Supporting Information

Tuning Structural Topologies of FourNi(II) Coordination Polymers Through Modifying the Substitute Group of Organic Ligand

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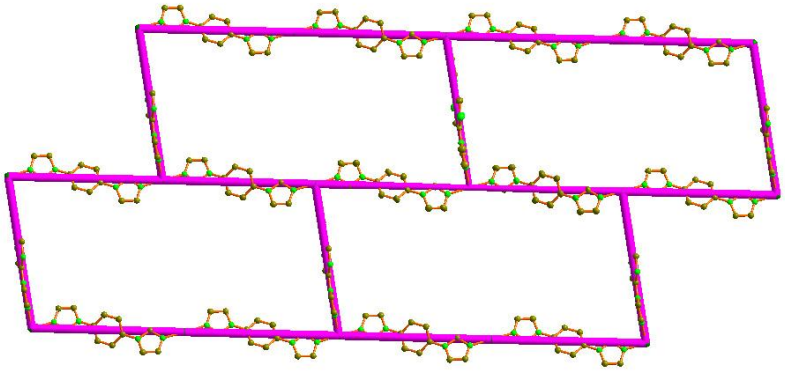


Fig.S1 The 2D hcb layer structure formed by L_1 ligands in 2

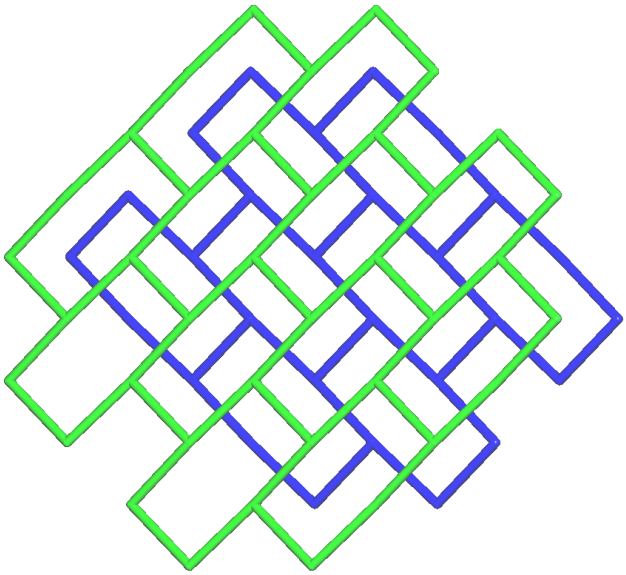


Fig. S2 the hcb layers adopt AB packed mode in 2

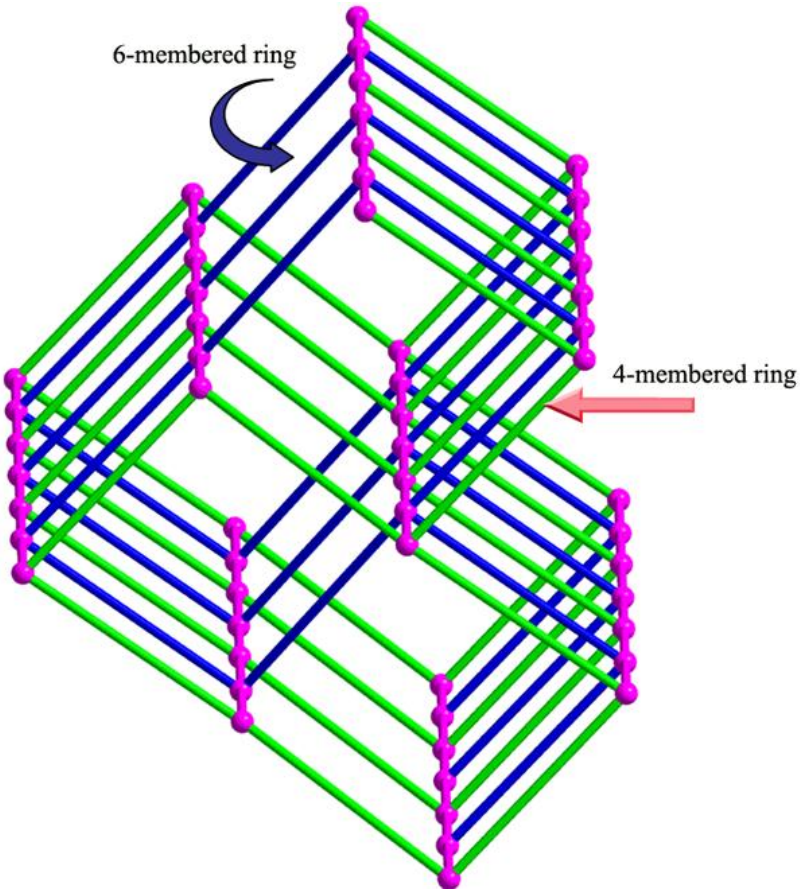


Fig. S3. Four- and six-membered rings in 2

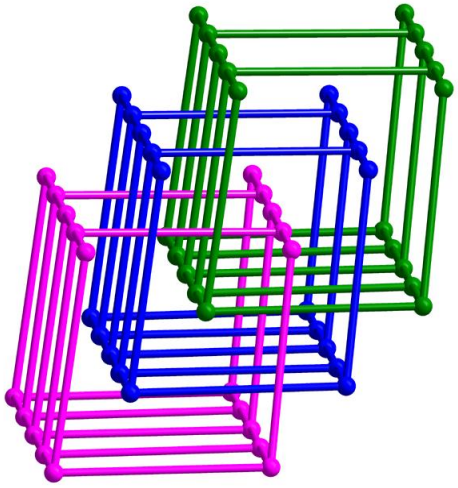


Fig.S4, the interpenetrating mode in 2

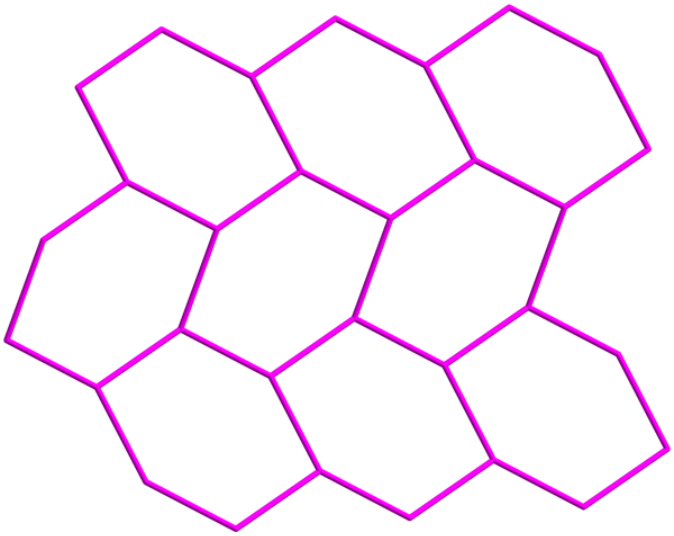


Fig.S5 the 2D hcb layer in 3

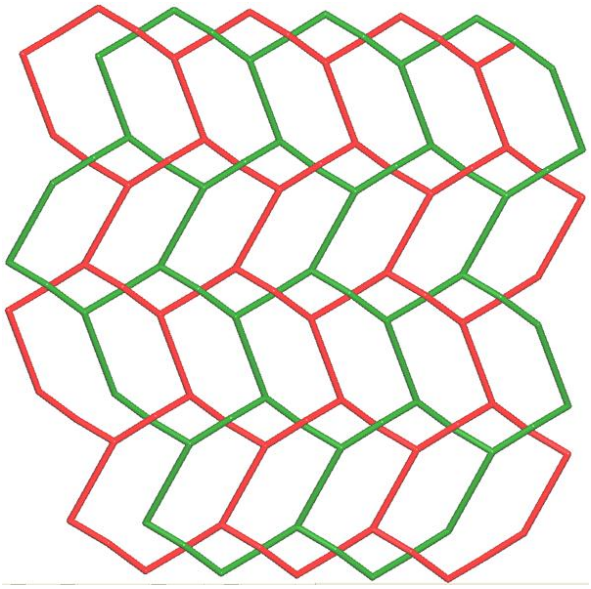


Fig. S6 The two-fold hcb topological net in 3

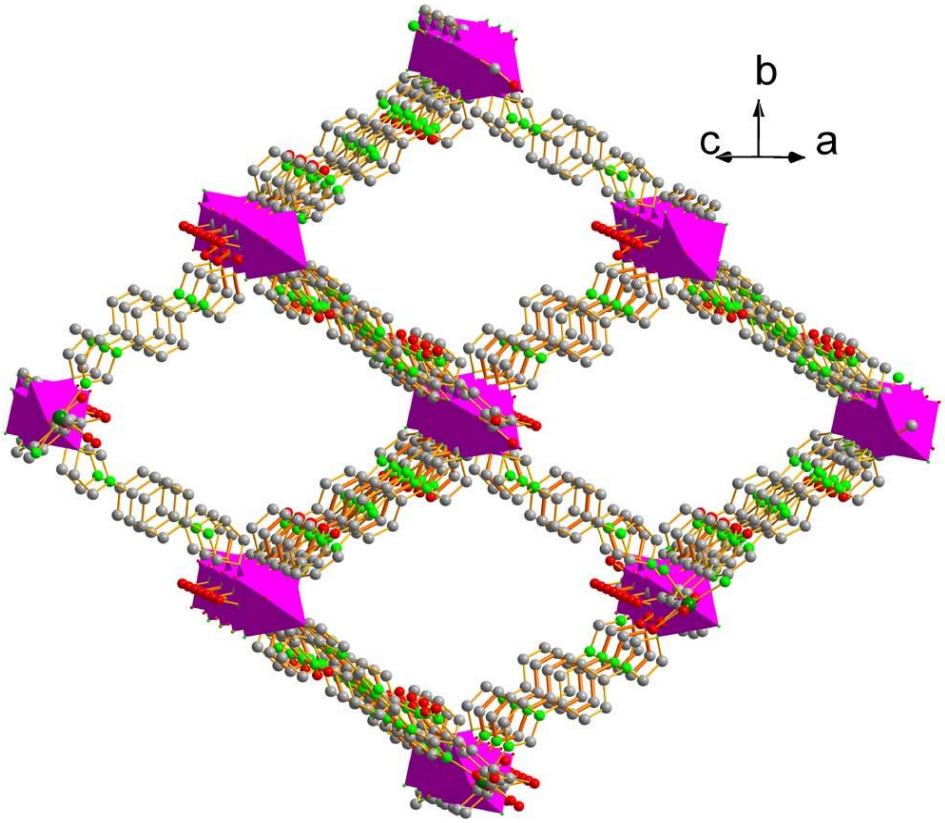


Fig. S7 The 3D structure for complex 3.

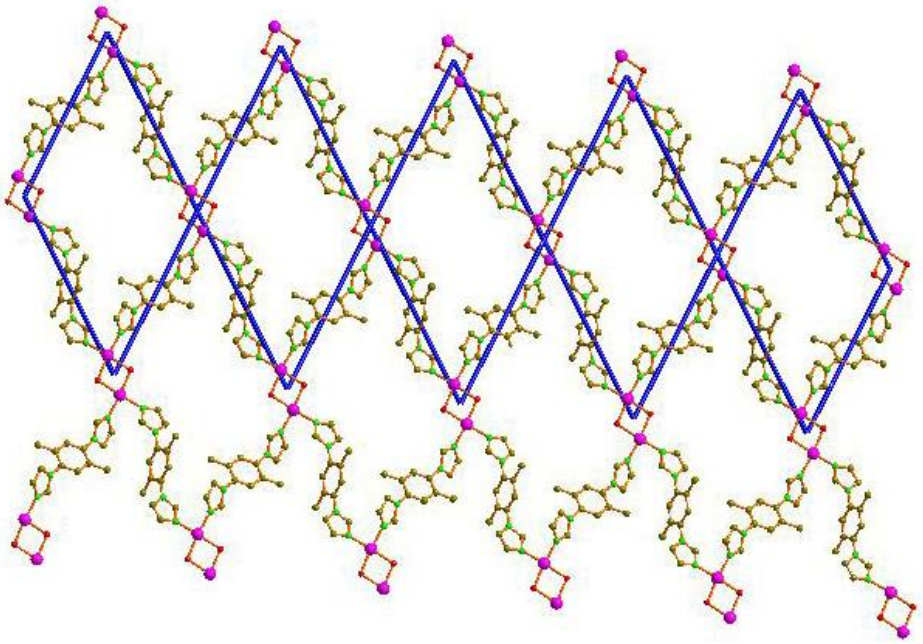
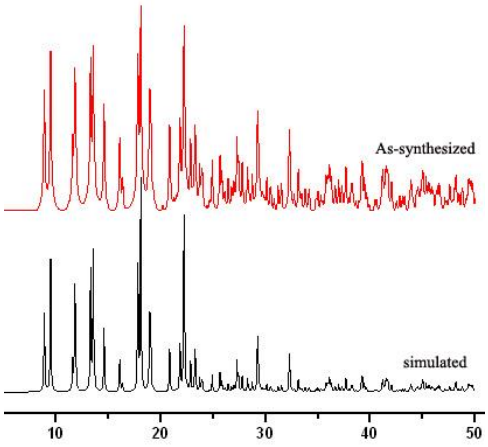
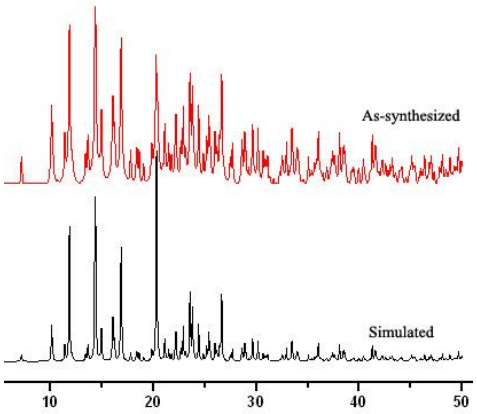


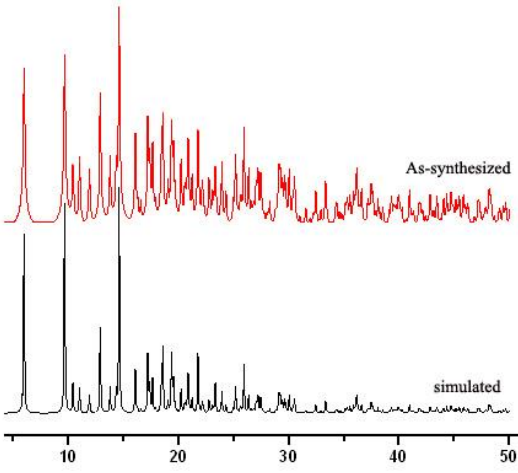
Fig. S8 The 2D layer formed by the L2 ligands and bridging coordination water molecules.



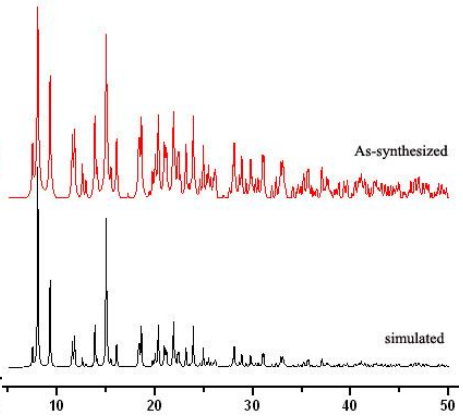
(a)



(b)



(c)



(d)

Fig.S9XRPD for complexes (a) complex 1; (b) complex 2; (c) complex 3; (d) complex 4.

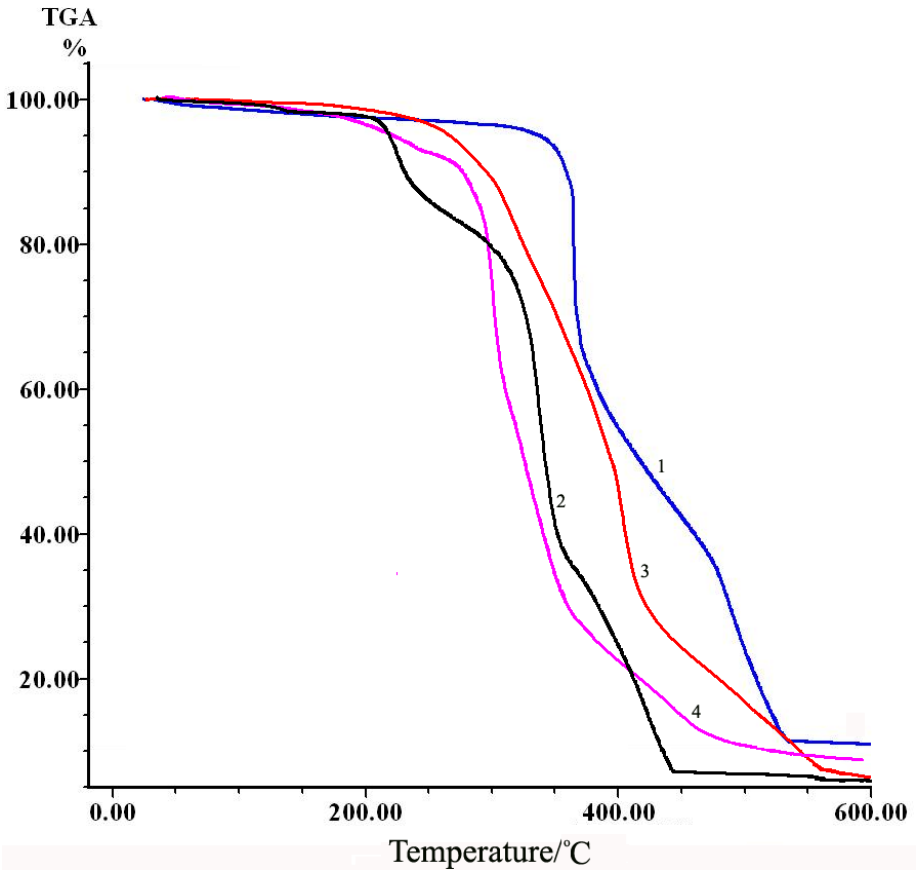


Fig. S10 The TG curves for complexes 1-4.

Table S1. Selected bond lengths (Å) and angles (°) for Complexes 1-4

Compound 1			
Ni(1)—O(1)	2.0411 (11)	Ni(1)—O(4A)^{i}	2.1054 (11)
Ni(1)—N(1)	2.0596 (13)	Ni(1)—O(5)	2.1173 (12)
Ni(1)—N(3)	2.0797 (14)	Ni(1)—O(3A)^{i}	2.1606 (11)
O(1)—Ni(1)—N(1)	92.91 (5)	O(4)^{i}—Ni(1)—O(5)	167.67 (5)
O(1)—Ni(1)—N(3)	87.79 (5)	O(1)—Ni(1)—O(3A)^{i}	157.84 (4)
N(1)—Ni(1)—N(3)	178.21 (5)	N(1)—Ni(1)—O(3A)^{i}	90.76 (5)
O(1)—Ni(1)—O(4A)^{i}	95.91 (4)	N(3)—Ni(1)—O(3A)^{i}	89.21 (5)
N(1)—Ni(1)—O(4A)^{i}	93.77 (5)	O(4A)^{i}—Ni(1)—O(3A)^{i}	62.03 (4)
N(3)—Ni(1)—O(4A)^{i}	87.80 (5)	O(5)—Ni(1)—O(3A)^{i}	106.20 (5)
O(1)—Ni(1)—O(5)	95.66 (5)	N(3)—Ni(1)—O(5)	88.41 (5)
N(1)—Ni(1)—O(5)	89.87 (5)		
Compound 2			
Ni(1)—O(4A)^{i}	2.0561 (16)	Ni(1)—N(3)	2.0715 (18)
Ni(1)—O(1)	2.0616 (15)	Ni(1)—N(1)	2.0936 (18)
Ni(1)—N(7)	2.0711 (17)	Ni(1)—O(7)	2.1331 (18)
O(4A)^{i}—Ni(1)—O(1)	178.26 (6)	N(3)—Ni(1)—N(1)	92.36 (7)
O(4A)^{i}—Ni(1)—N(7)	87.81 (7)	O(4A)^{i}—Ni(1)—O(7)	89.78 (8)
O(1)—Ni(1)—N(7)	91.90 (7)	O(1)—Ni(1)—O(7)	91.92 (7)
O(4A)^{i}—Ni(1)—N(3)	92.75 (7)	N(7)—Ni(1)—O(7)	87.14 (8)
O(1)—Ni(1)—N(3)	87.61 (7)	N(3)—Ni(1)—O(7)	90.49 (8)
N(7)—Ni(1)—N(3)	177.56 (7)	N(1)—Ni(1)—O(7)	177.12 (7)
O(4A)^{i}—Ni(1)—N(1)	90.57 (8)	N(7)—Ni(1)—N(1)	90.01 (7)
O(1)—Ni(1)—N(1)	87.71 (7)		
Compound 3			
Ni(1)—O(1)	2.0283 (12)	Ni(1)—N(3)	2.0850 (15)
Ni(1)—N(6A)^{i}	2.0605 (14)	Ni(1)—O(3A)^{ii}	2.1788 (12)
Ni(1)—N(1)	2.0733 (15)	Ni(1)—O(4A)^{ii}	2.2014 (14)
O(1)—Ni(1)—N(6A)^{i}	95.23 (6)	O(1)—Ni(1)—O(4A)^{ii}	101.07 (5)
O(1)—Ni(1)—N(1)	88.87 (6)	N(6A)^{i}—Ni(1)—O(4A)^{ii}	87.50 (6)
N(6A)^{i}—Ni(1)—N(1)	172.95 (6)	N(1)—Ni(1)—O(4A)^{ii}	86.08 (6)
O(1)—Ni(1)—N(3)	105.52 (6)	N(3)—Ni(1)—O(4A)^{ii}	152.94 (5)
N(6A)^{i}—Ni(1)—N(3)	94.98 (6)	O(3)^{ii}—Ni(1)—O(4A)^{ii}	60.19 (4)
N(1)—Ni(1)—N(3)	89.43 (6)	N(1)—Ni(1)—O(3A)^{ii}	87.77 (5)
O(1)—Ni(1)—O(3A)^{ii}	161.15 (5)	N(3)—Ni(1)—O(3A)^{ii}	93.00 (5)
N(6A)^{i}—Ni(1)—O(3)^{ii}	86.51 (5)		
Compound 4			
Ni(1)—O(1)	2.0175(12)	Ni(1)—N(3)	2.1073(16)
Ni(1)—O(4A)^{i}	2.0206(12)	Ni(1)—O(7)	2.1295(13)
Ni(1)—N(1)	2.0547(15)	Ni(1)—O(7A)^{ii}	2.1795(13)
O(1)—Ni(1)—O(4A)^{i}	179.11 (5)	O(1)—Ni(1)—O(7A)^{ii}	89.98 (6)

O(1)—Ni(1)—N(1)	89.37 (5)	O(4A)^{i}—Ni(1)—O(7A)^{ii}	89.13 (5)
O(4A)^{i}—Ni(1)—N(1)	90.49 (5)	N(1)—Ni(1)—O(7A)^{ii}	94.32 (6)
O(1)—Ni(1)—N(3)	90.11 (6)	N(3)—Ni(1)—O(7A)^{ii}	176.50 5)
O(4A)^{i}—Ni(1)—N(3)	90.76 (6)	O(7)—Ni(1)—O(7A)^{ii}	78.76 (6)
N(1)—Ni(1)—N(3)	89.18 (6)	N(1)—Ni(1)—O(7)	172.95 (6)
O(1)—Ni(1)—O(7)	89.29 (5)	N(3)—Ni(1)—O(7)	97.75 (6)
O(4A)^{i}—Ni(1)—O(7)	90.75 (5)		

Symmetry codes: 1: (i) *x*−1, *y*, *z*; 2: (i) *x*−1, −*y*+1/2, *z*−1/2; 3: (i) −*x*, *y*+1, −*z*+1/2; (ii) *x*−1/2, *y*−1/2; z; 4: (i) *x*−1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+1/2, −*y*+1/2, −*z*;

Topological analysis for complex 2:

####################
1:C20 N5 Ni2.50 O10
####################
Topology for Ni1

Atom Ni1 links by bridge ligands and has
Common vertex with R(A-A)

Ni 1	1.7997	0.2516	1.2621	(1 0 0)	11.022A	1
Ni 1	-0.2003	0.2516	0.2621	(-1 0-1)	11.022A	1
Ni 1	1.2003	-0.2484	0.2379	(2 0 1)	13.545A	1
Ni 1	0.2003	-0.2484	1.2379	(1 0 2)	13.657A	1
Ni 1	0.2003	0.7516	1.2379	(1 1 2)	13.727A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Ni
There are 3 interpenetrating nets
FIV: Full interpenetration vectors

[1,0,0] (8.40A)

PIC: [3,0,0][0,1,0][1,0,-1] (PICVR=3)
Zt=3; Zn=1
Class Ia Z=3
Coordination sequences

Ni1:	1	2	3	4	5	6	7	8	9	10
Num	5	16	35	62	98	142	194	254	322	398
Cum	6	22	57	119	217	359	553	807	1129	1527

TD10=1527
Vertex symbols for selected sublattice

Ni1 Point (Schlafli) symbol:{4^4.6^6}
Extended point symbol:[4.4.4.4.6.6(3).6(5).6(5).6(5).6(5)]

Point (Schlafli) symbol for net: {4^4.6^6}
5-c net; uninodal net
ATTENTION! If the name below is written in a long notation s/... or s-d-G-n, this net is a subnet of the net s (see Manual for details)
Topological type: pcu/P m -3 m->P b c n (a-b,-2c,2a+2b; 1/2,0,0);Bond sets: 2,3,4,5:pcu (uninodal.ttd) {4^4.6^6} - VS [4.4.4.4.6.6.6(3).6(5).6(5).6(5)] (71251 types in 10 databases)
Elapsed time: 7.33 sec.

Systre for complex 2
Structure #1 - "C20 N5 Ni2.50 O10".
Structure of dimension 3.
Given space group is P21/c.
4 nodes and 10 edges in repeat unit as given.
Structure is not connected.
Processing components separately.
==========
Processing component 1:
multiplicity = 3
Structure of dimension 3.
Given space group is P1.
4 nodes and 10 edges in repeat unit as given.
Given repeat unit is accurate.
Point group has 8 elements.
1 kind of node.
Equivalences for non-unique nodes:
V2 --> V1
V3 --> V1
V4 --> V1
Coordination sequences:
Node V1: 5 16 35 62 98 142 194 254 322 398
TD10 = 1527.0000
Ideal space group is Pmna.
Ideal group differs from given (Pmna vs P1).
Structure is new for this run.
Relaxed cell parameters:
a = 1.99713, b = 1.42194, c = 1.42227
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 4.03897

Relaxed positions:

Node V1: 0.00000 0.24647 0.25352

Edges:

0.00000 0.24647 0.25352 <-> 0.50000 0.24647 0.24648

0.00000 0.24647 0.25352 <-> -0.00000 0.75353 0.74648

0.00000 0.24647 0.25352 <-> -0.00000 -0.24647 0.74648

0.00000 0.24647 0.25352 <-> -0.00000 -0.24647 -0.25352

Edge centers:

0.25000 0.24647 0.25000

0.00000 0.50000 0.50000

0.00000 0.00000 0.50000

0.00000 0.00000 0.00000

Edge statistics: minimum = 0.99141, maximum = 1.00571, average = 1.00000

Angle statistics: minimum = 89.58849, maximum = 178.85225, average = 107.96411

Shortest non-bonded distance = 1.01976

Degrees of freedom: 5

Finished component 1.

Finished structure #1 - "C20 N5 Ni2.50 O10".

Toplogical analysis for complex 3

##################

1:C30 H27 N6 Ni O4

##################

Topology for Ni1

Atom Ni1 links by bridge ligands and has

Common vertex with					R(A-A)	
Ni 1	-0.4792	0.4963	0.1376	(-1-1 0)	10.225A	1
Ni 1	0.5208	1.4963	0.1376	(0 0 0)	10.225A	1
Ni 1	-0.0208	-0.0037	0.3624	(0-1 0)	12.922A	1
Ni 1	-0.0208	1.9963	0.3624	(0 1 0)	12.922A	1
Ni 1	0.4792	0.5037	-0.1376	(0 1 0)	13.595A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Ni

Coordination sequences

Ni1:	1	2	3	4	5	6	7	8	9	10
Num	5	18	52	108	176	258	358	474	606	754
Cum	6	24	76	184	360	618	976	1450	2056	2810

TD10=2810
Vertex symbols for selected sublattice

Ni1 Point (Schlafli) symbol:{4^2.6^8}
Extended point symbol:[4.4.6.6.6.6.6(2).6(2).6(2).6(3)]

Point (Schlafli) symbol for net: {4^2.6^8}
5-c net; uninodal net
New topology, please, contact the authors (71251 types in 10 databases)
Elapsed time: 7.92 sec.

Systre for complex 3
tructure #1 - "C30 H27 N6 Ni O4".
Structure of dimension 3.
Given space group is C2/c.
4 nodes and 10 edges in repeat unit as given.
Given repeat unit is accurate.
Point group has 8 elements.
1 kind of node.
Coordination sequences:
Node 1: 5 18 52 108 176 258 358 474 606 754
TD10 = 2810.0000
Ideal space group is Cccm.
Ideal group differs from given (Cccm vs C12/c1).
Structure is new for this run.
Relaxed cell parameters:
a = 1.82038, b = 0.82872, c = 3.11956
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 4.70609
Relaxed positions:
Node 1: 0.00000 0.00000 0.66063
Edges:
0.00000 0.00000 0.66063 <-> 0.00000 1.00000 0.83937
0.00000 0.00000 0.66063 <-> 0.00000 -0.00000 0.33937
0.00000 0.00000 0.66063 <-> 0.50000 -0.50000 0.66063
Edge centers:
0.00000 0.50000 0.75000
0.00000 -0.00000 0.50000
0.25000 -0.25000 0.66063
Edge statistics: minimum = 0.99884, maximum = 1.00219, average = 1.00000
Angle statistics: minimum = 69.89379, maximum = 180.00000, average = 108.00000
Shortest non-bonded distance = 0.55759

Degrees of freedom: 4

Finished structure #1 - "C30 H27 N6 Ni O4".

Toplogical analysis for complex 4

####################

2:C44 H36 N10 Ni2 O15

####################

Topology for Cr1

Atom Cr1 links by bridge ligands and has

Common vertex with					R(A-A)	
Cr 1	0.7500	0.2500	0.5000	(1 0 0)	9.674A	1
Cr 1	-0.2500	0.2500	-0.5000	(0 0-1)	9.674A	1
Cr 1	-0.2500	0.7500	-1.0000	(0 1-1)	15.642A	1
Cr 1	0.7500	-0.2500	1.0000	(1 0 1)	15.642A	1
Cr 1	0.2500	0.2500	-1.0000	(0 0-1)	16.465A	1
Cr 1	0.2500	0.2500	1.0000	(0 0 1)	16.465A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Cr

Coordination sequences

Cr1:	1	2	3	4	5	6	7	8	9	10
Num	6	22	56	110	182	272	380	506	650	812
Cum	7	29	85	195	377	649	1029	1535	2185	2997

TD10=2997

Vertex symbols for selected sublattice

Cr1 Point (Schlafli) symbol:{4^8.5^2.6^5}

Extended point symbol:[4.4.4.4.4.4.4.4.5(3).5(3).6(2).6(3).6(3).6(4).6(4)]

Point (Schlafli) symbol for net: {4^8.5^2.6^5}

6-c net; uninodal net

ATTENTION! If the name below is written in a long notation s/... or s-d-G-n, this net is a subnet of the net s (see Manual for details)

Topological type: bcu-x/ 14-conn;I m -3 m->C 2/c (-a-b,a-b,c; 0,1/2,0);Bond sets: 2,5,6:bcu-x (uninodal.ttd) {4^8.5^2.6^5} - VS [4.4.4.4.4.4.4.4.5(3).5(3).6.6.6(2).*.*] (71251 types in 10 databases)

Elapsed time: 8.16 sec.