

Electronic supplementary information (ESI)

Synthesis, structure, topology and magnetic properties of cobalt(II) coordination polymers with 2-nitrobiphenyl-4,4'-dicarboxylic acid and bis(pyridyl) ligands

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TOPOS outputs

Sc = Co₂(μ-COO)₂ for compound **1-3** and [Co₄(μ-COO)₆(μ-H₂O)₂] for **4**,

Ti = mononuclear Co₂ centers for **2**

Compound 1

Topology for Sc1

Atom Sc1 links by bridge ligands and has
Common vertex with

					R(A-A)	
Sc 1	0.5000	1.5000	0.0000	(0 1 0)	11.430A	1
Sc 1	0.5000	-0.5000	0.0000	(0-1 0)	11.430A	1
Sc 1	1.5000	1.5000	1.0000	(1 1 1)	15.743A	1
Sc 1	-0.5000	-0.5000	-1.0000	(-1-1-1)	15.743A	1
Sc 1	1.5000	0.5000	-1.0000	(1 0-1)	19.384A	1
Sc 1	-0.5000	0.5000	1.0000	(-1 0 1)	19.384A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Sc
There are 2 interpenetrating nets
FIV: Full interpenetration vectors

[1,0,0] (11.26A)

PIC: [2,0,0][0,1,0][1,0,1] (PICVR=2)

Zt=2; Zn=1

Class Ia Z=2

Coordination sequences

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-----
Sc1:  1  2  3  4  5  6  7  8  9 10
Num   6 18 38 66 102 146 198 258 326 402
Cum    7 25 63 129 231 377 575 833 1159 1561
-----
TD10=1561

Vertex symbols for selected sublattice
-----
Sc1 Point symbol:{4^12.6^3}
Extended point symbol:[4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]
-----
Point symbol for net: {4^12.6^3}
6-c net; uninodal net

Topological type: pcu alpha-Po primitive cubic; 6/4/c1; sqc1 (topos&RCSR.ttd) {4^12.6^3} - VS
[4.4.4.4.4.4.4.4.4.4.4.4.*.*] (72442 types in 11 databases)
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Compound 2

```
Topology for Sc1
-----
Atom Sc1 links by bridge ligands and has
Common vertex with
Sc 1   0.0000   0.0000   1.0000   ( 0 0 1)   R(A-A)   11.344A   1
Sc 1   0.0000   0.0000   0.0000   ( 0 0 0)   11.344A   1
Ti 1  -0.2500  -0.7500   0.5000  (-1-1 0)   14.730A   1
Ti 1   0.2500   0.7500   0.5000   ( 1 1 1)   14.730A   1
Sc 1   1.0000   0.0000   1.0000   ( 1 0 1)   19.193A   1
Sc 1  -1.0000   0.0000   0.0000  (-1 0 0)   19.193A   1
Topology for Ti1
-----
Atom Ti1 links by bridge ligands and has
Common vertex with
Ti 1   0.2500   0.2500   0.0000   ( 1 0 0)   R(A-A)   11.495A   1
Ti 1   1.2500   0.2500   1.0000   ( 2 0 1)   11.495A   1
Sc 1   0.5000  -0.5000   0.5000   ( 0-1 1)   14.730A   1
Sc 1   1.0000   1.0000   0.5000   ( 1 1 0)   14.730A   1
-----
Structural group analysis
-----

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Structural group No 1
-----
Structure consists of 3D framework with TiSc
There are 3 interpenetrating nets
FIV: Full interpenetration vectors
-----
[1/2,1/2,0] (14.14A)
[1/2,-1/2,0] (14.14A)
-----
PIC: [3/2,3/2,0][1,0,0][0,0,1] (PICVR=3)

Zt=3; Zn=1

Class Ia Z=3

Coordination sequences
-----
Sc1:  1  2  3  4  5  6  7  8  9 10
Num   6 18 42 76 120 174 238 312 396 490
Cum    7 25 67 143 263 437 675 987 1383 1873
-----
Ti1:  1  2  3  4  5  6  7  8  9 10
Num   4 12 32 62 106 156 220 290 374 464
Cum    5 17 49 111 217 373 593 883 1257 1721
-----
TD10=1797
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Vertex symbols for selected sublattice
-----
Sc1 Point symbol:{4^8.6^6.8}
Extended point symbol:[4.4.4.4.4.4.4.6(2).6(2).6(2).6(2).6(2).6(2).8(8)]
-----
Ti1 Point symbol:{4^4.6^2}
Extended point symbol:[4.4.4.4.6(2).6(4)]
-----
Point symbol for net: {4^4.6^2}{4^8.6^6.8}
4,6-c net with stoichiometry (4-c)(6-c); 2-nodal 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: tcj-4,6-Cccm-2 (binodal.ttd) {4^4.6^2}{4^8.6^6.8} - VS [4.4.4.4.6(2).8(36)]
[4.4.4.4.4.4.4.6.6.6.6.8(6).8(6).*] (72442 types in 11 databases)

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Compound 3

1) Considering only the organic bridges as linkers

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Topology for Sc1
-----
Atom Sc1 links by bridge ligands and has
Common vertex with
R(A-A)
Sc 1 0.5000 0.0000 0.0000 ( 1-1 0) 14.170A 1
Sc 1 0.5000 0.0000 1.0000 ( 1-1 1) 14.170A 1
Sc 1 0.5000 1.0000 0.0000 ( 1 0 0) 14.170A 1
Sc 1 0.5000 1.0000 1.0000 ( 1 0 1) 14.170A 1
Sc 1 1.5000 0.0000 1.0000 ( 2-1 1) 19.337A 1
Sc 1 1.5000 1.0000 1.0000 ( 2 0 1) 19.337A 1
Sc 1 -0.5000 1.0000 0.0000 ( 0 0 0) 19.337A 1
Sc 1 -0.5000 0.0000 0.0000 ( 0-1 0) 19.337A 1
Sc 1 1.5000 -1.5000 0.5000 ( 1-2 0) 22.034A 1
Sc 1 -0.5000 2.5000 0.5000 (-1 2 0) 22.034A 1
-----
Structural group analysis
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-----
Structural group No 1
-----
Structure consists of 3D framework with Sc

Coordination sequences
-----
Sc1: 1 2 3 4 5 6 7 8 9 10
Num 10 60 168 330 540 798 1104 1458 1860 2310
Cum 11 71 239 569 1109 1907 3011 4469 6329 8639
-----
TD10=8639

Vertex symbols for selected sublattice
-----
Sc1 Point symbol:{4^24.5^12.6^8.7}
Extended point
symbol:[4.4.4.4.4.4.4.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).5(2).
5(2).5(3).5(3).5(3).5(3).5(4).5(4).5(9).5(9).5(9).5(9).6(19).6(19).6(19).6(19).6(37).6(37).6(37).
6(37).7(24)]
-----
Point symbol for net: {4^24.5^12.6^8.7}
10-c net; uninodal net

Topological type: egg3 (personal.ttd) {4^24.5^12.6^8.7} - VS
[4.4.4.4.4.4.4.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).5(2).5(2).5(
3).5(3).5(3).5(3).5(4).5(4).5(9).5(9).5(9).5(9).6(10).6(10).6(10).6(10).6(28).6(28).6(28).6(28).*]
(72564 types in 11 databases)
Elapsed time: 8.42 sec.

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2) Including hydrogen bonds as additional linkers

Topology for Sc1

Atom Sc1 links by bridge ligands and has						
Common vertex with					R(A-A)	
Sc 1	0.5000	-0.5000	0.5000	(0-1 0)	7.908A	1
Sc 1	0.5000	1.5000	0.5000	(0 1 0)	7.908A	1
Sc 1	0.5000	0.0000	0.0000	(1-1 0)	14.170A	1
Sc 1	0.5000	0.0000	1.0000	(1-1 1)	14.170A	1
Sc 1	0.5000	1.0000	0.0000	(1 0 0)	14.170A	1
Sc 1	0.5000	1.0000	1.0000	(1 0 1)	14.170A	1
Sc 1	1.5000	0.0000	1.0000	(2-1 1)	19.337A	1
Sc 1	1.5000	1.0000	1.0000	(2 0 1)	19.337A	1
Sc 1	-0.5000	1.0000	0.0000	(0 0 0)	19.337A	1
Sc 1	-0.5000	0.0000	0.0000	(0-1 0)	19.337A	1
Sc 1	1.5000	-1.5000	0.5000	(1-2 0)	22.034A	1
Sc 1	-0.5000	2.5000	0.5000	(-1 2 0)	22.034A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Sc

Coordination sequences

Sc1:	1	2	3	4	5	6	7	8	9	10
Num	12	62	168	330	540	798	1104	1458	1860	2310
Cum	13	75	243	573	1113	1911	3015	4473	6333	8643

TD10=8643

Vertex symbols for selected sublattice

Sc1 Point symbol:{3^12.4^36.5^17.6}

Extended point

[illegible]

Point symbol for net: $\{3^{12}.4^{36}.5^{17}.6\}$

12-c net; uninodal net

Topological type: egg4 (personal.ttd) $\{3^{12}.4^{36}.5^{17}.6\}$ - VS

[3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).
4(2).4(2).4(2).4(2).4(3).4(3).4(3).4(3).5.5.5.5.5.5.5.5.5(2).5(2).5(4).6(2).6(2).6(5).6(5).6(5).6
(5).6(6).6(6).6(6).6(6).*] (72564 types in 11 databases)

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Elapsed time: 16.36 sec.
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Compound 4

Topology for Sc1

Atom Sc1 links by bridge ligands and has						
Common vertex with				R(A-A)		
Sc 1	0.3663	0.8308	-0.1089	(1 0 0)	12.919A	1
Sc 1	0.8663	0.6692	1.3911	(1 1 2)	13.906A	1
Sc 1	0.6337	1.8308	0.6089	(0 1 0)	14.343A	1
Sc 1	0.6337	-0.1692	0.6089	(0-1 0)	14.343A	1
Sc 1	0.1337	0.3308	0.6089	(-1-1 0)	18.713A	1
Sc 1	1.1337	1.3308	0.6089	(0 0 0)	18.713A	1

Structural group analysis

Structural group No 1

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

[0,0,1] (19.34A)
[0,1,1] (24.08A)
[0,1,-1] (24.08A)
[1,0,1] (31.45A)
[1,1,1] (34.56A)
[1,-1,1] (34.56A)
[1,0,-1] (46.36A)
[1,1,-1] (48.53A)
[1,-1,-1] (48.53A)

PIC: [0,0,3][0,1,0][1/2,1/2,0] (PICVR=3)

Zt=3; Zn=1

Class Ia Z=3

Coordination sequences

Sc1: 1 2 3 4 5 6 7 8 9 10
Num 6 20 46 84 136 202 280 370 472 586
Cum 7 27 73 157 293 495 775 1145 1617 2203
Rad 15.6(2.4) 24.8(5.8) 35.3(7.3) 46.5(8.7) 58.2(10.3) 70.0(11.9) 82.2(13.6) 94.6(15.4) 107.0(17.4) 119.4(19.5)
Cmp Sc6 Sc20 Sc46 Sc84 Sc136 Sc202 Sc280 Sc370 Sc472 Sc586

TD10=2203

Vertex symbols for selected sublattice

Sc1 Point symbol:{4¹⁰.5².6³}
Extended point symbol:[4.4.4.4.4.4.4.4.5(3).5(3).6(2).6(3).6(4)]
Vertex symbol: [4.4.4.4.4.4.4.4.5(3).5(3).*.*.]*
All rings (up to 10):
[(4,6(2)).(4,6(2)).(4,6(2)).(4,5).(4,5).(4,6).(4,5,6).(4,5,6).(4,6).5(3).5(3).*.*.]*
ATTENTION! Some rings * are bigger than 10, so likely no rings are contained in that angle
All circuits (up to 10):
[(4,6(10),7(4),8(83),9(151),10(955)).(4,6(10),7(4),8(83),9(151),10(955)).(4,6(9),7(6),8(81),9(135),10(952)).(4,6(9),7(6),8(81),9(135),10(952)).(4,5,6(4),7(17),8(49),9(214),10(741)).(4,5,6(4),7(17),8(49),9(214),10(741)).(4,6(7),7(7),8(68),9(127),10(879)).(4,5,6(7),7(12),8(80),9(158),10(1068)).(4,5,6(7),7(12),8(80),9(158),10(1068)).(4,6(7),7(7),8(68),9(127),10(879)).(5(3),6(2),7(21),8(42),9(248),10(704)).(5(3),6(2),7(21),8(42),9(248),10(704)).(6(2),7(12),8(32),9(204),10(618)).(6(3),7(2),8(67),9(72),10(951)).(6(4),7(6),8(71),9(124),10(993))]
Cycle sequence

Size 4 5 6 7 8 9 10
Num 10 10 87 154 976 2466 13160

Point symbol for net: {4¹⁰.5².6³}
6-c net; uninodal net

Topological type: **egg2** (CycleSeq=[4(10).5(10).6(87).7(154).8(976).9(2466).10(13160)])
(personal.ttd) {4¹⁰.5².6³} - VS [4.4.4.4.4.4.4.4.4.5(3).5(3).*.*.]* (72442 types in 11 databases)
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: **hex-6-P6222** (CycleSeq=[4(10).5(10).6(87).7(154).8(972).9(2484).10(13045)])
(uninodal.ttd) {4¹⁰.5².6³} - VS [4.4.4.4.4.4.4.4.4.5(3).5(3).*.*.]* (72442 types in 11 databases)
Use All Rings or Cycle Sequences to distinguish nets