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Poly[dichloridobis(μ_2-di-4-pyridyl sulfide-κ^2N,N')cobalt(II)]

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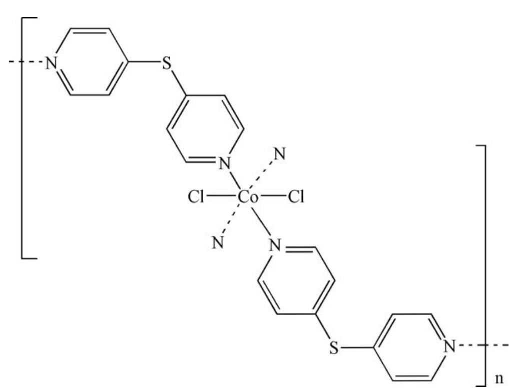
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.070; data-to-parameter ratio = 14.8.

In the title compound, $[CoCl_2(C_{10}H_8N_2S)_2]_n$, the Co^{II} atom is located on an inversion centre and is six-coordinated by four N atoms of four symmetry-related di-4-pyridyl sulfide ligands, and two Cl atoms in *trans* positions, in a distorted octahedral geometry. The bridging bidentate di-4-pyridyl sulfide ligands link the Co^{II} centres into a three-dimensional network. The four coordinating pyridine groups are donors and acceptors (N atoms) for intramolecular C—H···N and C—H···Cl hydrogen bonds.

Related literature

For di-4-pyridyl sulfide metal complexes, see: Jung *et al.* (1998, 1999); Kondo *et al.* (2004); Muthu *et al.* (2005).



Experimental

Crystal data

$[CoCl_2(C_{10}H_8N_2S)_2]$
M_r = 506.32
Monoclinic, $P2_1/c$
a = 7.4940 (11) Å
b = 15.355 (2) Å
c = 9.4009 (14) Å
β = 98.413 (2)°
V = 1070.1 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 296 (2) K
0.44 × 0.34 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.608, T_{max} = 0.747
5174 measured reflections
1969 independent reflections
1720 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.070
S = 1.05
1969 reflections
133 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.2185 (18)	Co1—Cl1	2.4221 (5)
Co1—N2^i	2.2822 (17)		
N1—Co1—N2^i	94.00 (6)	N1—Co1—Cl1	90.50 (5)

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···N2^{ii}	0.93	2.62	3.119 (3)	114
C6—H6···Cl1^{iii}	0.93	2.66	3.292 (2)	126
C10—H10···Cl1^{iv}	0.93	2.64	3.292 (2)	128

Symmetry codes: (ii) $x-1, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank Luo Yang Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2149).

References

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supplementary materials

Acta Cryst. (2009). E**65**, m247 [doi:10.1107/S1600536809001676]

Poly[dichloridobis(μ_2-di-4-pyridyl sulfide-κ^2*N*,*N*')cobalt(II)]

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Comment

As well known, di-4-pyridyl sulfide possesses a magic angle (C-S-C, ~100°) and conformational nonrigidity so it has some flexibility compared with other linear rigid ligands such as simple 4, 4'-bipyridine analogues. A number of metal complexes derived from di-4-pyridyl sulfide have been reported previously, such as the silver(I) complexes (Jung *et al.,* 1999), copper(II) complexes (Muthu *et al.,* 2005), nickel(II) complex (Kondo *et al.,* 2004), as well as the cobalt(II) complex that showing 2-fold interpenetrating structures (Jung *et al.,* 1998).

As shown in Fig. 1, the local geometry of the cobalt atoms is a distorted octahedral arrangement with two chlorine atoms in trans positions and four pyridine units in a propeller arrangement (Tab. 1). Each di-4-pyridyl sulfide ligand connects two cobalt(II) ions defining the edges of a 40-membered $[Co(II)]_4$ sheet (Fig. 2). The bent angle of the sulfur atom [C-S-C = 102.90 (10) °]. The Co-Co separation through a di-4-pyridyl sulfide ligand is 11.2646 (10) Å, and through the diagonal of the rhombus is 15.355 (2) Å. There are six intramolecular C—H···N and C—H···Cl hydrogen bonding contacts around the coordination sphere of the cobalt atom (Tab. 2). The packing of the layered structure is shown in Fig.3.

Experimental

To a stirred solution of di-4-pyridyl sulfide (0.5 mmol) in ethanol-H_2O 20 ml (v/v, 1:1) was added solid $CoCl_2$(0.5 mmol). Then the obtained mixture was basified with NaOH (0.5 mol/l) to a pH of 6.0 and stirred at 343K for 4h, filtrated. One week later, red crystals appeared.

Refinement

The H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å (CH) and *U*iso~(H) = 1.2Ueq(C).

Figures

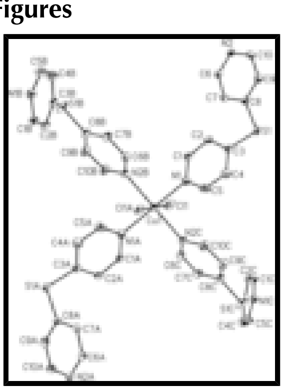


Fig. 1. A view of the local coordination of the Co(II) cation in the title compound. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (A) (-*x*, 1 - *y*, 1 - *z*); (B) (-1 + *x*, 3/2 - *y*, -1/2 + *z*); (C) (1 - *x*, -1/2 + *y*, 3/2 - *z*).

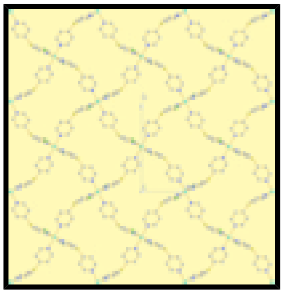


Fig. 2. A view of the two-dimensional network.

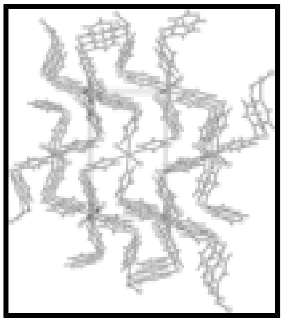


Fig. 3. A view of the compound packing down the *a* axis.

Poly[dichloridobis(μ_2-di-4-pyridyl sulfide-κ^2N,N')cobalt(II)]

Crystal data

$[CoCl_2(C_{10}H_8N_2S_1)_2]$	F_{000} = 514
M_r = 506.32	D_x = 1.571 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2498 reflections
a = 7.4940 (11) Å	θ = 2.6–29.0º
b = 15.355 (2) Å	μ = 1.26 mm^{-1}
c = 9.4009 (14) Å	T = 296 K
β = 98.413 (2)º	Block, red
V = 1070.1 (3) Å^3	0.44 × 0.34 × 0.24 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	1969 independent reflections
Radiation source: fine-focus sealed tube	1720 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 296 K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -9 \rightarrow 8$
T_{min} = 0.608, T_{max} = 0.747	$k = -14 \rightarrow 18$
5174 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.027$	H-atom parameters constrained
$wR(F^2) = 0.070$	$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2 + 0.5314P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
1969 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
133 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.0000	0.5000	0.5000	0.02605 (13)
Cl1	0.20061 (7)	0.43179 (4)	0.35327 (6)	0.04042 (16)
S1	0.46119 (10)	0.86590 (4)	0.38777 (6)	0.0496 (2)
N1	0.1375 (2)	0.62685 (11)	0.48432 (19)	0.0336 (4)
N2	0.8140 (2)	0.95816 (11)	0.79735 (18)	0.0295 (4)
C1	0.3135 (3)	0.63405 (14)	0.5315 (2)	0.0319 (5)
H1	0.3717	0.5866	0.5793	0.038*
C2	0.4148 (3)	0.70682 (14)	0.5143 (2)	0.0335 (5)
H2	0.5363	0.7088	0.5527	0.040*
C3	0.3335 (3)	0.77696 (14)	0.4393 (2)	0.0336 (5)
C4	0.1498 (3)	0.77243 (16)	0.3907 (3)	0.0485 (6)
H4	0.0894	0.8187	0.3410	0.058*
C5	0.0589 (3)	0.69710 (16)	0.4181 (3)	0.0492 (6)
H5	−0.0651	0.6952	0.3886	0.059*
C6	0.6455 (3)	0.92970 (14)	0.8003 (2)	0.0316 (5)
H6	0.6015	0.9310	0.8877	0.038*
C7	0.5337 (3)	0.89872 (14)	0.6820 (2)	0.0349 (5)
H7	0.4174	0.8803	0.6902	0.042*
C8	0.5962 (3)	0.89534 (14)	0.5507 (2)	0.0335 (5)
C9	0.7705 (3)	0.92370 (16)	0.5454 (2)	0.0433 (6)
H9	0.8182	0.9221	0.4595	0.052*
C10	0.8725 (3)	0.95443 (16)	0.6695 (2)	0.0411 (6)
H10	0.9889	0.9737	0.6640	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0256 (2)	0.0273 (2)	0.0247 (2)	0.00031 (16)	0.00196 (15)	0.00041 (15)
Cl1	0.0376 (3)	0.0546 (4)	0.0284 (3)	0.0153 (3)	0.0027 (2)	−0.0004 (2)

S1	0.0709 (4)	0.0438 (4)	0.0278 (3)	−0.0271 (3)	−0.0134 (3)	0.0079 (3)
N1	0.0322 (10)	0.0303 (10)	0.0371 (10)	−0.0001 (8)	0.0009 (8)	0.0009 (8)
N2	0.0310 (9)	0.0302 (10)	0.0261 (9)	−0.0020 (8)	0.0000 (7)	−0.0012 (7)
C1	0.0358 (12)	0.0290 (11)	0.0287 (11)	0.0006 (9)	−0.0023 (9)	0.0031 (9)
C2	0.0326 (11)	0.0336 (12)	0.0310 (11)	−0.0032 (9)	−0.0064 (9)	−0.0002 (9)
C3	0.0436 (13)	0.0287 (11)	0.0259 (10)	−0.0068 (9)	−0.0037 (9)	−0.0022 (9)
C4	0.0454 (14)	0.0302 (13)	0.0637 (17)	0.0008 (11)	−0.0125 (12)	0.0064 (12)
C5	0.0309 (12)	0.0374 (13)	0.0743 (18)	−0.0003 (10)	−0.0086 (12)	0.0023 (13)
C6	0.0339 (11)	0.0340 (11)	0.0265 (10)	−0.0025 (9)	0.0031 (9)	0.0002 (9)
C7	0.0345 (11)	0.0352 (12)	0.0333 (12)	−0.0093 (10)	−0.0004 (9)	0.0005 (10)
C8	0.0437 (13)	0.0265 (11)	0.0269 (11)	−0.0063 (9)	−0.0058 (9)	0.0022 (9)
C9	0.0495 (14)	0.0531 (15)	0.0280 (12)	−0.0121 (12)	0.0079 (10)	−0.0043 (11)
C10	0.0346 (12)	0.0550 (15)	0.0340 (12)	−0.0127 (11)	0.0061 (10)	−0.0060 (11)

Geometric parameters (Å, °)

Co1—N1^{i}	2.2184 (18)	C2—C3	1.379 (3)
Co1—N1	2.2185 (18)	C2—H2	0.9300
Co1—N2^{ii}	2.2822 (17)	C3—C4	1.388 (3)
Co1—N2^{iii}	2.2822 (17)	C4—C5	1.386 (3)
Co1—Cl1	2.4221 (5)	C4—H4	0.9300
Co1—Cl1^{i}	2.4222 (5)	C5—H5	0.9300
S1—C8	1.766 (2)	C6—C7	1.376 (3)
S1—C3	1.775 (2)	C6—H6	0.9300
N1—C1	1.334 (3)	C7—C8	1.384 (3)
N1—C5	1.338 (3)	C7—H7	0.9300
N2—C10	1.340 (3)	C8—C9	1.385 (3)
N2—C6	1.340 (3)	C9—C10	1.381 (3)
N2—Co1^{iv}	2.2822 (17)	C9—H9	0.9300
C1—C2	1.373 (3)	C10—H10	0.9300
C1—H1	0.9300		
N1^{i}—Co1—N1	180.0	C1—C2—H2	120.5
N1^{i}—Co1—N2^{ii}	94.00 (6)	C3—C2—H2	120.5
N1—Co1—N2^{ii}	86.00 (6)	C2—C3—C4	118.2 (2)
N1^{i}—Co1—N2^{iii}	86.00 (6)	C2—C3—S1	121.68 (17)
N1—Co1—N2^{iii}	94.00 (6)	C4—C3—S1	119.80 (17)
N2^{ii}—Co1—N2^{iii}	180.00 (8)	C5—C4—C3	118.1 (2)
N1^{i}—Co1—Cl1	89.50 (5)	C5—C4—H4	120.9
N1—Co1—Cl1	90.50 (5)	C3—C4—H4	120.9
N2^{ii}—Co1—Cl1	90.03 (4)	N1—C5—C4	124.4 (2)
N2^{iii}—Co1—Cl1	89.97 (4)	N1—C5—H5	117.8
N1^{i}—Co1—Cl1^{i}	90.50 (5)	C4—C5—H5	117.8
N1—Co1—Cl1^{i}	89.50 (5)	N2—C6—C7	124.10 (19)
N2^{ii}—Co1—Cl1^{i}	89.97 (4)	N2—C6—H6	118.0
N2^{iii}—Co1—Cl1^{i}	90.03 (4)	C7—C6—H6	118.0

Cl1—Co1—Cl1^{i}	179.999 (1)	C6—C7—C8	119.2 (2)
C8—S1—C3	102.90 (10)	C6—C7—H7	120.4
C1—N1—C5	115.77 (19)	C8—C7—H7	120.4
C1—N1—Co1	119.81 (14)	C7—C8—C9	117.7 (2)
C5—N1—Co1	124.16 (15)	C7—C8—S1	123.87 (17)
C10—N2—C6	115.96 (18)	C9—C8—S1	118.24 (16)
C10—N2—Co1^{iv}	121.39 (14)	C10—C9—C8	119.1 (2)
C6—N2—Co1^{iv}	122.47 (13)	C10—C9—H9	120.5
N1—C1—C2	124.4 (2)	C8—C9—H9	120.5
N1—C1—H1	117.8	N2—C10—C9	124.0 (2)
C2—C1—H1	117.8	N2—C10—H10	118.0
C1—C2—C3	119.0 (2)	C9—C10—H10	118.0
N2^{ii}—Co1—N1—C1	−149.12 (16)	S1—C3—C4—C5	172.1 (2)
N2^{iii}—Co1—N1—C1	30.88 (16)	C1—N1—C5—C4	3.4 (4)
Cl1—Co1—N1—C1	−59.12 (16)	Co1—N1—C5—C4	−170.7 (2)
Cl1^{i}—Co1—N1—C1	120.88 (16)	C3—C4—C5—N1	−2.4 (4)
N2^{ii}—Co1—N1—C5	24.8 (2)	C10—N2—C6—C7	−0.6 (3)
N2^{iii}—Co1—N1—C5	−155.2 (2)	Co1^{iv}—N2—C6—C7	−175.65 (16)
Cl1—Co1—N1—C5	114.8 (2)	N2—C6—C7—C8	0.6 (3)
Cl1^{i}—Co1—N1—C5	−65.2 (2)	C6—C7—C8—C9	0.0 (3)
C5—N1—C1—C2	−1.0 (3)	C6—C7—C8—S1	−174.41 (17)
Co1—N1—C1—C2	173.43 (16)	C3—S1—C8—C7	−41.6 (2)
N1—C1—C2—C3	−2.4 (3)	C3—S1—C8—C9	144.02 (19)
C1—C2—C3—C4	3.3 (3)	C7—C8—C9—C10	−0.6 (4)
C1—C2—C3—S1	−169.79 (17)	S1—C8—C9—C10	174.20 (19)
C8—S1—C3—C2	−51.6 (2)	C6—N2—C10—C9	0.0 (4)
C8—S1—C3—C4	135.4 (2)	Co1^{iv}—N2—C10—C9	175.13 (19)
C2—C3—C4—C5	−1.0 (4)	C8—C9—C10—N2	0.6 (4)

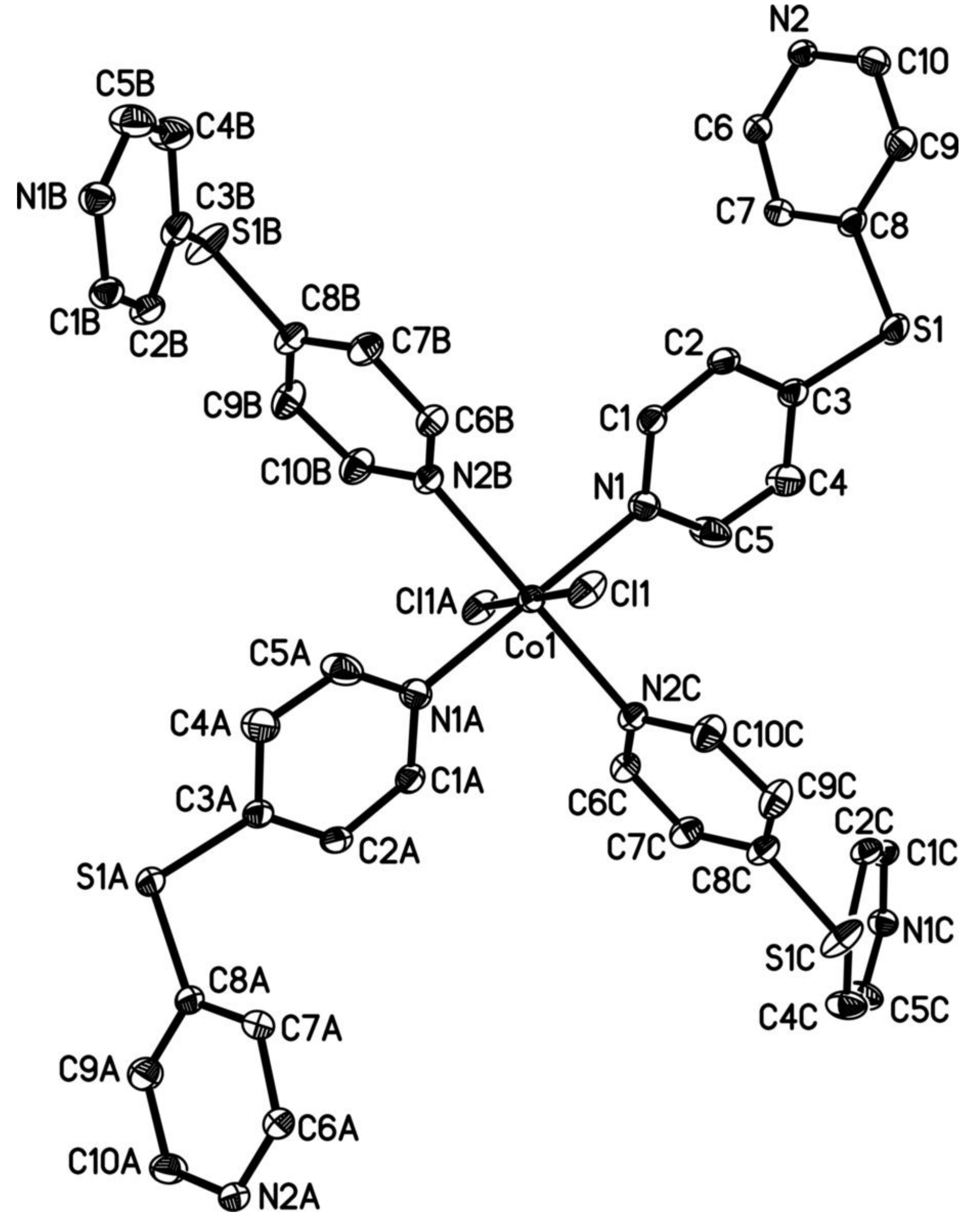
Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x-1, -y+3/2, z-1/2$; (iii) $-x+1, y-1/2, -z+3/2$; (iv) $-x+1, y+1/2, -z+3/2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···N2^{ii}	0.93	2.62	3.119 (3)	114
C6—H6···Cl1^{iv}	0.93	2.66	3.292 (2)	126
C10—H10···Cl1^{v}	0.93	2.64	3.292 (2)	128

Symmetry codes: (ii) $x-1, -y+3/2, z-1/2$; (iv) $-x+1, y+1/2, -z+3/2$; (v) $x+1, -y+3/2, z+1/2$.

Fig. 1


N2
C10
C6
C9
C7
C8
S1
C2
C3
C1
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N1
C5
Cl1
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C5B
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C8A
C7A
C9A
C6A
C10A
N2A
N2C
C10C
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C9C
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C4C
C5C

Fig. 2

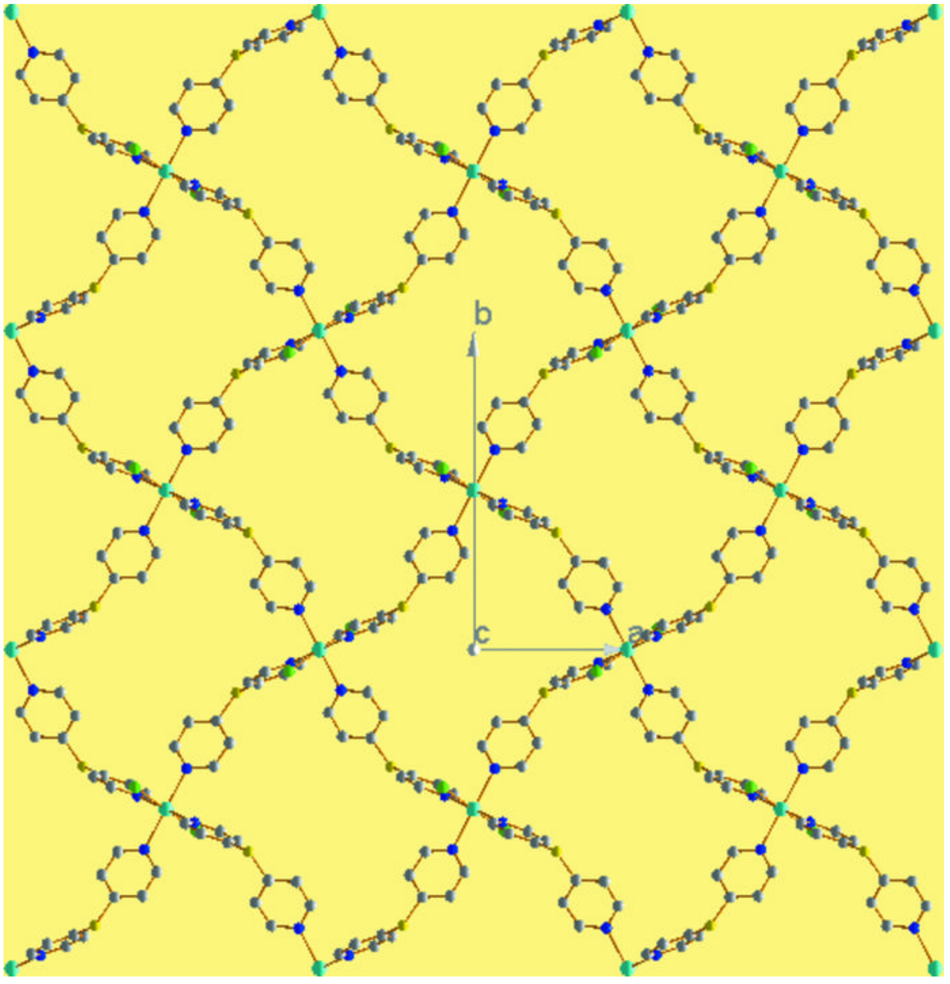

Fig. 3