```
#############
12:kate1ideal
#############

Structure consists of molecules (ZD1). The composition of molecule is O
Structure consists of molecules (ZE1). The composition of molecule is Si
Topology for ZD1
--------------------
Atom ZD1 links by bridge ligands and has
Common vertex with                          R(A-A)       f Total SA
ZE 1    0.0774    0.2769    0.0647   ( 0 0 0)    0.999A       1  14.99
ZE 1    0.2231    0.4226    0.0647   ( 0 0-1)    0.999A       1  14.99
ZE 1    0.2769    0.0774    0.5647   ( 0 0 0)    0.999A       1  15.18
ZE 1    0.4226    0.2231    0.5647   ( 0 0 0)    0.999A       1  15.18
ZE 1   -0.0774    0.2769    0.5647   ( 0 0 0)    1.001A       1  19.84
ZE 1    0.2231    0.5774    0.5647   ( 0 0 0)    1.001A       1  19.84
Topology for ZE1
--------------------
Atom ZE1 links by bridge ligands and has
Common vertex with                          R(A-A)       f Total SA
ZD 1    0.1804    0.3196    0.4229   ( 0 0 0)    0.999A       1  29.97
ZD 1    0.3196    0.1804   -0.0771   ( 0 0-1)    0.999A       1  30.35
ZD 1   -0.1804    0.3196   -0.0771   ( 0 0-1)    1.001A       1  39.68
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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 ZE2ZD

Coordination sequences
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ZD1:  1  2  3  4   5   6   7   8   9   10
Num   6 10 38 36 106  80 210 140 346  218
Cum   7 17 55 91 197 277 487 627 973 1191
Rad 1.0(0.0) 1.8(0.2) 2.3(0.3) 3.0(0.4) 3.6(0.4) 4.4(0.4) 5.0(0.5) 5.8(0.5) 6.4(0.5) 7.2(0.5)
Cmp ZE6 ZD10 ZE38 ZD36 ZE106 ZD80 ZE210 ZD140 ZE346 ZD218
----------------------
ZE1:  1  2  3   4   5   6   7   8   9   10
Num   3 14 19  64  53 148 105 268 173  420
Cum   4 18 37 101 154 302 407 675 848 1268
Rad 1.0(0.0) 1.6(0.3) 2.3(0.4) 2.8(0.4) 3.6(0.4) 4.2(0.5) 5.0(0.5) 5.6(0.5) 6.4(0.5) 7.0(0.6)
Cmp ZD3 ZE14 ZD19 ZE64 ZD53 ZE148 ZD105 ZE268 ZD173 ZE420
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TD10=1242

Vertex symbols for selected sublattice
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ZD1 Point (Schlafli) symbol:{4^2;6^10;8^3}
Extended point symbol:[4.4.6.6.6.6.6.6.6.6.6(2).6(2).8(4).8(4).8(8)]
Vertex symbol: [4.4.6.6.6.6.6.6.6.6.6(2).6(2).8(2).8(2).8(7)]
All rings (up to 10):
[(4,8(4)).(4,8(3)).(6,10(2)).6.6.(6,10(2)).(6,8,10(5)).(6,10).(6,10).(6,8,10(5)).(6(2),8,10).(6(2),8,10).(8(2),10).(8(2),10).8(7)]

ZE1 Point (Schlafli) symbol:{4;6^2}
Extended point symbol:[4.6(2).6(2)]
Rings coincide with circuits
All rings (up to 10): [(4,6(2),10(2)).(6(2),8(7),10(2)).(6(2),8(4),10(6))]

Point (Schlafli) symbol for net: {4;6^2}2{4^2;6^10;8^3}
3,6-c net with stoichiometry (3-c)2(6-c); 2-nodal net

Topological type: scu/P 4/m m m->I 4 c m (-2b,2a,2c; 1/2,1/2,0);Bond sets: 2,3,4:scu
{4;6^2}2{4^2;6^10;8^3} - VS [4.6(2).6(2)] [4.4.6.6.6.6.6.6.6.6.6(2).6(2).8(2).8(2).8(7)]
(66909 types in 9 databases)
Elapsed time: 248.91 sec.

##############
11:kate2ideal
##############

Structure consists of molecules (ZD1). The composition of molecule is O
Topology for ZD1

Atom ZD1 links by bridge ligands and has

Common vertex with					R(A-A)	f	Total SA
ZE 1	0.0000	0.1925	-0.2142	(-1 0-1)	0.999A	1	18.64
ZE 1	0.5000	0.3075	0.2858	(0 0 0)	0.999A	1	20.18
ZE 1	-0.5000	0.3075	0.2858	(-1 0 0)	0.999A	1	20.18
ZD 1	0.0000	0.5772	-0.3808	(0 1-1)	1.002A	1	20.50
ZD 1	0.0000	0.5772	0.6192	(0 1 0)	1.002A	1	20.50

Topology for ZE1

Atom ZE1 links by bridge ligands and has

Common vertex with					R(A-A)	f	Total SA
ZD 1	0.5000	0.0772	0.6192	(0 0 0)	0.999A	1	31.60
ZD 1	1.0000	0.4228	0.1192	(1 0 0)	0.999A	1	34.20
ZD 1	0.0000	0.4228	0.1192	(0 0 0)	0.999A	1	34.20

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZEZD

Coordination sequences

ZD1: 1 2 3 4 5 6 7 8 9 10
Num 5 14 30 55 82 114 165 210 254 335
Cum 6 20 50 105 187 301 466 676 930 1265
Rad 1.0(0.0) 1.7(0.2) 2.2(0.3) 2.9(0.4) 3.6(0.4) 4.3(0.5) 5.0(0.5) 5.7(0.6) 6.4(0.6) 7.1(0.7)
Cmp ZD2ZE3 ZD8ZE6 ZD18ZE12 ZD24ZE31 ZD42ZE40 ZD66ZE48 ZD74ZE91 ZD104ZE106 ZD146ZE108 ZD152ZE183

ZE1: 1 2 3 4 5 6 7 8 9 10
Num 3 12 28 47 80 120 147 202 276 303
Cum 4 16 44 91 171 291 438 640 916 1219
Rad 1.0(0.0) 1.5(0.2) 2.2(0.4) 2.8(0.4) 3.5(0.4) 4.2(0.4) 4.9(0.5) 5.6(0.5) 6.3(0.6) 7.0(0.6)
Cmp ZD3 ZD6ZE6 ZD12ZE16 ZD31ZE16 ZD40ZE40 ZD48ZE72 ZD91ZE56 ZD106ZE96 ZD108ZE168 ZD183ZE120

TD10=1242

Vertex symbols for selected sublattice

ZD1 Point (Schlafli) symbol:{6^9;8}
Extended point symbol:[6.6.6.6(2).6(2).6(2).6(2).6(2).6(2).8(4)]
Vertex symbol: [6.6.6.6(2).6(2).6(2).6(2).6(2).6(2).*]
All rings (up to 14): coincide with rings
All rings with types: [6a.6c.6c.(6a,6b).(6a,6b).6b(2).(6b,6c).(6b,6c).6b(2).*]
ATTENTION! Some rings * are bigger than 14, so likely no rings are contained in that angle
---
ZE1 Point (Schlafli) symbol:{6^3}
Extended point symbol:[6(3).6(3).6(3)]
Rings coincide with circuits
All rings (up to 14): coincide with rings
All rings with types: [(6a,6b(2)).(6a,6b(2)).(6a,6c(2))]

Point (Schlafli) symbol for net: {6^3}{6^9;8}
3,5-c net with stoichiometry (3-c)(5-c); 2-nodal net

Topological type: seh-3,5-Cmc21 {6^3}{6^9;8} - VS [6.6.6.6(2).6(2).6(2).6(2).6(2).6(2).*] [6(3).6(3).6(3)] (66909 types in 9 databases)

Non-equivalent circuits

Circuit No 1; Type=6a; Centroid: (0.500,0.269,0.953)

Atom	x	y	z
ZD1	0.0000	0.4228	1.1192
ZE1	0.0000	0.1925	0.7858
ZD1	0.5000	0.0772	0.6192
ZE1	1.0000	0.1925	0.7858

ZD1 1.0000 0.4228 1.1192
ZE1 0.5000 0.3075 1.2858

Circuit No 2; Type=6b; Centroid: (0.333,0.167,0.091)

Atom	x	y	z
ZD1	0.0000	0.4228	0.1192
ZE1	0.0000	0.1925	-0.2142
ZD1	0.5000	0.0772	-0.3808
ZD1	0.5000	-0.0772	0.1192
ZD1	0.5000	0.0772	0.6192
ZE1	0.5000	0.3075	0.2858

Circuit No 3; Type=6c; Centroid: (0.500,0.500,0.925)

Atom	x	y	z
ZE1	0.5000	0.3075	1.2858
ZD1	1.0000	0.4228	1.1192
ZD1	1.0000	0.5772	0.6192
ZE1	0.5000	0.6925	0.7858
ZD1	0.0000	0.5772	0.6192

Elapsed time: 10.22 sec.

Structure #1 - "MOFCJ3".

Structure of dimension 3.
Given space group is I4cm.
12 nodes and 24 edges in repeat unit as given.

Given repeat unit is accurate.
Point group has 8 elements.
2 kinds of node.

Coordination sequences:
Node 1: 3 14 19 64 53 148 105 268 173 420
Node 2: 6 10 38 36 106 80 210 140 346 218

TD10 = 1242.3333

Ideal space group is I4cm.

Structure is new for this run.

Relaxed cell parameters:

a = 3.57081, b = 3.57081, c = 2.55967
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 32.63757
Relaxed positions:
Node 1: 0.07703 0.27682 0.23067
Node 2: 0.31936 0.18064 0.08842
Edges:
0.07703 0.27682 0.23067 <-> 0.18064 0.31936 0.58842
0.07703 0.27682 0.23067 <-> 0.31936 0.18064 0.08842
0.07703 0.27682 0.23067 <-> -0.18064 0.31936 0.08842
Edge centers:
0.12884 0.29809 0.40954
0.19820 0.22873 0.15954
-0.05180 0.29809 0.15954

Edge statistics: minimum = 0.99924, maximum = 1.00113, average = 1.00000
Angle statistics: minimum = 43.32442, maximum = 135.65923, average = 106.63495
Shortest non-bonded distance = 0.73799

Degrees of freedom: 6

Finished structure #1 - "MOFCJ3".

Finished data file "/Applications/Che/systre/MOFCJ3.cgd".

Data file "/Applications/Che/systre/katezn1.cgd".

Structure #1 - "kateZn1".

Structure of dimension 3.
Given space group is Cmc21.
24 nodes and 48 edges in repeat unit as given.

Ideal repeat unit smaller than given (24 vs 48 edges).
Point group has 8 elements.
2 kinds of node.

Equivalences for non-unique nodes:
2 --> 1
3 --> 1
4 --> 1
6 --> 5
7 --> 5

Coordination sequences:
Node 5: 6 10 38 36 106 80 210 140 346 218
Node 1: 3 14 19 64 53 148 105 268 173 420

TD10 = 1242.3333

Ideal space group is I4cm.
Ideal group differs from given (I4cm vs Cmc21).

Structure already seen in this run.
Name: MOFCJ3

Relaxed cell parameters:
a = 3.57099, b = 3.57099, c = 2.55944
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 32.63792
Relaxed positions:
Node 5: 0.18065 0.31935 0.25059
Node 1: 0.27654 0.07695 0.39293
Edges:
0.18065 0.31935 0.25059 <-> 0.07695 0.27654 -0.10707
0.18065 0.31935 0.25059 <-> 0.27654 0.07695 0.39293
0.18065 0.31935 0.25059 <-> 0.22346 0.57695 0.39293
Edge centers:
0.12880 0.29794 0.07176
0.22860 0.19815 0.32176
0.20206 0.44815 0.32176

Edge statistics: minimum = 0.99924, maximum = 1.00116, average = 1.00000
Angle statistics: minimum = 43.44165, maximum = 135.67105, average = 106.63958

Shortest non-bonded distance = 0.73987

Degrees of freedom: 6

Finished structure #1 - "kateZn1".

Finished data file "/Applications/Che/systre/katezn1.cgd".

Data file "/Applications/Che/systre/katezn2.cgd".

Structure #1 - "kateZn2".

Structure of dimension 3.
Given space group is P21.
4 nodes and 8 edges in repeat unit as given.

Given repeat unit is accurate.
Point group has 4 elements.
2 kinds of node.

Coordination sequences:
Node 2: 3 12 28 47 80 120 147 202 276 303
Node 1: 5 14 30 55 82 114 165 210 254 335

TD10 = 1242.0000

Ideal space group is Cmc21.
Ideal group differs from given (Cmc21 vs P1211).

Structure is new for this run.

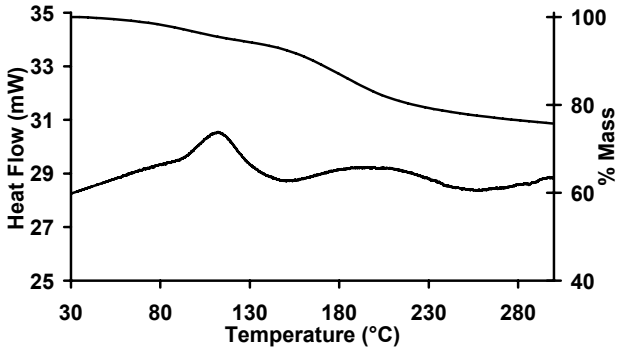
Relaxed cell parameters:
a = 1.73055, b = 3.60698, c = 1.66591
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 10.39874
Relaxed positions:
Node 2: 0.50000 0.30752 0.28583
Node 1: 0.00000 0.42283 0.11919
Edges:
0.00000 0.42283 0.11919 <-> 0.50000 0.30752 0.28583
0.00000 0.42283 0.11919 <-> 0.00000 0.19248 -0.21417
0.00000 0.42283 0.11919 <-> 0.00000 0.57717 -0.38081
Edge centers:
0.25000 0.36518 0.20251
0.00000 0.30765 -0.04749
0.00000 0.50000 -0.13081

Edge statistics: minimum = 0.99937, maximum = 1.00186, average = 1.00000
Angle statistics: minimum = 78.95149, maximum = 157.51507, average = 108.68836
Shortest non-bonded distance = 1.27072

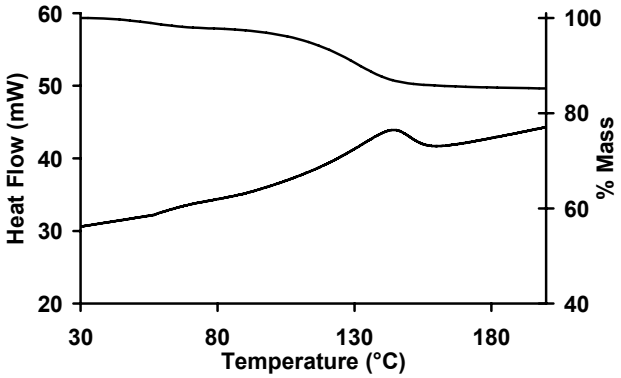
Degrees of freedom: 6

Finished structure #1 - "kateZn2".

Finished data file "/Applications/Che/systre/katezn2.cgd".



TG and DSC curves for **1**.



TG and DSC curves for **2**.