

catena-Poly[[bis(thiocyanato- κN)-cobalt(II)]- μ -di-4-pyridylamine- $\kappa^2 N:N'$]

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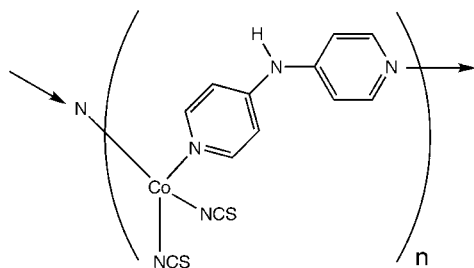
Received 25 September 2007; accepted 8 October 2007

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.064; wR factor = 0.125; data-to-parameter ratio = 19.4.

In the title compound, $[Co(NCS)_2(C_{10}H_9N_3)]_n$, a Co^{II} atom with tetrahedral coordination is bound by two N -donor thiocyanate anions and two N -donor atoms from two crystallographically distinct di-4-pyridylamine (dpa) ligands whose central NH units lie on twofold axes. The dpa ligands link the Co atoms into one-dimensional $[Co(NCS)_2(dpa)]_n$ coordination polymer chains that propagate along the b -axis direction.

Related literature

For related literature, see: Knapp *et al.* (2007); Montney *et al.* (2007); Zapf *et al.* (1998).



Experimental

Crystal data

$[Co(NCS)_2(C_{10}H_9N_3)]$

$M_r = 346.31$

Orthorhombic, $Pccn$

$a = 11.3975$ (9) Å

$b = 14.8905$ (12) Å

$c = 17.0136$ (14) Å

$V = 2887.5$ (4) Å³

$Z = 8$

Mo $K\alpha$ radiation

$\mu = 1.47$ mm⁻¹

$T = 173$ (2) K

$0.22 \times 0.10 \times 0.06$ mm

Data collection

Bruker SMART 1K diffractometer

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.764$, $T_{\max} = 0.915$

33685 measured reflections

3576 independent reflections

2384 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.117$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$

$wR(F^2) = 0.125$

$S = 1.06$

3576 reflections

184 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.35$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.53$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2N\cdots S1^i$	0.88 (2)	2.775 (12)	3.367 (4)	125.6 (3)
$N2-H2N\cdots S1^{ii}$	0.88 (2)	2.775 (12)	3.367 (4)	125.6 (3)
$N4-H4N\cdots S2^{iii}$	0.876 (19)	2.943 (15)	3.621 (4)	135.6 (3)
$N4-H4N\cdots S2^{iv}$	0.876 (19)	2.943 (15)	3.621 (4)	135.6 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalMaker* (CrystalMaker Software, 2005); software used to prepare material for publication: *SHELXL97*.

We gratefully acknowledge Michigan State University for funding of this work. CHS thanks the MSU Honors College for his Professorial Assistantship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2052).

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supplementary materials

Acta Cryst. (2007). E63, m2705 [doi:10.1107/S1600536807049276]

***catena*-Poly[[bis(thiocyanato- κ N)cobalt(II)]- μ -di-4-pyridylamine- κ^2 N:N']**

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Comment

In comparison to the wide variety of coordination polymers incorporating the rigid rod tethering ligand 4,4'-bipyridine, metal-organic materials based on di-4-pyridylamine (dpa) are much less common (Montney *et al.*, 2007). The title compound was prepared during our continuing attempts to prepare metal pseudohalide/dpa coordination polymers (Knapp *et al.*, 2007). The title compound possesses an asymmetric unit (Fig. 1) consisting of one cobalt atom, two N-bound isothiocyanate anions, and two halves of two crystallographically distinct dpa moieties. Both atoms of each dpa central N–H unit are situated on crystallographic 2-fold rotation axes.

Extension of the structure along the *b* crystal direction reveals an undulating 1-D chain coordination polymer of formulation [Co(NCS)₂(dpa)]_n, constructed *via* the linkage of [CoN₄] coordination tetrahedra through the tethering, kinked dpa ligands. The Co–N_{NCS} bond lengths are slightly shorter than the Co–N_{dpa} bond lengths, likely indicating a modicum of π -donation by the isothiocyanate ligands. The marked undulations in the 1-D chains are imparted by the varied amounts of torsional twisting within the dpa ligands as well as the tetrahedral coordination at cobalt. For one dpa ligand, the inter-ring torsion was measured as 19.6 (3)° *via* the through-bond/through-space torsion angle C4–C3–C3A–C4A, while the other exhibited a much more pronounced torsional twist of 39.4 (3)° (*via* the four-atom angle C7–C8–C8A–C7A). Within the 1-D chain motif, the Co–Co distances alternate between 11.464 (1) and 10.985 (1) Å.

As seen in Fig. 2, the 1-D [Co(NCS)₂(dpa)]_n chains aggregate into discrete *pseudo* 2-D layers through extensive cooperative π – π stacking interactions between the pyridyl rings of dpa units in neighboring chains (centroid-to-centroid distance = 3.693 (2) Å). Due to this arrangement, the through-space Co–Co distance between neighboring chain motifs within a *pseudo* 2-D layer is 5.767 (1) Å, over 5 Å closer than the through-ligand Co–Co distance within each chain. The central dpa N–H subunits and pendant sulfur atoms of the isothiocyanate ligands project into the interlamellar regions (Fig. 3), thereby permitting weak bifurcated N–H...S hydrogen bonding interactions between the layers, and propagating the full *pseudo* 3-D structure of the title compound. The closest Co–Co through-space distances between neighboring *pseudo* 2-D layers is 11.070 (1) Å.

Experimental

Cobalt thiocyanate was obtained commercially. di-4-pyridylamine (dpa) was prepared *via* a published procedure (Zapf *et al.*, 1998). Cobalt thiocyanate (58 mg, 0.33 mmol) and dpa (114 mg, 0.66 mmol) were added to 10 ml H₂O in a 23 ml a Teflon-lined Parr acid digestion bomb. The mixture was then heated under autogenous pressure at 393 K for 48 h., whereupon it was cooled slowly to 293 K. Small dark blue crystals of the title compound were produced, entrained in a pink polycrystalline powder.

Refinement

All H atoms bound to C atoms were placed in calculated positions, with C—H = 0.93 Å and refined in riding mode with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$. Both of the H atoms bound to N within the dpa ligands were found *via* Fourier difference map, restrained with N—H = 0.88 (2) Å, and refined with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{N})$.

Figures

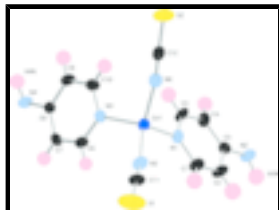


Fig. 1. Asymmetric unit of the title compound, showing 50% probability ellipsoids and partial atom numbering scheme. Color codes: light-blue N, yellow S, black C, pink H, dark blue Co.

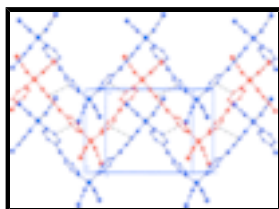


Fig. 2. Aggregation of individual $[\text{Co}(\text{NCS})_2(\text{dpa})]_n$ chains by π - π stacking, shown as dashed lines.

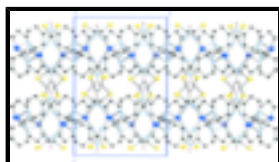


Fig. 3. Packing diagram illustrating the stacking of the *pseudo* two-dimensional layers by bifurcated hydrogen bonding patterns (shown as dashed lines) to form the three-dimensional crystal structure of the title compound.

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$M_r = 346.31$

Orthorhombic, *Pccn*

Hall symbol: -P 2ab 2ac

$a = 11.3975$ (9) Å

$b = 14.8905$ (12) Å

$c = 17.0136$ (14) Å

$V = 2887.5$ (4) Å³

$Z = 8$

$F_{000} = 1400$

$D_x = 1.593$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 33685 reflections

$\theta = 2.3$ – 28.3°

$\mu = 1.47$ mm⁻¹

$T = 173$ (2) K

Block, blue

$0.22 \times 0.10 \times 0.06$ mm

Data collection

Bruker SMART 1K
diffractometer

3576 independent reflections

Radiation source: fine-focus sealed tube	2384 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.117$
$T = 173(2)$ K	$\theta_{\text{max}} = 28.3^\circ$
ω scans	$\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 15$
$T_{\text{min}} = 0.764$, $T_{\text{max}} = 0.915$	$k = -19 \rightarrow 19$
33685 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 5.2183P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
3576 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
184 parameters	$\Delta\rho_{\text{max}} = 0.35 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -0.53 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The small crystal size resulted in relatively weak diffraction and an R_{int} value in excess of 0.10 despite collection of 30 second frames. Nevertheless, refinement was satisfactory.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.11826 (4)	0.01219 (3)	0.27376 (3)	0.02166 (15)
S1	0.38959 (13)	0.14244 (13)	0.44325 (9)	0.0688 (5)
S2	0.32324 (12)	-0.12349 (10)	0.06501 (8)	0.0517 (4)
N1	0.0002 (3)	-0.0711 (2)	0.32258 (19)	0.0224 (7)
N2	-0.2500	-0.2500	0.4099 (3)	0.0350 (13)
H2N	-0.2500	-0.2500	0.4619 (12)	0.042*

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N3	0.0200 (3)	0.1031 (2)	0.21497 (18)	0.0213 (7)
N4	-0.2500	0.2500	0.1100 (3)	0.0286 (11)
H4N	-0.2500	0.2500	0.0585 (12)	0.034*
N5	0.2067 (3)	0.0673 (2)	0.3582 (2)	0.0307 (8)
N6	0.2040 (3)	-0.0515 (2)	0.1925 (2)	0.0289 (8)
C1	-0.0077 (4)	-0.0918 (3)	0.3989 (2)	0.0333 (10)
H1	0.0447	-0.0653	0.4338	0.040*
C2	-0.0899 (4)	-0.1506 (3)	0.4279 (2)	0.0370 (12)
H2	-0.0923	-0.1629	0.4815	0.044*
C3	-0.1695 (3)	-0.1919 (3)	0.3779 (2)	0.0244 (9)
C4	-0.1645 (4)	-0.1677 (3)	0.3001 (2)	0.0291 (10)
H4	-0.2188	-0.1907	0.2646	0.035*
C5	-0.0789 (4)	-0.1094 (3)	0.2748 (2)	0.0298 (9)
H5	-0.0758	-0.0957	0.2215	0.036*
C6	-0.0327 (3)	0.1699 (3)	0.2534 (2)	0.0222 (8)
H6	-0.0078	0.1827	0.3042	0.027*
C7	-0.1216 (3)	0.2210 (2)	0.2220 (2)	0.0250 (8)
H7	-0.1558	0.2668	0.2513	0.030*
C8	-0.1597 (3)	0.2033 (2)	0.1464 (2)	0.0209 (8)
C9	-0.1012 (3)	0.1368 (3)	0.1044 (2)	0.0290 (9)
H9	-0.1215	0.1250	0.0525	0.035*
C10	-0.0133 (4)	0.0888 (3)	0.1400 (2)	0.0276 (9)
H10	0.0248	0.0445	0.1112	0.033*
C11	0.2825 (4)	0.0991 (3)	0.3950 (2)	0.0335 (10)
C12	0.2527 (4)	-0.0810 (3)	0.1386 (2)	0.0266 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0196 (3)	0.0225 (3)	0.0229 (3)	0.0014 (2)	-0.0008 (2)	0.0028 (2)
S1	0.0426 (8)	0.1086 (13)	0.0550 (9)	-0.0084 (9)	-0.0107 (7)	-0.0464 (9)
S2	0.0493 (8)	0.0760 (10)	0.0300 (7)	0.0062 (7)	0.0046 (6)	-0.0156 (7)
N1	0.0203 (16)	0.0222 (17)	0.0247 (18)	0.0004 (13)	-0.0033 (14)	0.0042 (14)
N2	0.052 (3)	0.036 (3)	0.017 (2)	-0.023 (3)	0.000	0.000
N3	0.0194 (16)	0.0207 (16)	0.0239 (18)	0.0029 (13)	0.0009 (13)	0.0017 (14)
N4	0.030 (3)	0.039 (3)	0.017 (2)	0.015 (2)	0.000	0.000
N5	0.0284 (19)	0.039 (2)	0.0252 (19)	-0.0045 (16)	0.0029 (15)	0.0024 (16)
N6	0.0259 (19)	0.0292 (19)	0.032 (2)	0.0061 (15)	0.0004 (16)	0.0018 (16)
C1	0.041 (3)	0.036 (3)	0.023 (2)	-0.014 (2)	-0.0052 (19)	-0.0010 (19)
C2	0.049 (3)	0.045 (3)	0.017 (2)	-0.021 (2)	-0.0003 (19)	0.0030 (19)
C3	0.029 (2)	0.021 (2)	0.024 (2)	-0.0043 (17)	-0.0012 (17)	-0.0015 (17)
C4	0.026 (2)	0.030 (2)	0.031 (2)	-0.0062 (18)	-0.0109 (18)	0.0061 (19)
C5	0.032 (2)	0.038 (2)	0.019 (2)	-0.0061 (18)	-0.0036 (18)	0.0115 (19)
C6	0.0190 (19)	0.029 (2)	0.0185 (19)	-0.0017 (16)	-0.0017 (15)	-0.0005 (16)
C7	0.0249 (19)	0.0211 (18)	0.029 (2)	0.0047 (17)	0.0031 (19)	-0.0037 (17)
C8	0.0181 (18)	0.022 (2)	0.022 (2)	0.0018 (15)	0.0025 (15)	0.0017 (16)
C9	0.031 (2)	0.039 (2)	0.018 (2)	0.0145 (19)	0.0007 (17)	0.0001 (17)
C10	0.029 (2)	0.029 (2)	0.024 (2)	0.0078 (18)	0.0016 (17)	-0.0040 (18)

C11	0.032 (2)	0.045 (3)	0.024 (2)	0.000 (2)	0.0040 (19)	-0.008 (2)
C12	0.023 (2)	0.028 (2)	0.030 (2)	-0.0010 (18)	-0.0059 (18)	0.0064 (18)

Geometric parameters (Å, °)

Co1—N5	1.937 (4)	N6—C12	1.157 (5)
Co1—N6	1.942 (4)	C1—C2	1.375 (6)
Co1—N1	2.010 (3)	C1—H1	0.9300
Co1—N3	2.022 (3)	C2—C3	1.388 (5)
S1—C11	1.606 (5)	C2—H2	0.9300
S2—C12	1.617 (4)	C3—C4	1.373 (6)
N1—C1	1.337 (5)	C4—C5	1.375 (5)
N1—C5	1.342 (5)	C4—H4	0.9300
N2—C3 ⁱ	1.374 (4)	C5—H5	0.9300
N2—C3	1.374 (4)	C6—C7	1.375 (5)
N2—H2N	0.88 (2)	C6—H6	0.9300
N3—C6	1.333 (5)	C7—C8	1.383 (5)
N3—C10	1.348 (5)	C7—H7	0.9300
N4—C8	1.388 (4)	C8—C9	1.391 (5)
N4—C8 ⁱⁱ	1.388 (4)	C9—C10	1.371 (5)
N4—H4N	0.876 (19)	C9—H9	0.9300
N5—C11	1.167 (5)	C10—H10	0.9300
N5—Co1—N6	118.24 (14)	C4—C3—N2	125.1 (4)
N5—Co1—N1	107.65 (14)	C4—C3—C2	116.7 (4)
N6—Co1—N1	109.26 (14)	N2—C3—C2	118.1 (4)
N5—Co1—N3	111.84 (14)	C3—C4—C5	119.8 (4)
N6—Co1—N3	104.70 (14)	C3—C4—H4	120.1
N1—Co1—N3	104.29 (13)	C5—C4—H4	120.1
C1—N1—C5	116.5 (3)	N1—C5—C4	123.7 (4)
C1—N1—Co1	126.1 (3)	N1—C5—H5	118.1
C5—N1—Co1	117.5 (3)	C4—C5—H5	118.1
C3 ⁱ —N2—C3	133.3 (5)	N3—C6—C7	123.7 (4)
C3 ⁱ —N2—H2N	113.4 (2)	N3—C6—H6	118.2
C3—N2—H2N	113.4 (2)	C7—C6—H6	118.2
C6—N3—C10	117.1 (3)	C6—C7—C8	119.1 (3)
C6—N3—Co1	120.4 (3)	C6—C7—H7	120.4
C10—N3—Co1	121.2 (3)	C8—C7—H7	120.4
C8—N4—C8 ⁱⁱ	127.0 (5)	C7—C8—N4	123.5 (4)
C8—N4—H4N	116.5 (2)	C7—C8—C9	117.6 (3)
C8 ⁱⁱ —N4—H4N	116.5 (2)	N4—C8—C9	118.9 (4)
C11—N5—Co1	162.7 (3)	C10—C9—C8	119.6 (4)
C12—N6—Co1	172.1 (3)	C10—C9—H9	120.2
N1—C1—C2	122.8 (4)	C8—C9—H9	120.2
N1—C1—H1	118.6	N3—C10—C9	122.8 (4)
C2—C1—H1	118.6	N3—C10—H10	118.6
C1—C2—C3	120.4 (4)	C9—C10—H10	118.6
C1—C2—H2	119.8	N5—C11—S1	178.2 (4)
C3—C2—H2	119.8	N6—C12—S2	178.3 (4)

supplementary materials

N5—Co1—N1—C1	-6.3 (4)	C1—C2—C3—C4	-2.8 (7)
N6—Co1—N1—C1	123.3 (4)	C1—C2—C3—N2	-179.9 (4)
N3—Co1—N1—C1	-125.2 (4)	N2—C3—C4—C5	-179.4 (3)
N5—Co1—N1—C5	173.2 (3)	C2—C3—C4—C5	3.8 (6)
N6—Co1—N1—C5	-57.3 (3)	C1—N1—C5—C4	-0.6 (6)
N3—Co1—N1—C5	54.2 (3)	Co1—N1—C5—C4	179.9 (3)
N5—Co1—N3—C6	-37.7 (3)	C3—C4—C5—N1	-2.2 (7)
N6—Co1—N3—C6	-166.9 (3)	C10—N3—C6—C7	3.3 (5)
N1—Co1—N3—C6	78.4 (3)	Co1—N3—C6—C7	-164.0 (3)
N5—Co1—N3—C10	155.5 (3)	N3—C6—C7—C8	-0.2 (6)
N6—Co1—N3—C10	26.3 (3)	C6—C7—C8—N4	178.9 (3)
N1—Co1—N3—C10	-88.4 (3)	C6—C7—C8—C9	-3.0 (6)
N6—Co1—N5—C11	21.6 (13)	C8 ⁱⁱ —N4—C8—C7	-23.5 (3)
N1—Co1—N5—C11	145.9 (12)	C8 ⁱⁱ —N4—C8—C9	158.4 (4)
N3—Co1—N5—C11	-100.1 (12)	C7—C8—C9—C10	3.2 (6)
C5—N1—C1—C2	1.5 (6)	N4—C8—C9—C10	-178.7 (3)
Co1—N1—C1—C2	-179.0 (3)	C6—N3—C10—C9	-3.1 (6)
N1—C1—C2—C3	0.2 (7)	Co1—N3—C10—C9	164.1 (3)
C3 ⁱ —N2—C3—C4	11.4 (3)	C8—C9—C10—N3	-0.1 (6)
C3 ⁱ —N2—C3—C2	-171.7 (4)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2N \cdots S1 ⁱⁱⁱ	0.88 (2)	2.775 (12)	3.367 (4)	125.6 (3)
N2—H2N \cdots S1 ^{iv}	0.88 (2)	2.775 (12)	3.367 (4)	125.6 (3)
N4—H4N \cdots S2 ^v	0.876 (19)	2.943 (15)	3.621 (4)	135.6 (3)
N4—H4N \cdots S2 ^{vi}	0.876 (19)	2.943 (15)	3.621 (4)	135.6 (3)

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

Fig. 1

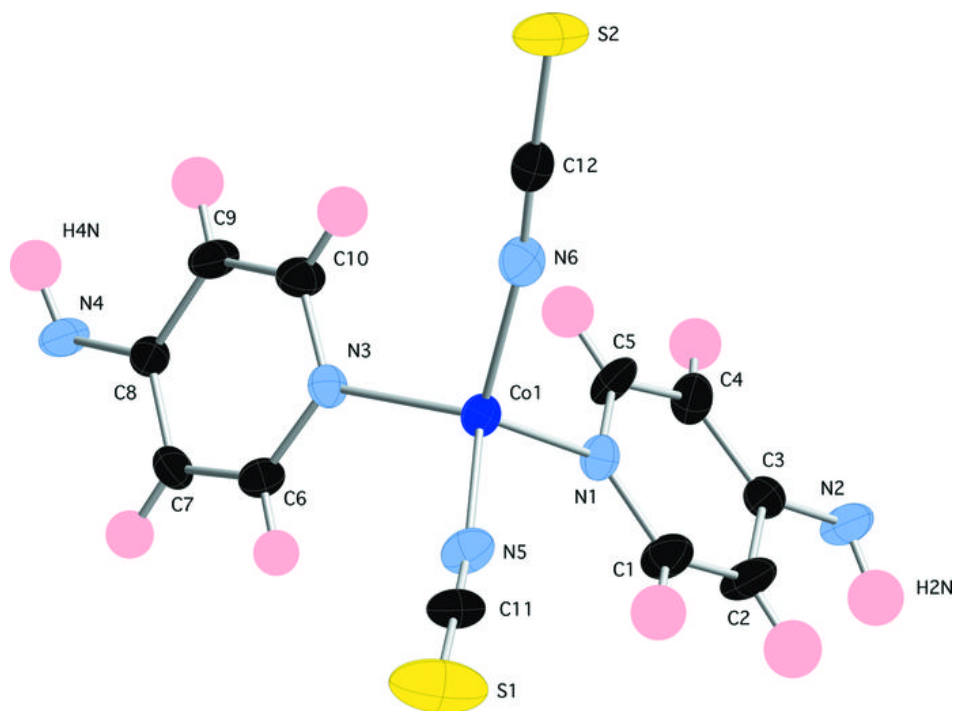


Fig. 2

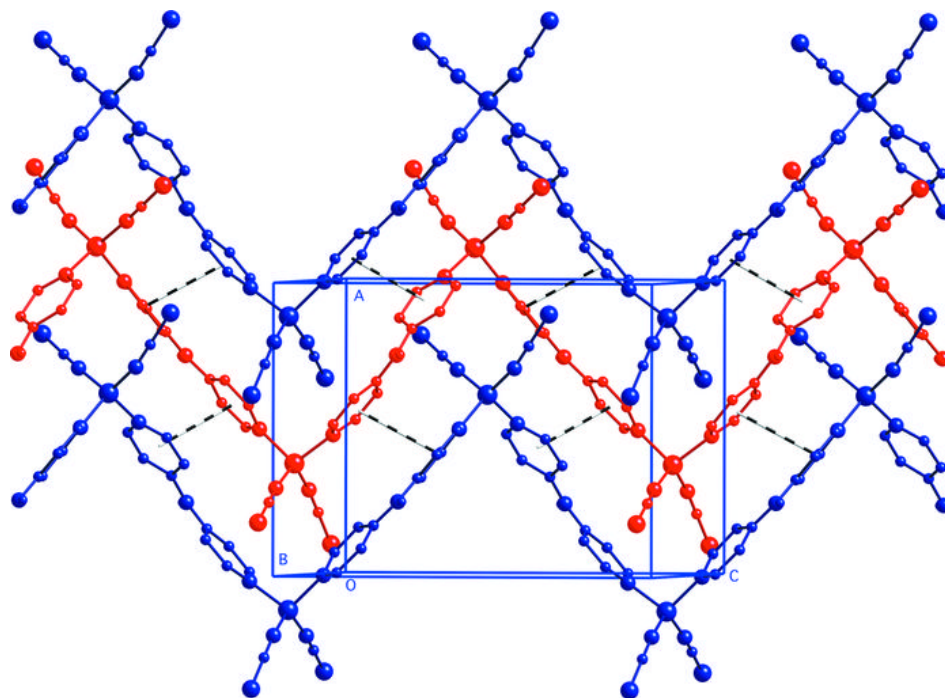


Fig. 3

