

Synthesis and Crystal Structure of N-(2-Pyridylmethyl)-L-Alanine) Isothiocyanate Cobalt(III)

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Abstract

The title compound, [N-(2-pyridylmethyl)-(L)-alanine]Co(III) thiocyanate (**1**) was obtained from the reaction of Co(OOCH₃)₂·H₂O with the tridentate reduced Schiff base ligand, N-(2-pyridylmethyl)-(L)-alanine (L) and NH₄SCN and characterized by elemental analysis, IR, UV-visible, TGA and single-crystal X-ray diffraction. Structural and spectroscopic analyses reveal [Co(L)₂]SCN to be monomeric with Cobalt(III) adopting a pseudo-octahedral geometry, coordinating to two reduced Schiff base ligands. In the crystal lattice, the thiocyanate anion forms an intermolecular SCN...HN_{amine} hydrogen bond, while adjacent monomers are linked by intermolecular O_{carboxyl}...HN_{amine}...H-bonds to form a supramolecular network. This work is therefore undertaken in an attempt to construct coordination framework structures of varying properties using the mixed-ligand strategy involving reduced Schiff bases and the thiocyanate ion.

Keywords

Cobalt(III), (L)-Alanine, Thiocyanate, Tridentate Reduced Schiff Base, Crystal Structure

1. Introduction

Cobalt complexes of Schiff base ligands are an important class of coordination compounds due to their structural diversity which display geometries ranging from tetrahedral, bipyramidal, square pyramidal to octahedral [1] [2] [3]. Co-

balt(III) complexes are generally prepared by air oxidation of Co(II) ion in the presence of relatively oxidation-inert ligands, which exhibit relatively strong co-ordinating abilities [4] [5]. An effective method for the construction of coordination frameworks with interesting structures and properties is through mixed-ligand assemblies and reduced Schiff base ligands have been found to form flexible and multidentate network structures because of the reduction of the imine group, (-C=N-) of the Schiff base, thus overcoming ligand instability in complexes [6] [7].

Reduced Schiff base ligands have been found to be relatively inert towards air oxidation and are strongly coordinating due to the reduction of the N=C bond, giving rise to flexible multidentate ligands [8] [9]. Pseudohalides possess versatile bonding modes, which result in the formation of complexes with various dimensionalities. The thiocyanate ions have therefore been found to possess versatile coordination abilities which result in the formation of metal complexes of varied structures. Thiocyanate-containing metal complexes have attracted much attention due to their versatile binding modes and its propensity to coordinate using either the nitrogen or/and the sulphur donor-atom, thus affording a number of homo- and hetero-metallic discrete structural assemblies with specific structural features and properties [10].

Recent attention has been focused on the study of the coordination compounds of cobalt due to its varied oxidation states and their interesting structural, magnetic, electronic and optoelectronic properties [11]. Our focus has been on the synthesis of mixed ligand complexes involving tridentate reduced Schiff bases and the thiocyanate ion. The crystal structure of one such compound is reported here.

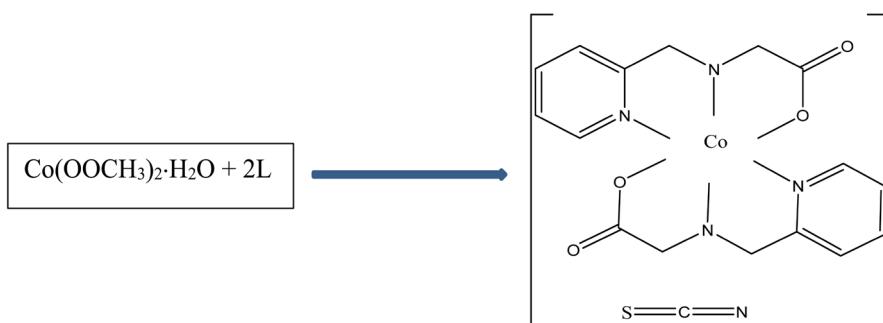
2. Experimental

2.1. Physical Measurements

Elemental analysis for carbon, nitrogen and hydrogen were carried out on a FLASH 2000 Organic Elemental Analyzer, CHNS-O analyser by Thermo Scientific. Thermo Scientific iCAP 6000 SERIES duo ICAP Spectrometer was used to determine the metal content. Thermogravimetric analysis was investigated using a Mettler Toledo TGA/DSC1 STAR System; Infrared spectra were recorded on a Perkin-Elmer model IR-457 spectrometer and a spectrum 100 FT-IR Perkin Elmer spectrometer, while the UV/Vis spectrum was recorded using an Agilent HP8453 Diode Array UV/Vis Spectrometer. The magnetic susceptibility measurement was made using the Sherwood Scientific magnetic susceptibility balance; while X-ray diffraction was carried using a Bruker APEX diffractometer.

2.2. Synthesis and Crystallization

N-(2-pyridylmethyl)-(L)-alanine (L)(0.361 g, 2 mmol) in 10 mL aqueous ethanol was added drop wise to a 5 ml aqueous solution of $\text{Co}(\text{OOCH}_3)_2\text{H}_2\text{O}$ (0.249 g, 1 mmol,) while stirring at room temperature. After stirring for a further 10 minutes,



Scheme 1. Synthesis and structure of N-(2-pyridylmethyl)-L-alanine) isothiocyanate Cobalt(III).

NH_4SCN , (0.16 g, 2 mmol,) in 2 mL distilled water was added drop wise and stirring continued for a further two hours. Rectangular reddish brown crystals suitable for X-ray analysis were obtained from the solution by slow evaporation. Yield: 81%; anal. Calc. (Found) for $\text{C}_{19}\text{H}_{22}\text{N}_5\text{O}_4\text{SCo}$; C:48.00 (47.92); H:4.66 (4.78); N: 14.73 (14.72); S: 6.74 (6.69); Co: 12.40 (12.28). The synthesis of N-(2-pyridylmethyl)-L-alanine) isothiocyanate Cobalt(III) is summarized in **Scheme 1**.

2.3. Crystal Structure Determination

A suitable single crystal of the title compound was mounted on a glass fiber on the goniometer head of a Bruker APEX diffractometer and data were collected using graphite monochromated $\text{Cu}-K_\alpha$ radiation ($\lambda = 1.54178 \text{ \AA}$, operating at 50 kV and 40 mA) at a temperature of 100 K. Crystal data, data collection and structure refinement details are summarized in **Table 1**.

The structure was solved by direct methods and refined by full-matrix least squares on F^2 [12]. All non-Hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions, assigned isotropic thermal parameters and allowed to ride on their parent carbon atoms. All calculations were carried out using the SHELXTL package [13]. CCDC 1419814 contains the supplementary crystallographic data for this paper.

3. Results and Discussion

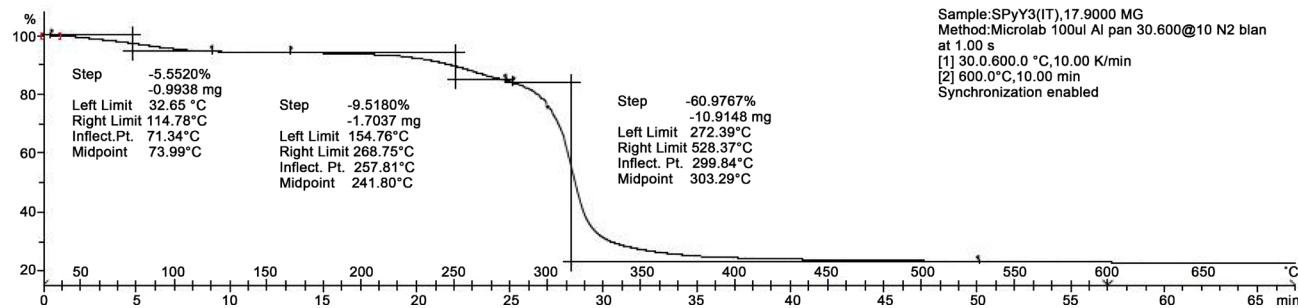
3.1. Spectroscopic and Other Analysis

In the IR spectrum of the Co(III) complex, a very strong infrared absorption band at 1609 cm^{-1} is attributed to $\nu_{\text{C}=\text{C}}$ and $\nu_{\text{C}=\text{N}}$ of the pyridyl ring, while the strong band at 2098 cm^{-1} suggest the presence of $\text{N}=\text{C}=\text{S}$ stretch [14] [15] [16], as confirmed by the single crystal structure of the compound. Two distinct peaks at 362 nm and 497 nm are observed in the UV-Visible spectrum of the complex and attributed to spin allowed $d-d$ transitions.

The thermal behaviour of the title compound (**Figure 1**), recorded under an N_2 atmosphere, in the temperature range of 25°C to 600°C at a heating rate of $25^\circ\text{C min}^{-1}$ shows a one-step decomposition patterns at 310°C though with a small shoulder at 240°C which probably accounts for the decomposition of the

Table 1. Experimental details.

Empirical formula	C ₁₉ H ₂₂ CoN ₅ O ₄ S
Formula weight	475.41
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 9.8179(4) Å α = 90°. b = 7.3412(3) Å β = 106.813(3)°. c = 14.4414(6) Å γ = 90°.
Volume	996.37(7) Å ³
Z	2
Density (calculated)	1.585 Mg/m ³
Absorption coefficient	8.064 mm ⁻¹
F(000)	492
Crystal size	0.20 × 0.08 × 0.03 mm ³
Theta range for data collection	3.20° to 72.11°.
Index ranges	-12 ≤ h ≤ 10, -9 ≤ k ≤ 8, -17 ≤ l ≤ 17
Reflections collected	4709
Independent reflections	3009 [R(int) = 0.0497]
Completeness to theta = 67.00°	98.4%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7939 and 0.584652
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	3009/1/281
Goodness-of-fit on F ²	0.776
Final R indices [I > 2sigma(I)]	R ₁ = 0.0408, wR ₂ = 0.0819
R indices (all data)	R ₁ = 0.0539, wR ₂ = 0.0861
Absolute structure parameter	-0.010(5)
Largest diff. peak and hole	0.587 and -0.350 e.Å ⁻³

**Figure 1.** Thermal Analysis of the Title compound.

organic ligands [calc. 75.2% (found 75.8%)]. The final residue of [24.15% (calc. 24.61%)] represents a mixture of Cobalt oxides, CoO and Co₂O₃.

The peak at m/z = 474.1 corresponds to C₁₉H₂₂N₅O₄SCo (calc. 475.41) which confirms the molecular weight of the compound. The effective magnetic moment, μ_{eff} was found to be consistent with a d⁶ low-spin configuration with some

degree of spin-orbit coupling.

3.2. Crystal Structure Determination

The structure of the title compound (I) is represented in **Scheme 1** and comprise the $[\text{Co}(\text{L})_2]^+$ cation and the NCS^- anion with the resulting complex having the composition $[\text{Co}(\text{L})_2]^+\text{NCS}^-$. The two L ligands are bonded to the cobalt centre via their two pyridyl nitrogen atoms ($\text{Co}(1)\text{-N}(1)$, 1.931(3) Å; $\text{Co}(1)\text{-N}(3)$, 1.929(3) Å), two secondary amine nitrogen atoms ($\text{Co}(1)\text{-N}(2)$, 1.971(4) Å; $\text{Co}(1)\text{-N}(4)$, 1.967(3) Å) and two carboxylate oxygen atoms ($\text{Co}(1)\text{-O}(2)$, 1.884(3) Å; $\text{Co}(1)\text{-O}(4)$, 1.891(3) Å) to give a pseudo octahedral geometry around the cobalt atom (**Figure 2** and **Table 2**). The X-ray crystal structure reveals that the thiocyanate anion in the crystal lattice is not bonded to the Co(III) centre but forms interionic hydrogen bonds [17] [18], through the nitrogen atom of the NCS^- anion, [$\text{N}(4)\text{-H}(4\text{A})\dots\text{N}(5)\#1$ (**Figure 3**, **Table 3**)]. A second intermolecular hydrogen bond, [$\text{N}(2)\text{-H}(2\text{A})\dots\text{O}(3)\#2$ (**Table 3**)] is observed linking two different monomeric centres. The crystallographic indicators show a good-quality data set [$R(\text{int}) = 0.0497$ and $R1(\text{all data}) = 0.0539$]. Comparable bonds lengths and bond angles are observed. The average Co-N bond length (1.950 Å) is longer than the average Co-O bond length (1.886 Å) as expected, and these values are in good agreement with those of similar cobalt(III) complexes [19]. The *trans* bond angles around the cobalt center, [$\text{N}(3)\text{-Co}(1)\text{-N}(1)$ (174.18(16)°), $\text{O}(2)\text{-Co}(1)\text{-N}(4)$ (171.62(16)°), $\text{O}(4)\text{-Co}(1)\text{-N}(2)$ (172.66(16)°)] deviates slightly from the theoretical value of 180°, some of the *cis* bond angles deviated considerably from the theoretical value of 90° [$\text{N}(1)\text{-Co}(1)\text{-N}(2)$ bond angle of 94.30(18)° [19]]. The bond angle of the N-C-S thiocyanate anion is within the expected range of 178° - 182° [18]. The packing diagramme of the title compound is shown in **Figure 4**.

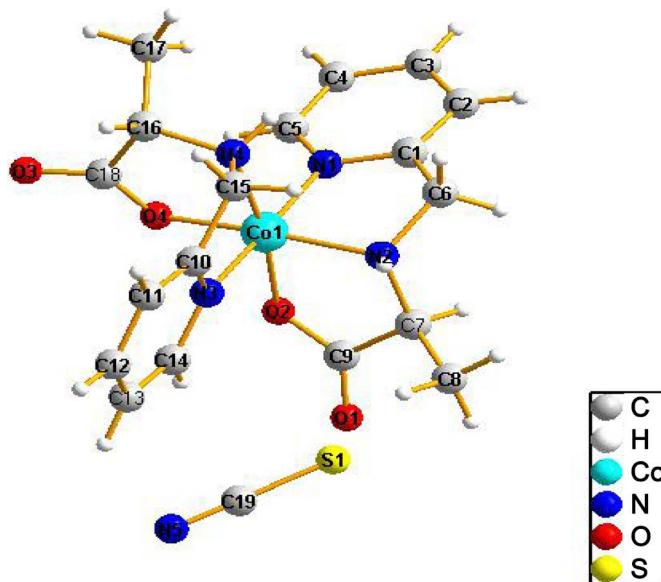
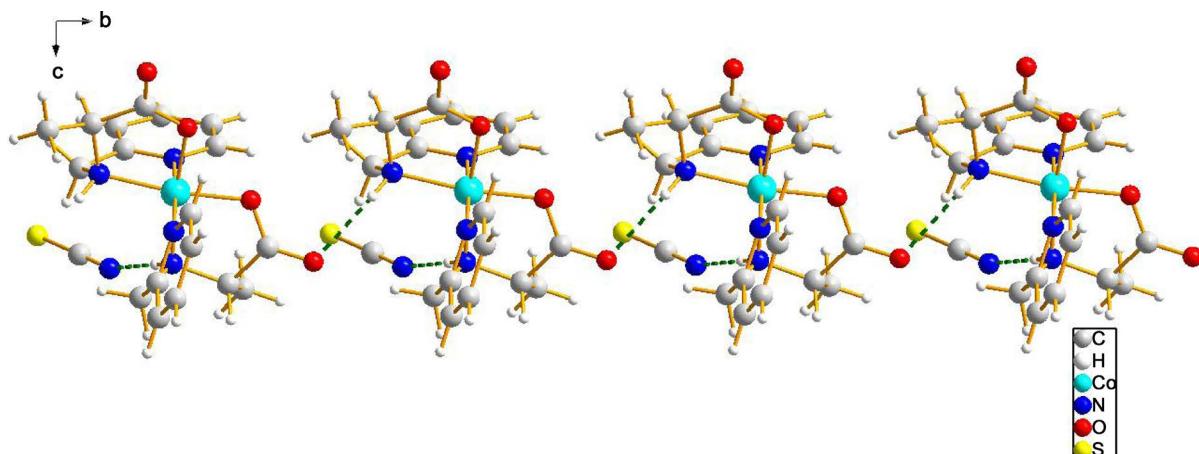


Figure 2. Ortep drawing of the Monomer of the titled compound (I) showing the atom numbering scheme.

Table 2. Selected bond parameters (\AA , $^{\circ}$).

Co(1)-O(2)	1.884(3)
Co(1)-O(4)	1.891(3)
Co(1)-N(3)	1.929(3)
Co(1)-N(1)	1.931(3)
Co(1)-N(4)	1.967(3)
Co(1)-N(2)	1.971(4)
O(3)-C(18)-O(4)	122.9(4)
N(5)-C(19)-S(1)	178.9(4)
O(2)-Co(1)-O(4)	86.73(14)
O(2)-Co(1)-N(3)	91.93(13)
O(4)-Co(1)-N(3)	88.55(17)
O(2)-Co(1)-N(1)	93.53(13)
O(4)-Co(1)-N(1)	93.77(18)
N(3)-Co(1)-N(1)	174.18(16)
O(2)-Co(1)-N(4)	171.62(16)
O(4)-Co(1)-N(4)	86.88(17)
N(3)-Co(1)-N(4)	82.50(14)
N(1)-Co(1)-N(4)	92.29(14)
O(2)-Co(1)-N(2)	86.41(15)
O(4)-Co(1)-N(2)	172.66(16)
N(3)-Co(1)-N(2)	94.30(18)
N(1)-Co(1)-N(2)	84.03(18)
N(4)-Co(1)-N(2)	100.19(18)

**Figure 3.** Ortep diagram showing hydrogen bonding.**Table 3.** Hydrogen bonds (\AA and $^{\circ}$).

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
N(4)-H(4A)...N(5) ^{#1}	0.87(4)	2.03(5)	2.892(5)	174(4)
N(2)-H(2A)...O(3) ^{#2}	0.88(5)	2.26(5)	2.997(5)	141(4)

Symmetry transformations used to generate equivalent atoms: #1 $x - 1, y, z$ #2 $x, y - 1, z$.

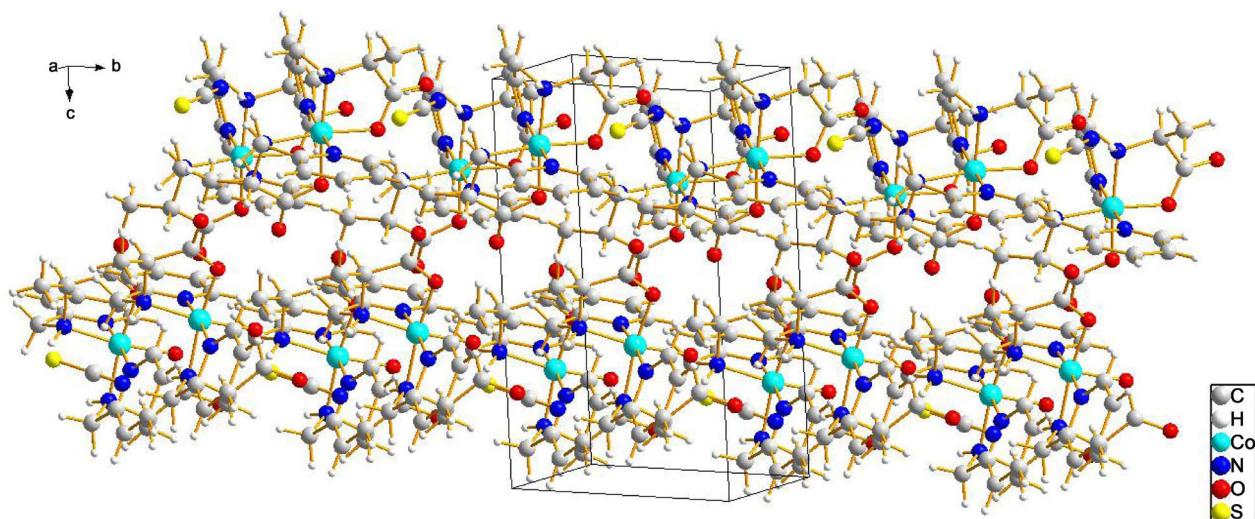


Figure 4. Packing diagram the title compound.

4. Conclusion

We have isolated a Co(III) Isothiocyanate metal-organic framework containing the chiral ligand, N-(2-pyridylmethyl)-L-alanine (pyala). Spectroscopic studies and the x-ray structure show that the compound is a monomer in which Cobalt(III) adopts a pseudo octahedral geometry, coordinating to two molecules of the ligand. Adjacent monomeric centres are linked by N-H...O, N-H...S hydrogen bonds which stabilize the compound thus forming a 3D supramolecular networks.

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Conflict of Interest

The authors declare that there is no conflict of interest.

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Supplementary Materials

[N-(2-pyridylmethyl)-(L)-alanine] Co(III) thiocyanate

Computing details

Data collection: Bruker Apex diffractometer; Data collection: Graphite monochromated Cu- κ radiation ($\lambda = 1.54178 \text{ \AA}$); structure solved by: Direct methods; refined by: Full matrix least square method; all calculations were carried out by: SHELXTL package.

Crystal data

$C_{19}H_{22}N_5O_4SCo$	$F(000) = 492$
$Mr = 475.41$	$Dx = 1.585 \text{ Mg/m}^3$
Monoclinic, P2(1)	$MoK\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
$a = 9.8179(4) \text{ \AA}$	Cell parameters from 4709 reflections
$b = 7.3412(3) \text{ \AA}$	$\theta = 3.20$ to 72.11° .
$c = 14.4414(6) \text{ \AA}$	$\mu = 8.064 \text{ mm}^{-1}$
$V = 996.37(7) \text{ \AA}^3$	$T = 100(2) \text{ K}$
$Z = 2$	$0.20 \times 0.08 \times 0.03 \text{ mm}^3$

Data collection

Bruker APEX diffractometer	3009 Independent reflections
Radiation source: graphite monochromated Cu- $K\alpha$ radiation	3009 reflections with $I > 2 \sigma(I)$ $R(\text{int}) = 0.0497$
Absorption correction: Semi-empirical from equivalents	$\theta_{\max} = 72.11^\circ$, $\theta_{\min} = 3.20^\circ$
$T_{\min} = 0.584652$, $T_{\max} = 0.7939$	$h = -12 \rightarrow 10$
4709 measured reflections	$k = -9 \rightarrow 8$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	3009 reflections
Full-matrix least-squares	281 parameters
$R_1 = 0.0539$, $wR_2 = 0.0861$	1 restraints
$S = -0.010(5)$	

Table S1. Atomic coordinates ($\times 104$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 103$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	1690(5)	4175(7)	3505(3)	15(1)
C(2)	583(5)	3899(7)	3909(3)	21(1)
C(3)	-123(5)	5428(7)	4109(3)	22(1)
C(4)	331(5)	7165(8)	3942(3)	22(1)
C(5)	1451(5)	7319(7)	3555(3)	19(1)

Continued

C(6)	2428(4)	2659(6)	3169(3)	14(1)
C(7)	5010(5)	3078(7)	3978(3)	17(1)
C(8)	6004(5)	1571(6)	3869(3)	23(1)
C(9)	5752(5)	4892(7)	4298(3)	18(1)
C(10)	4486(4)	5285(6)	1065(3)	16(1)
C(11)	5308(5)	5304(6)	431(3)	19(1)
C(12)	6703(4)	5895(8)	772(3)	19(1)
C(13)	7235(5)	6450(6)	1727(3)	20(1)
C(14)	6361(4)	6430(6)	2313(3)	18(1)
C(15)	2951(4)	4702(7)	800(3)	16(1)
C(16)	1945(5)	7696(6)	1036(3)	18(1)
C(17)	404(5)	8204(7)	948(4)	21(1)
C(18)	2918(5)	9048(6)	1701(3)	16(1)
C(19)	9040(5)	2628(7)	1589(3)	20(1)
Co(1)	3622(1)	5922(1)	2717(1)	12(1)
N(1)	2112(3)	5869(7)	3327(2)	15(1)
N(2)	3808(4)	3315(5)	3055(3)	14(1)
N(3)	5000(3)	5844(6)	2000(2)	15(1)
N(4)	2268(3)	5787(6)	1414(2)	14(1)
N(5)	9758(4)	3657(6)	1330(3)	23(1)
O(1)	6903(3)	4966(5)	4911(2)	20(1)
O(2)	5048(3)	6324(4)	3892(2)	14(1)
O(3)	3036(3)	10,609(5)	1433(2)	21(1)
O(4)	3549(3)	8482(4)	2563(2)	15(1)
S(1)	8003(1)	1191(2)	1938(1)	29(1)

Table S2. Hydrogen coordinates ($\times 104$) and isotropic displacement parameters ($\text{\AA}^2 \times 103$).

	x	y	z	U(eq)
H(2)	317	2706	4045	25
H(3)	-912	5289	4359	26
H(4)	-124	8219	4093	26
H(5)	1766	8501	3445	23
H(6A)	1821	2191	2543	17
H(6B)	2603	1651	3645	17
H(7)	4574	2689	4493	21
H(8A)	5467	433	3699	35
H(8B)	6754	1410	4481	35
H(8C)	6434	1892	3358	35
H(11)	4924	4923	-221	23
H(12)	7294	5920	354	23
H(13)	8195	6841	1972	24
H(14)	6723	6841	2962	22

Continued

H(15A)	2479	4941	106	20
H(15B)	2881	3384	923	20
H(16)	2097	7774	381	21
H(17A)	-238	7380	489	32
H(17B)	225	9460	716	32
H(17C)	236	8097	1582	32
H(4A)	1490(50)	5220(60)	1400(30)	7(11)
H(2A)	4030(50)	2630(80)	2620(40)	20(15)

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 103$). The anisotropic displacement factor exponent takes the form: $-2p_2 [h_2a * U_{11} + \dots + 2 h_ka * b * U_{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	17(2)	15(3)	11(2)	2(2)	2(2)	0(2)
C(2)	23(2)	17(3)	21(2)	5(2)	5(2)	1(2)
C(3)	19(2)	30(3)	16(2)	-4(2)	5(2)	-4(2)
C(4)	25(2)	22(3)	17(2)	-6(2)	5(2)	3(2)
C(5)	21(2)	12(2)	21(2)	-3(2)	2(2)	-2(2)
C(6)	16(2)	10(2)	18(2)	2(2)	7(2)	3(2)
C(7)	17(2)	15(3)	18(2)	6(2)	3(2)	0(2)
C(8)	21(2)	14(3)	29(2)	-6(2)	0(2)	5(2)
C(9)	21(2)	22(3)	15(2)	-2(2)	8(2)	3(2)
C(10)	17(2)	9(2)	22(2)	2(2)	5(2)	0(2)
C(11)	23(2)	13(2)	22(2)	2(2)	6(2)	4(2)
C(12)	22(2)	16(2)	24(2)	3(2)	14(2)	6(2)
C(13)	15(2)	20(3)	25(2)	1(2)	5(2)	0(2)
C(14)	17(2)	20(3)	18(2)	3(2)	6(2)	-1(2)
C(15)	19(2)	13(2)	16(2)	-4(2)	3(2)	-2(2)
C(16)	21(2)	13(2)	19(2)	3(2)	7(2)	2(2)
C(17)	19(2)	18(3)	28(2)	3(2)	9(2)	-1(2)
C(18)	22(2)	13(2)	16(2)	1(2)	8(2)	2(2)
C(19)	15(2)	26(3)	17(2)	-3(2)	3(2)	4(2)
Co(1)	14(1)	10(1)	13(1)	0(1)	4(1)	0(1)
N(1)	14(2)	16(2)	17(2)	0(2)	6(1)	-3(2)
N(2)	18(2)	11(2)	16(2)	-1(2)	6(2)	-1(2)
N(3)	16(2)	11(2)	18(2)	2(2)	6(1)	0(2)
N(4)	10(1)	14(2)	16(2)	-2(2)	4(1)	-4(2)
N(5)	19(2)	29(3)	20(2)	-2(2)	6(2)	-3(2)
O(1)	22(2)	19(2)	16(2)	2(1)	-2(1)	1(1)
O(2)	18(1)	12(2)	12(1)	0(1)	4(1)	-1(1)
O(3)	32(2)	12(2)	20(1)	2(1)	9(1)	-1(1)
O(4)	19(2)	10(2)	16(2)	0(1)	6(1)	1(1)
S(1)	35(1)	24(1)	32(1)	-2(1)	18(1)	-8(1)

Table S4. Bond lengths [\AA] and angles [$^\circ$].

C(1)-N(1)	1.359(6)
C(1)-C(2)	1.388(7)
C(1)-C(6)	1.484(6)
C(2)-C(3)	1.393(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.394(7)
C(3)-H(3)	0.9500
C(4)-C(5)	1.375(6)
C(4)-H(4)	0.9500
C(5)-N(1)	1.337(6)
C(5)-H(5)	0.9500
C(6)-N(2)	1.491(5)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-N(2)	1.513(5)
C(7)-C(8)	1.513(6)
C(7)-C(9)	1.524(6)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-O(1)	1.218(5)
C(9)-O(2)	1.301(6)
C(10)-N(3)	1.361(5)
C(10)-C(11)	1.384(6)
C(10)-C(15)	1.505(6)
C(11)-C(12)	1.385(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.387(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.369(6)
C(13)-H(13)	0.9500
C(14)-N(3)	1.350(5)
C(14)-H(14)	0.9500
C(15)-N(4)	1.489(6)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-N(4)	1.505(6)
C(16)-C(18)	1.514(6)
C(16)-C(17)	1.527(6)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800

Continued

C(17)-H(17C)	0.9800
C(18)-O(3)	1.226(5)
C(18)-O(4)	1.288(5)
C(19)-N(5)	1.166(6)
C(19)-S(1)	1.643(5)
Co(1)-O(2)	1.884(3)
Co(1)-O(4)	1.891(3)
Co(1)-N(3)	1.929(3)
Co(1)-N(1)	1.931(3)
Co(1)-N(4)	1.967(3)
Co(1)-N(2)	1.971(4)
N(2)-H(2A)	0.88(5)
N(4)-H(4A)	0.87(4)
N(1)-C(1)-C(2)	122.1(4)
N(1)-C(1)-C(6)	114.8(4)
C(2)-C(1)-C(6)	122.9(4)
C(1)-C(2)-C(3)	117.8(5)
C(1)-C(2)-H(2)	121.1
C(3)-C(2)-H(2)	121.1
C(2)-C(3)-C(4)	119.8(4)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	120.1
C(5)-C(4)-C(3)	118.6(5)
C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7
N(1)-C(5)-C(4)	122.5(5)
N(1)-C(5)-H(5)	118.8
C(4)-C(5)-H(5)	118.8
C(1)-C(6)-N(2)	109.8(4)
C(1)-C(6)-H(6A)	109.7
N(2)-C(6)-H(6A)	109.7
C(1)-C(6)-H(6B)	109.7
N(2)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
N(2)-C(7)-C(8)	110.8(4)
N(2)-C(7)-C(9)	110.4(4)
C(8)-C(7)-C(9)	113.9(4)
N(2)-C(7)-H(7)	107.2
C(8)-C(7)-H(7)	107.2
C(9)-C(7)-H(7)	107.2
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5

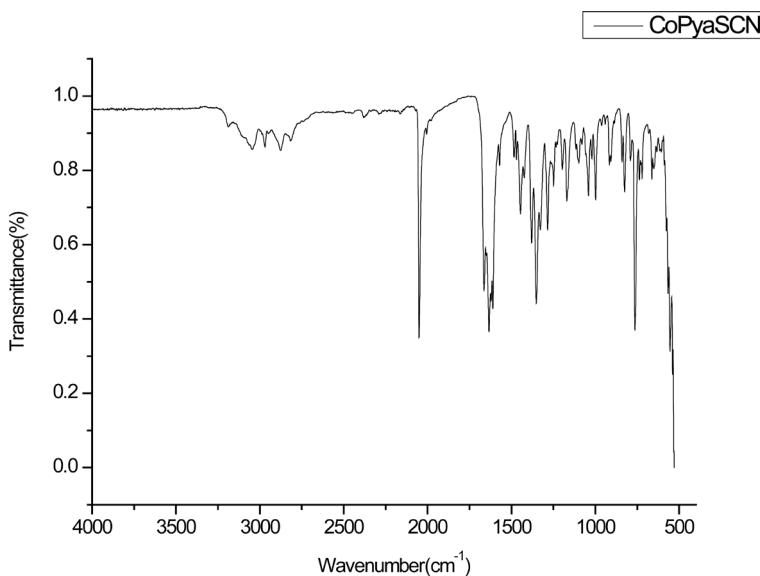
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H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(1)-C(9)-O(2)	123.5(5)
O(1)-C(9)-C(7)	121.3(4)
O(2)-C(9)-C(7)	115.1(4)
N(3)-C(10)-C(11)	122.2(4)
N(3)-C(10)-C(15)	113.3(4)
C(11)-C(10)-C(15)	124.5(4)
C(10)-C(11)-C(12)	118.3(4)
C(10)-C(11)-H(11)	120.8
C(12)-C(11)-H(11)	120.8
C(11)-C(12)-C(13)	119.6(4)
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2
C(14)-C(13)-C(12)	119.3(4)
C(14)-C(13)-H(13)	120.4
C(12)-C(13)-H(13)	120.4
N(3)-C(14)-C(13)	122.1(4)
N(3)-C(14)-H(14)	118.9
C(13)-C(14)-H(14)	118.9
N(4)-C(15)-C(10)	106.7(4)
N(4)-C(15)-H(15A)	110.4
C(10)-C(15)-H(15A)	110.4
N(4)-C(15)-H(15B)	110.4
C(10)-C(15)-H(15B)	110.4
H(15A)-C(15)-H(15B)	108.6
N(4)-C(16)-C(18)	110.6(4)
N(4)-C(16)-C(17)	110.9(4)
C(18)-C(16)-C(17)	108.7(4)
N(4)-C(16)-H(16)	108.9
C(18)-C(16)-H(16)	108.9
C(17)-C(16)-H(16)	108.9
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(3)-C(18)-O(4)	122.9(4)
O(3)-C(18)-C(16)	120.8(4)
O(4)-C(18)-C(16)	116.2(4)
N(5)-C(19)-S(1)	178.9(4)
O(2)-Co(1)-O(4)	86.73(14)
O(2)-Co(1)-N(3)	91.93(13)

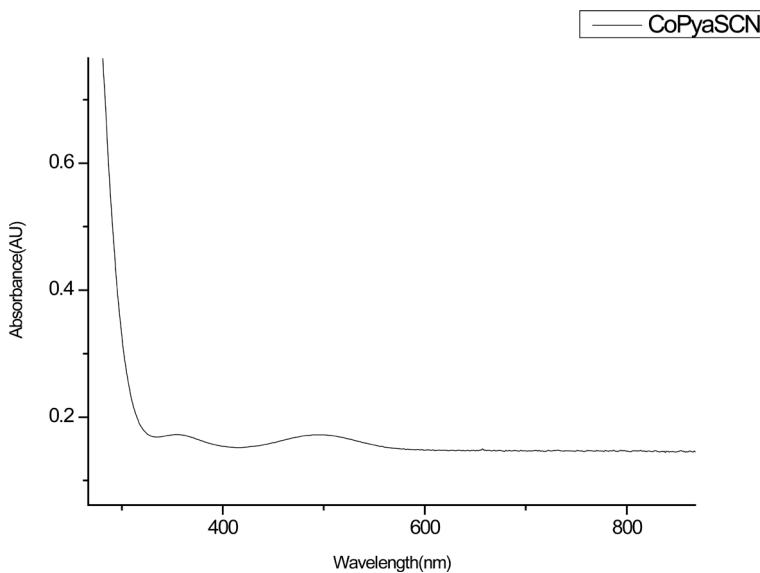
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O(4)-Co(1)-N(3)	88.55(17)
O(2)-Co(1)-N(1)	93.53(13)
O(4)-Co(1)-N(1)	93.77(18)
N(3)-Co(1)-N(1)	174.18(16)
O(2)-Co(1)-N(4)	171.62(16)
O(4)-Co(1)-N(4)	86.88(17)
N(3)-Co(1)-N(4)	82.50(14)
N(1)-Co(1)-N(4)	92.29(14)
O(2)-Co(1)-N(2)	86.41(15)
O(4)-Co(1)-N(2)	172.66(16)
N(3)-Co(1)-N(2)	94.30(18)
N(1)-Co(1)-N(2)	84.03(18)
N(4)-Co(1)-N(2)	100.19(18)
C(5)-N(1)-C(1)	119.0(4)
C(5)-N(1)-Co(1)	126.0(4)
C(1)-N(1)-Co(1)	114.9(3)
C(6)-N(2)-C(7)	111.6(3)
C(6)-N(2)-Co(1)	108.6(3)
C(7)-N(2)-Co(1)	108.8(3)
C(6)-N(2)-H(2A)	108(3)
C(7)-N(2)-H(2A)	106(3)
Co(1)-N(2)-H(2A)	114(4)
C(14)-N(3)-C(10)	118.5(4)
C(14)-N(3)-Co(1)	126.1(3)
C(10)-N(3)-Co(1)	115.1(3)
C(15)-N(4)-C(16)	111.5(3)
C(15)-N(4)-Co(1)	107.5(2)
C(16)-N(4)-Co(1)	108.3(3)
C(15)-N(4)-H(4A)	106(3)
C(16)-N(4)-H(4A)	110(3)
Co(1)-N(4)-H(4A)	113(3)
C(9)-O(2)-Co(1)	116.0(3)
C(18)-O(4)-Co(1)	115.2(3)

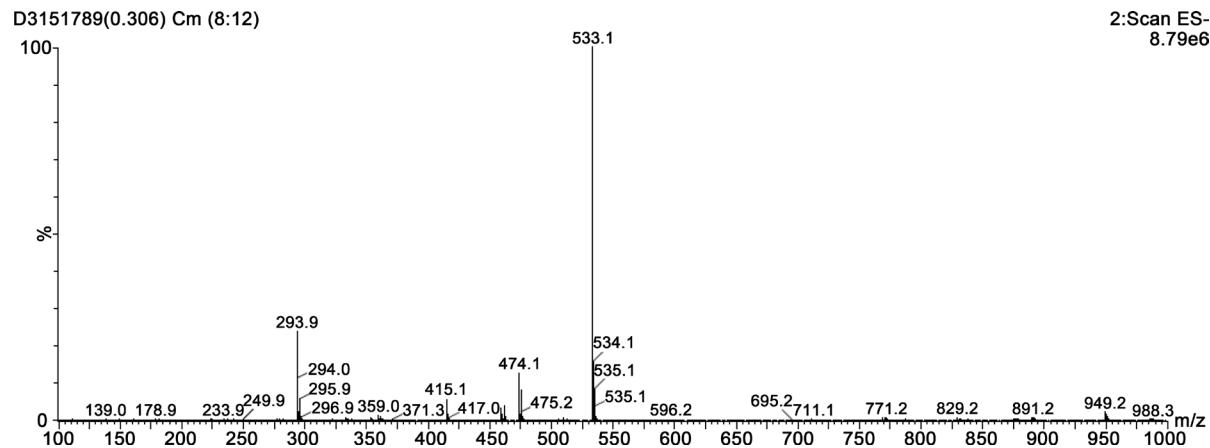
Symmetry transformations used to generate equivalent atoms.



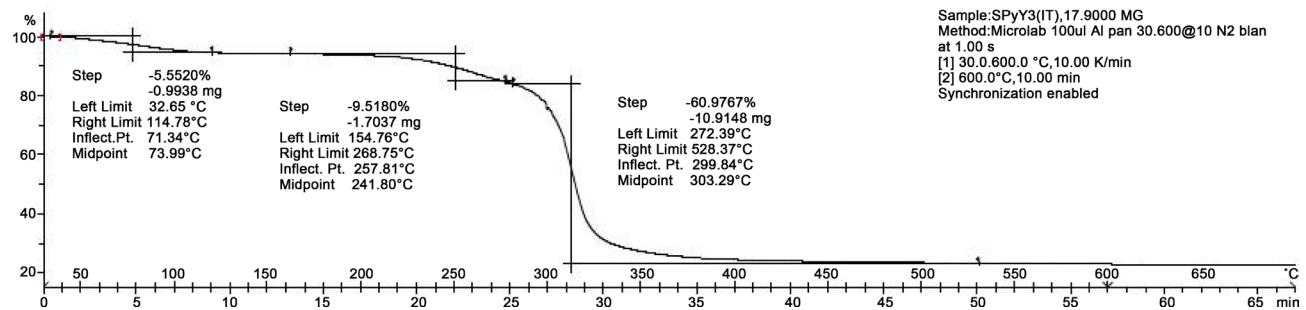
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