 351 567 859 1241 1721

TD10=1820

Vertex symbols for selected sublattice

ZD1 Point (Schlafli) symbol:{4^8;6^6;8}
Extended point symbol:[4.4.4.4.4(2).4(2).4(2).4(2).6(2).6(2).6(2).6(2).6(3).6(3).8(12)]

ZD2 Point (Schlafli) symbol:{4^2;6^3;8}
Extended point symbol:[4(2).4(2).6(2).8(32).6(3).6(3)]

ZE1 Point (Schlafli) symbol:{4^8;6^6;8}
Extended point symbol:[4.4.4.4.4.4.4(2).4(2).6.6.6(3).6(3).6(4).6(4).8(6)]

ZE2 Point (Schlafli) symbol:{4^5;6}

Point (Schlafli) symbol for net: {4²;6³;8}{4⁵;6}{4⁸;6⁶;8}2
4,6-c net with stoichiometry (4-c)(6-c); 4-nodal net

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

Non-equivalent circuits

Circuit No 1; Type=4a; Centroid: (0.000,0.523,0.688)

Atom x y z

ZD1 -0.5000 0.5000 0.5000
ZE2 0.0000 0.5938 0.7500
ZD1 0.5000 0.5000 1.0000
ZE1 0.0000 0.5000 0.5000

Circuit No 2; Type=4b; Centroid: (0.813,0.586,0.563)

Atom x y z

ZD1 0.5000 0.5000 0.5000
ZE2 1.0000 0.5938 0.7500
ZD2 0.7500 0.7500 0.5000
ZE1 1.0000 0.5000 0.5000

Circuit No 3; Type=4c; Centroid: (0.000,0.500,0.750)

Atom x y z

ZD1 -0.5000 0.5000 0.5000
ZE1 0.0000 0.5000 1.0000
ZD1 0.5000 0.5000 1.0000
ZE1 0.0000 0.5000 0.5000

Circuit No 4; Type=4d; Centroid: (0.500,0.500,0.250)

Atom x y z

ZD1 0.5000 0.5000 0.5000
ZE1 0.0000 0.5000 0.0000
ZD1 0.5000 0.5000 0.0000
ZE1 1.0000 0.5000 0.5000

Circuit No 5; Type=4e; Centroid: (0.938,0.586,0.813)

Atom x y z

ZD1 0.5000 0.5000 0.5000
ZE1 1.0000 0.5000 1.0000
ZD2 1.2500 0.7500 1.0000
ZE2 1.0000 0.5938 0.7500

Circuit No 6; Type=6a; Centroid: (0.750,0.500,0.750)

Atom x y z

ZD1 0.5000 0.5000 0.5000
ZE1 1.0000 0.5000 0.5000
ZD1 1.5000 0.5000 1.0000
ZE1 1.0000 0.5000 1.0000
ZD1 0.5000 0.5000 1.0000
ZE1 0.0000 0.5000 0.5000

Circuit No 7; Type=6b; Centroid: (0.250,0.484,0.208)

Atom x y z

ZD1 0.5000 0.5000 0.5000
ZE1 1.0000 0.5000 0.5000
ZD1 0.5000 0.5000 0.0000
ZE1 0.0000 0.5000 0.0000
ZD1 -0.5000 0.5000 0.0000
ZE2 0.0000 0.4062 0.2500

Circuit No 8; Type=6c; Centroid: (0.292,0.443,0.208)

Atom x y z

ZD1 0.5000 0.5000 0.5000
ZE1 1.0000 0.5000 0.5000
ZD1 0.5000 0.5000 0.0000
ZE1 0.0000 0.5000 0.0000

ZD2 -0.2500 0.2500 0.0000
ZE2 0.0000 0.4062 0.2500

Circuit No 9; Type=6d; Centroid: (0.500,0.667,0.333)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	1.0000	0.5938	0.7500
ZD2	0.7500	0.7500	0.5000
ZE2	0.5000	0.9062	0.2500
ZD2	0.2500	0.7500	0.0000
ZE1	0.0000	0.5000	0.0000

Circuit No 10; Type=6e; Centroid: (0.750,0.516,0.458)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	1.0000	0.5938	0.7500
ZD1	1.5000	0.5000	1.0000
ZE1	1.0000	0.5000	0.5000
ZD1	0.5000	0.5000	0.0000
ZE1	0.0000	0.5000	0.0000

Circuit No 11; Type=6f; Centroid: (0.625,0.557,0.375)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	1.0000	0.5938	0.7500
ZD2	0.7500	0.7500	0.5000
ZE1	1.0000	0.5000	0.5000
ZD1	0.5000	0.5000	0.0000
ZE1	0.0000	0.5000	0.0000

Circuit No 12; Type=6g; Centroid: (0.750,0.500,0.500)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE1	1.0000	0.5000	1.0000
ZD1	1.5000	0.5000	1.0000
ZE1	1.0000	0.5000	0.5000
ZD1	0.5000	0.5000	0.0000
ZE1	0.0000	0.5000	0.0000

Circuit No 13; Type=6h; Centroid: (0.000,0.849,0.792)

Atom	x	y	z
ZD2	-0.2500	0.7500	0.5000
ZE2	0.0000	0.5938	0.7500
ZD2	0.2500	0.7500	1.0000
ZE1	0.5000	1.0000	1.0000
ZD1	0.0000	1.0000	1.0000
ZE1	-0.5000	1.0000	0.5000

Circuit No 14; Type=6i; Centroid: (0.083,0.401,0.292)

Atom	x	y	z
ZE2	0.0000	0.4062	0.2500
ZD2	-0.2500	0.2500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.5000
ZE1	0.0000	0.5000	0.5000
ZD2	0.2500	0.2500	0.5000

Circuit No 15; Type=8a; Centroid: (0.313,0.613,0.281)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	0.0000	0.4062	0.2500
ZD1	-0.5000	0.5000	0.0000
ZE1	0.0000	0.5000	0.0000
ZD2	0.2500	0.7500	0.0000
ZE2	0.5000	0.9062	0.2500
ZD2	0.7500	0.7500	0.5000
ZE2	1.0000	0.5938	0.7500

Circuit No 16; Type=8b; Centroid: (0.344,0.582,0.281)

Atom	x	y	z
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ZD1	0.5000	0.5000	0.5000
ZE2	0.0000	0.4062	0.2500
ZD2	-0.2500	0.2500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD2	0.2500	0.7500	0.0000
ZE2	0.5000	0.9062	0.2500
ZD2	0.7500	0.7500	0.5000
ZE2	1.0000	0.5938	0.7500

Circuit No 17; Type=8c; Centroid: (0.500,0.500,0.375)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	0.0000	0.4062	0.2500
ZD1	-0.5000	0.5000	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000
ZD1	1.5000	0.5000	1.0000
ZE2	1.0000	0.5938	0.7500

Circuit No 18; Type=8d; Centroid: (0.531,0.469,0.375)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	0.0000	0.4062	0.2500
ZD2	-0.2500	0.2500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000
ZD1	1.5000	0.5000	1.0000
ZE2	1.0000	0.5938	0.7500

Circuit No 19; Type=8e; Centroid: (0.406,0.531,0.313)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	0.0000	0.4062	0.2500
ZD1	-0.5000	0.5000	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000
ZD2	0.7500	0.7500	0.5000
ZE2	1.0000	0.5938	0.7500

Circuit No 20; Type=8f; Centroid: (0.438,0.500,0.313)

Atom	x	y	z
ZD1	0.5000	0.5000	0.5000
ZE2	0.0000	0.4062	0.2500
ZD2	-0.2500	0.2500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000
ZD2	0.7500	0.7500	0.5000
ZE2	1.0000	0.5938	0.7500

Circuit No 21; Type=8g; Centroid: (0.250,0.762,0.531)

Atom	x	y	z
ZD2	-0.2500	0.7500	0.5000
ZE1	-0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.5000
ZE1	0.5000	1.0000	0.5000
ZD2	0.7500	0.7500	0.5000
ZE2	1.0000	0.5938	0.7500
ZD1	0.5000	0.5000	0.5000
ZE1	0.0000	0.5000	0.5000

Circuit No 22; Type=8h; Centroid: (0.250,0.750,0.500)

Atom	x	y	z
ZD2	-0.2500	0.7500	0.5000
ZE1	-0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.5000
ZE1	0.5000	1.0000	0.5000
ZD2	0.7500	0.7500	0.5000
ZE1	1.0000	0.5000	0.5000

ZD1 0.5000 0.5000 0.5000
 ZE1 0.0000 0.5000 0.5000

Circuit No 23; Type=8i; Centroid: (0.250,0.750,0.000)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.0000
ZE1	-0.5000	1.0000	-0.5000
ZD2	-0.2500	0.7500	-0.5000
ZE1	0.0000	0.5000	-0.5000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
* 1	ZD2	0.2500	0.7500	0.0000	ZE2	0.0000	0.5938	-0.2500	5.991	4e/1 6c/1 8b/1 8d/1 8f
* 1	ZD2	0.2500	0.7500	0.0000	ZE2	0.5000	0.9062	0.2500	5.991	4e/1 6c/1 8b/1 8d/1 8f
* 2	ZD2	0.2500	0.7500	0.0000	ZE1	0.0000	0.5000	0.0000	7.927	4e/1 6c/1 8b/1 8d/1 8f
* 2	ZD2	0.2500	0.7500	0.0000	ZE1	0.5000	1.0000	0.0000	7.927	4e/1 6c/1 8b/1 8d/1 8f

Circuit No 24; Type=8j; Centroid: (0.250,0.762,0.031)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.0000
ZE1	-0.5000	1.0000	-0.5000
ZD2	-0.2500	0.7500	-0.5000
ZE2	0.0000	0.5938	-0.2500
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Crossed with bonds

No	Atom	x	y	z	Atom	x	y	z	Dist.	N Cycles
* 2	ZD2	0.2500	0.7500	0.0000	ZE1	0.0000	0.5000	0.0000	7.927	8i/1 8i/1 8j/1 8j/1 8j

Circuit No 25; Type=8k; Centroid: (0.438,0.750,0.188)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.0000
ZE2	0.5000	0.9062	0.2500
ZD2	0.2500	0.7500	0.0000
ZE2	0.0000	0.5938	-0.2500
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Circuit No 26; Type=8l; Centroid: (0.563,0.750,0.250)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	1.0000	1.0000	0.5000
ZE2	0.5000	0.9062	0.2500
ZD2	0.2500	0.7500	0.0000
ZE2	0.0000	0.5938	-0.2500
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Circuit No 27; Type=8m; Centroid: (0.438,0.762,0.156)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.0000
ZE1	0.5000	1.0000	0.0000
ZD2	0.2500	0.7500	0.0000
ZE2	0.0000	0.5938	-0.2500
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Circuit No 28; Type=8n; Centroid: (0.563,0.762,0.219)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	1.0000	1.0000	0.5000
ZE1	0.5000	1.0000	0.0000
ZD2	0.2500	0.7500	0.0000
ZE2	0.0000	0.5938	-0.2500
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Circuit No 29; Type=8o; Centroid: (0.438,0.738,0.219)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.0000
ZE2	0.5000	0.9062	0.2500
ZD2	0.2500	0.7500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Circuit No 30; Type=8p; Centroid: (0.563,0.738,0.281)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	1.0000	1.0000	0.5000
ZE2	0.5000	0.9062	0.2500
ZD2	0.2500	0.7500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Circuit No 31; Type=8q; Centroid: (0.438,0.738,0.281)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.0000
ZE2	0.5000	0.9062	0.2500
ZD2	0.2500	0.7500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.5000
ZE1	1.0000	0.5000	0.5000

Circuit No 32; Type=8r; Centroid: (0.563,0.738,0.344)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	1.0000	1.0000	0.5000
ZE2	0.5000	0.9062	0.2500
ZD2	0.2500	0.7500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.5000
ZE1	1.0000	0.5000	0.5000

Circuit No 33; Type=8s; Centroid: (0.438,0.750,0.188)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	0.0000	1.0000	0.0000
ZE1	0.5000	1.0000	0.0000
ZD2	0.2500	0.7500	0.0000
ZE1	0.0000	0.5000	0.0000
ZD1	0.5000	0.5000	0.0000
ZE1	1.0000	0.5000	0.5000

Circuit No 34; Type=8t; Centroid: (0.563,0.750,0.250)

Atom	x	y	z
ZD2	0.7500	0.7500	0.5000
ZE1	0.5000	1.0000	0.5000
ZD1	1.0000	1.0000	0.5000
ZE1	0.5000	1.0000	0.0000
ZD2	0.2500	0.7500	0.0000

```
ZE1 0.0000 0.5000 0.0000
ZD1 0.5000 0.5000 0.0000
ZE1 1.0000 0.5000 0.5000
```

Circuit No 35; Type=8u; Centroid: (0.250,0.500,0.625)

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-----
Atom      x      y      z
-----
ZE1      0.0000  0.5000  0.5000
ZD2      0.2500  0.2500  0.5000
ZE2      0.0000  0.4062  0.2500
ZD1      0.5000  0.5000  0.5000
ZE1      1.0000  0.5000  1.0000
ZD1      0.5000  0.5000  1.0000
ZE2      0.0000  0.5938  0.7500
ZD2     -0.2500  0.7500  0.5000
```

Circuit No 36; Type=8v; Centroid: (0.344,0.430,0.750)

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-----
Atom      x      y      z
-----
ZE1      0.0000  0.5000  0.5000
ZD2      0.2500  0.2500  0.5000
ZE2      0.5000  0.0938  0.7500
ZD2      0.7500  0.2500  1.0000
ZE1      1.0000  0.5000  1.0000
ZD1      0.5000  0.5000  1.0000
ZE2      0.0000  0.5938  0.7500
ZD2     -0.2500  0.7500  0.5000
```

Ring links

```
-----
Cycle 1 | Cycle 2 | Chain | Cross | Link | Hopf | Mult
-----
8i | 8i | 1 | 1 | 1 | * | 2
8i | 8j | 1 | 1 | 1 | * | 4
8j | 8i | 1 | 1 | 1 | * | 2
8j | 8j | 1 | 1 | 1 | * | 3
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```

Elapsed time: 30.02 sec.