



[Tpy₂Co][Co(CO)₄]: a mixed-valent cobalt(III)/cobalt(–I) complex based on phenyltris(pyridin-2-yl)borate (Tpy[–])

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Received 2 February 2026

Accepted 17 April 2026

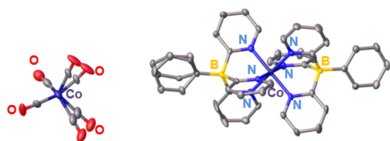
Edited by J. Reibenspies, Texas A & M University, USA

Keywords: crystal structure; scorpionate; tris(pyridin-2-yl)borate; mixed valence.**CCDC reference:** 2547200**Supporting information:** this article has supporting information at journals.iucr.org/e

Tris(pyridin-2-yl)borates are an emerging class of scorpionate ligands. Distinguished by their robustness and nucleophilicity, they have promise as alternatives to tris(pyrazolyl)borates in coordination chemistry, materials applications, and catalysis. In this article, bis[phenyltris(pyridin-2-yl)borato]-cobalt(III) tetracarbonylcobalt(–I) dichloromethane monosolvate, [Co(C₂₁H₁₇BN₃)₂][Co(CO)₄]·CH₂Cl₂ or [Tpy₂Co][Co(CO)₄]·CH₂Cl₂, was prepared by the reaction of hydrogen phenyltris(pyridin-2-yl)borate (TpyH), triethylamine, and Co(CO)₄I. Single-crystal X-ray diffraction resulted in a homoleptic complex consisting of the diamagnetic [Tpy₂Co]⁺ cation and the tetracarbonylcobaltate {[Co(CO)₄][–]} counter-ion. The unusual Co^{III}/Co^{–I} mixed-valence composition presumably results from disproportionation. [Tpy₂Co][Co(CO)₄] represents the first mixed-valence tris(pyridin-2-yl)borate complex.

1. Chemical context

Scorpionate ligands have a wide range of applications in inorganic chemistry and are typified by the tris(pyrazolyl)borate ligands introduced by Trofimenko (Calabrese *et al.*, 1986; Trofimenko, 1966; Trofimenko, 1967; Trofimenko, 1993; Santini *et al.*, 2010). A notable weakness of tris(pyrazolyl)borates is the vulnerability of their metal complexes to hydrolysis and borotropic shifts (Albinati *et al.*, 1997; Biagini *et al.*, 2006; Chisholm *et al.*, 1996; Darensbourg *et al.*, 1996; Kunrath *et al.*, 2003; Lee & Jordan, 2005; Michiue & Jordan, 2004; Trofimenko *et al.*, 1989). In this context, aryltris(pyridin-2-yl)borates have emerged as more robust and electron-donating alternatives (McQuade & Jäkle, 2023; Pawar *et al.*, 2016), which lack the labile B–N and B–H bonds of tris(pyrazolyl)borates and offer advantages for catalysis or coordination studies under demanding conditions. Analogous to tris(pyrazolyl)borates, aryltris(pyridin-2-yl)borates are anionic tripodal ligands with a tendency for facial κ^3 -coordination geometries. Also like tris(pyrazolyl)borates (Abernethy *et al.*, 2008; O'Reilly *et al.*, 1996), aryltris(pyridin-2-yl)borates show a strong preference for octahedral coordination geometries in metal complexes, often as 2:1 homoleptic complexes. Jäkle introduced (Cui *et al.*, 2012) and subsequently studied (Cui *et al.*, 2013; Goura *et al.*, 2022; Jeong *et al.*, 2016; Pawar *et al.*, 2015; Shipman *et al.*, 2013) the aryltris(pyridin-2-yl)borates as octahedral 2:1 homoleptic complexes of divalent and trivalent metal ions (Mg²⁺, Mn²⁺, Fe²⁺, Fe³⁺, Cu²⁺, and Ru²⁺). Our laboratory reported 1:1 complexes of phenyltris(pyridin-2-yl)borate (Tpy[–]) of V⁵⁺ and V³⁺ that are also octahedral (Qian & Comito, 2021; Qian & Comito, 2023). We did obtain tetrahedral organozinc, organoaluminum, and



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organogallium complexes by reaction of TpyH (**1**) with diethylzinc, with trialkylaluminums, and with trimethylgallium (Qian *et al.*, 2024). However, the reaction of TpyH (**1**) with metal amides $M(\text{HMDS})_2$; $M^{2+} = \text{Mg}^{2+}$, Zn^{2+} , or Ca^{2+} ; $\text{HMDS}^- = ^-\text{N}(\text{SiMe}_3)_2$] instead gave homoleptic complexes Tpy_2M (Qian & Comito, 2022).

Consequently, all other metal tris(pyridin-2-yl)borate complexes with coordination numbers less than 6 have used ligands with sterically hindered six-substituted pyridin-2-yl units, which sterically inhibit homoleptic complex formation. Our group introduced the hydrogen phenyltris(6-*R*-pyridin-2-yl)borate Tpy^RH proligands ($R^- = \text{mesityl}$, *tert*-butyl, and isopropyl). From them we prepared the four-coordinate and distorted tetrahedral complexes $\text{Tpy}^{\text{iPr}}\text{Mg}(\text{HMDS})$, $\text{Tpy}^{\text{iPr}}\text{Zn}(\text{HMDS})$, $\text{Tpy}^{\text{iPr}}\text{Ca}(\text{HMDS})$, and $\text{Tpy}^{\text{tBu}}\text{Ca}(\text{HMDS})$ (Qian & Comito, 2022). Hikichi reported the more ideally tetrahedral complex $\text{Tpy}^{\text{Me}}\text{NiBr}$, prepared from hydrogen phenyltris(6-methylpyridin-2-yl)borate ($\text{Tpy}^{\text{Me}}\text{H}$) (Fujiwara *et al.* 2022). Dias studied low-coordinate tris(6-trifluoromethylpyridin-2-yl)borate complexes of coinage metals (Vanga *et al.*, 2022; Watson *et al.*, 2023; Vanga *et al.*, 2024) and of thallium (Vanga *et al.*, 2023), comparing and contrasting them to trifluoromethylated tris(pyrazolyl)borate complexes that they also reported (Dias *et al.*, 1996; Dias & Kim, 1996; Dias & Lovely, 2008; Dias & Jin, 2003) (Fig. 1).

In this context, we targeted a five-coordinate complex $\text{TpyCo}(\text{CO})_2$ as a platform for coordination chemistry and catalysis. Transition-metal carbonyl complexes of Tpy^- would be analogs of the well-known ‘piano-stool’ complexes of

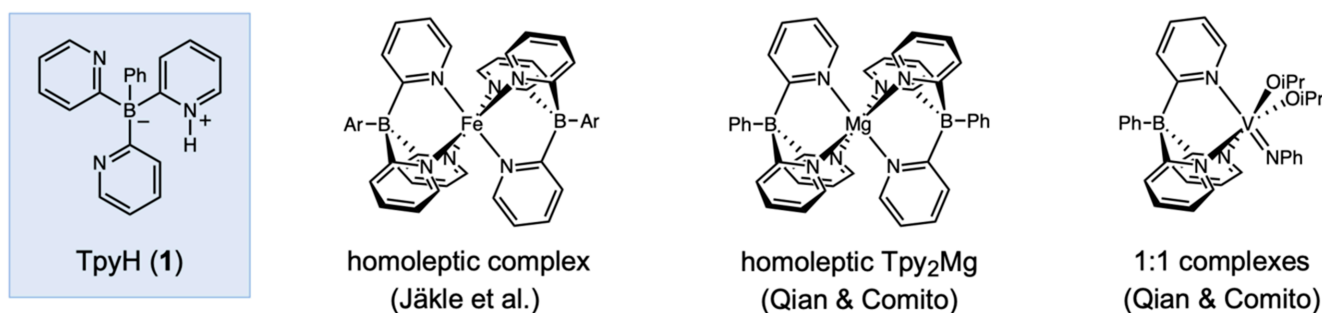
cyclopentadienides (Poli, 1990; Kuo *et al.*, 2018), which often have coordination numbers higher or lower than 6. Given the structural analogy to $\text{CpCo}(\text{CO})_2$ (Nafady *et al.*, 2006) and given that $\text{TpyCo}(\text{CO})_2$ would be 18-electron at cobalt, we reasoned that this complex would be stable despite the lower coordination number. However, the reaction of TpyH (**1**) and triethylamine with $\text{Co}(\text{CO})_4\text{I}$ (**2**), prepared freshly from $\text{Co}_2(\text{CO})_8$ and I_2 , instead gave complex $[\text{Tpy}_2\text{Co}][\text{Co}(\text{CO})_4]$ (**3**) in 81% yield (Fig. 2). ^1H and ^{13}C NMR analysis of this complex results in diamagnetic signals for the Tpy^- unit, indicating a low-spin d^6 $[\text{Tpy}_2\text{Co}]^+$ cation. IR spectroscopy identifies a $\nu(\text{C}=\text{O})$ stretch at 1980 cm^{-1} , consistent with the $\text{Co}(\text{CO})_4^-$ anion (Brennessel & Ellis, 2014). That would make $[\text{Tpy}_2\text{Co}][\text{Co}(\text{CO})_4]$ (**3**) the first mixed-valent tris(pyridin-2-yl)borate complex. The $\text{Co}^{\text{III}}/\text{Co}^{-\text{I}}$ mixed valence is rare, although mixed-valent cobalt complexes with a $\text{Co}(\text{CO})_4^-$ anion are known (see *Database survey*) (Fig. 2).

The structures we obtained reinforce the notion of tris(pyridin-2-yl)borates as ‘octahedral enforcers’, which like tris(pyrazolyl)borates show a much stronger preference for octahedral coordination geometries than do cyclopentadienides.

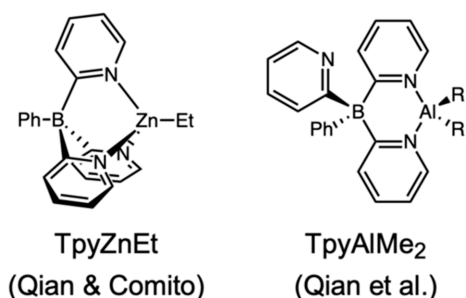
2. Structural commentary

The $[\text{Tpy}_2\text{Co}]^+$ complex showed nearly ideal octahedral coordination, with six N–Co bond lengths between 1.939 (6) and 1.979 (5) Å, and six intraligand N–Co–N bond angles between 90.4 (2) and 91.2 (2)°. The nearly linear N–Co–N

A) Coordination chemistry of aryl tris(2-pyridyl)borates: κ^3 -coordination and pseudo-octahedral geometry.



B) Lower coordination numbers



C) Sterically hindered tris(2-pyridyl)borates:

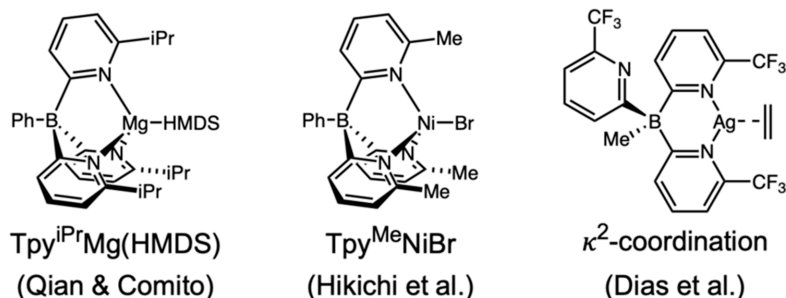


Figure 1

Published aryltris(pyridin-2-yl)borates: (a) octahedral tris(pyridin-2-yl)borate metal complexes, (b) tetrahedral organometallic tris(pyridin-2-yl)borate complexes and (c) sterically hindered tris(pyridin-2-yl)borates with lower coordination numbers.

angles of $\sim 179^\circ$ confirms the symmetry of the complex (Fig. 3).

3. Supramolecular features

There are no significant intermolecular interactions between the $[\text{Tpy}_2\text{Co}]^+$ and $[\text{Co}(\text{CO})_4]^-$ ions.

4. Database survey

A database survey found many single-crystal X-ray diffraction structures of mixed-valent $\text{Co}^{\text{I}}/\text{Co}^{-\text{I}}$ (Hollingsworth *et al.*, 2018; Adamczyk *et al.*, 2011; Azhakar *et al.*, 2012; Luque-Gómez *et al.*, 2023; Luque-Gómez *et al.*, 2025; Chen *et al.*, 2025) and $\text{Co}^{\text{II}}/\text{Co}^{-\text{I}}$ (Uehara *et al.*, 2005; Wang *et al.*, 2022; Kaefer *et al.*, 2021) complexes with a $[\text{Co}(\text{CO})_4]^-$ ion (not an exhaustive list). $\text{Co}^{\text{III}}/\text{Co}^{-\text{I}}$ complexes with a $[\text{Co}(\text{CO})_4]^-$ ion are rare (Petz *et al.*, 2006) with the closest analog being $[\text{Cp}_2\text{Co}][\text{Co}(\text{CO})_4]$ (Cp^- = cyclopentadienide) (Bockman & Kochi, 1988). Interestingly the published $[\text{Cp}_2\text{Co}][\text{Co}(\text{CO})_4]$ salt is pale yellow like $[\text{Tpy}_2\text{Co}][\text{Co}(\text{CO})_4]$ (**3**) reported here.

5. Synthesis and crystallization

5.1. General comments

All manipulations were performed in a nitrogen glovebox using dry degassed solvents unless otherwise noted. Hydrogen phenyltris(pyridin-2-yl)borate (TpyH, **1**) was prepared according to our previous report (Qian & Comito, 2021). NMR spectra were recorded on a JEOL 400 MHz spectrometer. ^1H NMR signals are internally referenced relative to residual proton solvent signals (chloroform-*d* at $\delta = 7.26$ ppm). ^{13}C NMR signals are internally referenced relative to the solvent signal (chloroform-*d* at $\delta = 77.16$). Data for ^1H NMR are reported as follows: chemical shift (δ , ppm), multiplicity (*s* = singlet, *d* = doublet), integration, and coupling constant (Hz). Data for ^{13}C NMR are reported in terms of chemical shift and multiplicity where appropriate. IR spectra were recorded on a Bruker Platinum ATR spectrometer with monolithic diamond crystal plate and are reported in terms of wavenumber of absorption (cm^{-1}). X-ray diffraction data were collected on a Bruker DUO platform diffractometer equipped with a 4K CCD APEXII detector and an Incoatec 30 W Cu microsource with compact multilayer optics. Data were collected using a narrow-frame algorithm with scan widths of 0.50° in ω and a θ

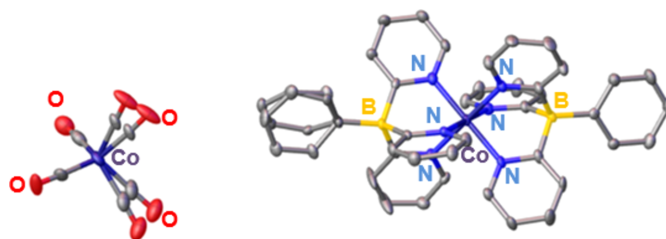


Figure 3
SCXRD structure of $[\text{Tpy}_2\text{Co}][\text{Co}(\text{CO})_4]$ (**3**), with displacement ellipsoids drawn at the 50% probability level for all atoms except hydrogen and the solvent (CH_2Cl_2). All atoms are labeled except for carbon.

dependent exposure time of 10–30 s/frame at 4 cm detector distance.

5.2. Bis[phenyltris(pyridin-2-yl)borato]cobalt(II) tetracarbonylcobalt(−I), $[\text{Tpy}_2\text{Co}][\text{Co}(\text{CO})_4]$ (**3**)

A solution of I_2 (10 mg, 0.039 mmol, 0.66 equiv.) and tetrahydrofuran (2.0 ml) was added to a solution of $\text{Co}_2(\text{CO})_8$ (11 mg, 0.032 mmol, 0.54 equiv.) and tetrahydrofuran (2.0 ml). The combination resulted in a green color. After 2 h in the dark, the solution was concentrated under vacuum to a green solid. The solid was redissolved in CH_2Cl_2 (2.0 ml) and transferred to a solution of hydrogen phenyltris(pyridin-2-yl)borate (TpyH, **1**; 19.4 mg, 0.061 mmol, 1.0 equiv.), triethylamine (9.0 μl , 0.065 mmol, 1.1 equiv.), and CH_2Cl_2 (2.0 ml). After stirring for 18 h in the dark, the reaction was concentrated under vacuum, giving a bright-yellow solid. Crude ^1H NMR analysis resulted in a mixture of the isolated product and a triethylamine-derived product, presumably triethylammonium iodide. The crude product was then removed from the glovebox and partitioned between CH_2Cl_2 (10 ml) and H_2O (10 ml) in a separatory funnel. The aqueous phase was then extracted with CH_2Cl_2 (3×10 ml). The combined CH_2Cl_2 solution was dried over anhydrous Na_2SO_4 and then filtered. Vacuum drying yielded the title compound as a dark-green powder (yield: 0.073 g, 0.081 mmol, 81%). ^1H NMR (400 MHz, CDCl_3): δ 8.08 (*s*, 4H), 7.88 (*s*, 6H), 7.59 (*d*, $J = 54.6$ Hz, 12H), 6.79 (*d*, $J = 49.5$ Hz, 12H). These NMR data matched those of the crude product, before exposure to air and water. ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 137.5, 136.0, 129.7, 128.5, 126.4, 123.6. The two *ipso*-C atoms (B–C) were not observed. IR 2934, 2761, 2679, 2477, 1980, 1900, 1593, 1459, 1419, 1272, 1217, 1163, 1069, 1031, 887, 765, 739, 713, 639,

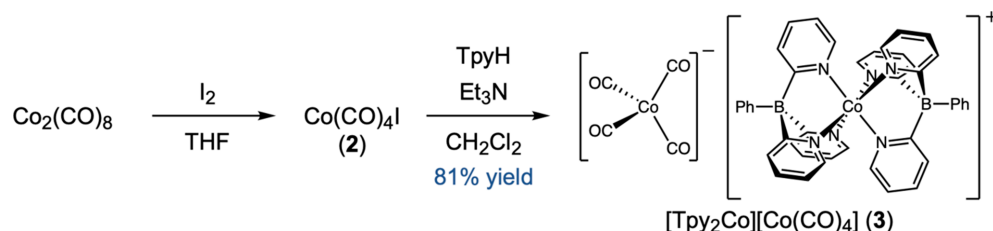


Figure 2
The synthesis of the title compound (**3**).

Table 1
Experimental details.

Crystal data	
Chemical formula	[Co(C ₂₁ H ₁₇ BN ₃) ₂][Co(CO) ₄]-CH ₂ Cl ₂
<i>M_r</i>	959.20
Crystal system, space group	Monoclinic, <i>Cc</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.2341 (5), 22.3721 (13), 20.8218 (14)
β (°)	97.593 (3)
<i>V</i> (Å ³)	4263.8 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.96
Crystal size (mm)	0.27 × 0.25 × 0.01
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Empirical (using intensity measurements) (<i>SADABS</i> ; Bruker, 2025)
<i>T_{min}</i> , <i>T_{max}</i>	0.643, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	45755, 10229, 7481
<i>R_{int}</i>	0.117
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.667
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.061, 0.125, 1.01
No. of reflections	10229
No. of parameters	732
No. of restraints	293
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.83, -0.51
Absolute structure	Flack <i>x</i> determined using 2647 quotients [(<i>I</i> ⁺)-(<i>I</i> ⁻)]/[(<i>I</i> ⁺)+(<i>I</i> ⁻)] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	-0.015 (13)

Computer programs: *APEX6* (Bruker, 2025), *SAINT* (Bruker, 2025), *SHELXT2018* (Sheldrick, 2015a) and *SHELXL2025* (Sheldrick, 2015b).

548, 468 cm⁻¹. Elemental analysis for C₄₀H₂₄B₂N₆O₄CO₂, calculated (%): C 60.55, H 3.05, N 10.61; found (%): C 59.66, H 3.5, N 9.52; difference (%) C 0.89, H 0.45, N 1.09. A crystal suitable for single-crystal X-ray diffraction was obtained as a green needle by vapor diffusion of hexane into a dichloromethane solution of **3** at room temperature in the glovebox.

6. Refinement

All of the H atoms were calculated in idealized positions and refined riding on their parent atoms. Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

The X-ray diffraction data were collected and refined by Dr Xiqu Wang. We also appreciate guidance and discussion by Dr Liton Seikh.

Funding information

Funding for this research was provided by: Welch Foundation (award No. E-2135-20230405); National Science Foundation,

Directorate for Mathematical and Physical Sciences (grant No. 2337696).

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supporting information

Acta Cryst. (2026). E82, 712-716 [https://doi.org/10.1107/S2056989026004093]

[Tpy₂Co][Co(CO)₄]: a mixed-valent cobalt(III)/cobalt(-I) complex based on phenyltris(pyridin-2-yl)borate (Tpy⁻)

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Computing details

Bis[phenyltris(pyridin-2-yl)borato]cobalt(III) tetracarbonylcobalt(-I) dichloromethane monosolvate

Crystal data

[Co(C₂₁H₁₇BN₃)₂][Co(CO)₄]·CH₂Cl₂

M_r = 959.20

Monoclinic, *Cc*

a = 9.2341 (5) Å

b = 22.3721 (13) Å

c = 20.8218 (14) Å

β = 97.593 (3)°

V = 4263.8 (4) Å³

Z = 4

F(000) = 1960

D_x = 1.494 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 4368 reflections

θ = 2.4–20.0°

μ = 0.96 mm⁻¹

T = 100 K

Plate, brown

0.27 × 0.25 × 0.01 mm

Data collection

Bruker D8 Venture
diffractometer

φ and ω scans

Absorption correction: empirical (using
intensity measurements)

(SADABS; Bruker, 2025)

T_{min} = 0.643, *T_{max}* = 0.746

45755 measured reflections

10229 independent reflections

7481 reflections with *I* > 2σ(*I*)

R_{int} = 0.117

θ_{max} = 28.3°, θ_{min} = 2.1°

h = -12→12

k = -29→29

l = -27→26

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.061

wR (*F*²) = 0.125

S = 1.01

10229 reflections

732 parameters

293 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0305*P*)² + 7.1252*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.83 e Å⁻³

Δρ_{min} = -0.51 e Å⁻³

Absolute structure: Flack *x* determined using

2647 quotients [(*I*⁺)-(*I*⁻)]/[(*I*⁺)+(*I*⁻)] (Parsons *et al.*, 2013)

Absolute structure parameter: -0.015 (13)

Special details

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

Refinement. All measurements were made with a Bruker D8 Venture four-circle diffractometer equipped with a Photon III detector, Oxford Cryostream 1000 cooling device and Cu/Mo Incoatec microfocus $I\mu S$ 3.0 sources with HELIOS mirror optics. The data were integrated using the Bruker SAINT program, with the intensities corrected for Lorentz factor, polarization, and background effects. The data were scaled, and an absorption correction was applied using SADABS. The structure was solved with the program SHELXT 2018, and refined with SHELXL 2025 using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters, and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co1	0.16619 (10)	0.42442 (4)	0.39521 (6)	0.01777 (19)	
N1	0.0949 (6)	0.3467 (2)	0.4175 (3)	0.0207 (12)	
N2	-0.0339 (5)	0.4516 (2)	0.3639 (3)	0.0193 (12)	
N3	0.1904 (5)	0.3961 (2)	0.3078 (3)	0.0173 (12)	
N4	0.2414 (5)	0.5026 (2)	0.3731 (3)	0.0202 (12)	
N5	0.1423 (5)	0.4522 (2)	0.4814 (3)	0.0200 (12)	
N6	0.3672 (5)	0.3969 (2)	0.4258 (3)	0.0192 (12)	
C1	-0.1833 (6)	0.3069 (3)	0.2660 (3)	0.0177 (13)	
C2	-0.3318 (7)	0.3067 (3)	0.2743 (4)	0.0260 (16)	
H2	-0.365424	0.335361	0.302539	0.031*	
C3	-0.4314 (8)	0.2663 (3)	0.2432 (4)	0.0316 (17)	
H3	-0.531168	0.268373	0.249736	0.038*	
C4	-0.3867 (8)	0.2236 (3)	0.2029 (4)	0.0325 (18)	
H4	-0.455041	0.196443	0.180791	0.039*	
C5	-0.2410 (8)	0.2206 (3)	0.1951 (4)	0.0263 (16)	
H5	-0.208222	0.190819	0.167864	0.032*	
C6	-0.1422 (7)	0.2608 (3)	0.2266 (3)	0.0199 (14)	
H6	-0.041971	0.256948	0.221243	0.024*	
C7	-0.0093 (7)	0.3194 (3)	0.3766 (3)	0.0192 (14)	
C8	-0.0670 (8)	0.2648 (3)	0.3957 (4)	0.0294 (17)	
H8	-0.140322	0.244886	0.367158	0.035*	
C9	-0.0180 (9)	0.2399 (3)	0.4554 (4)	0.0328 (18)	
H9	-0.058591	0.203528	0.468251	0.039*	
C10	0.0908 (8)	0.2685 (3)	0.4962 (4)	0.0336 (18)	
H10	0.127383	0.251900	0.537098	0.040*	
C11	0.1444 (8)	0.3216 (3)	0.4759 (4)	0.0252 (15)	
H11	0.218763	0.341629	0.503728	0.030*	
C12	-0.1236 (7)	0.4176 (3)	0.3225 (4)	0.0221 (16)	
C13	-0.2555 (7)	0.4430 (3)	0.2936 (4)	0.0285 (17)	
H13	-0.316736	0.420800	0.261935	0.034*	
C14	-0.2982 (7)	0.4997 (3)	0.3102 (4)	0.0301 (17)	
H14	-0.388184	0.516220	0.290682	0.036*	
C15	-0.2077 (7)	0.5315 (3)	0.3553 (4)	0.0285 (17)	

H15	-0.235382	0.569845	0.368976	0.034*	
C16	-0.0758 (7)	0.5066 (3)	0.3805 (4)	0.0240 (15)	
H16	-0.011791	0.529120	0.410727	0.029*	
C17	0.0776 (6)	0.3673 (3)	0.2711 (3)	0.0202 (14)	
C18	0.3124 (7)	0.4105 (3)	0.2816 (4)	0.0229 (15)	
H18	0.390211	0.429587	0.308338	0.027*	
C19	0.3291 (7)	0.3989 (3)	0.2185 (4)	0.0254 (16)	
H19	0.417417	0.408224	0.201853	0.030*	
C20	0.2116 (8)	0.3731 (3)	0.1795 (4)	0.0291 (16)	
H20	0.217064	0.365863	0.134917	0.035*	
C21	0.0883 (7)	0.3580 (3)	0.2057 (3)	0.0228 (15)	
H21	0.008142	0.340852	0.178669	0.027*	
C22	0.1941 (7)	0.5283 (3)	0.3151 (4)	0.0237 (15)	
H22	0.114435	0.510501	0.288261	0.028*	
C23	0.2566 (7)	0.5790 (3)	0.2935 (4)	0.0267 (16)	
H23	0.220306	0.596237	0.252841	0.032*	
C24	0.3736 (8)	0.6044 (3)	0.3324 (4)	0.0275 (16)	
H24	0.422351	0.638299	0.318170	0.033*	
C25	0.4178 (6)	0.5793 (3)	0.3922 (3)	0.0193 (14)	
H25	0.496906	0.596920	0.419516	0.023*	
C26	0.3498 (6)	0.5285 (3)	0.4140 (3)	0.0170 (14)	
C27	0.2516 (6)	0.4826 (3)	0.5166 (3)	0.0164 (13)	
C28	0.2354 (7)	0.4966 (3)	0.5807 (3)	0.0220 (15)	
H28	0.312779	0.516530	0.606831	0.026*	
C29	0.1107 (7)	0.4822 (3)	0.6072 (4)	0.0285 (16)	
H29	0.101608	0.492171	0.650882	0.034*	
C30	-0.0007 (7)	0.4530 (3)	0.5686 (4)	0.0274 (16)	
H30	-0.088733	0.443125	0.585157	0.033*	
C31	0.0173 (7)	0.4388 (3)	0.5073 (4)	0.0224 (15)	
H31	-0.059511	0.418612	0.481070	0.027*	
C32	0.4590 (6)	0.4319 (3)	0.4654 (3)	0.0157 (14)	
C33	0.5985 (8)	0.4097 (4)	0.4851 (5)	0.052 (3)	
H33	0.665919	0.433211	0.512878	0.062*	
C34	0.6412 (9)	0.3542 (4)	0.4653 (6)	0.059 (3)	
H34	0.736993	0.339843	0.479238	0.070*	
C35	0.5451 (7)	0.3205 (3)	0.4258 (4)	0.0255 (16)	
H35	0.572332	0.282100	0.411915	0.031*	
C36	0.4093 (8)	0.3426 (3)	0.4065 (4)	0.0212 (15)	
H36	0.341834	0.319158	0.378721	0.025*	
B1	-0.0656 (7)	0.3510 (3)	0.3071 (4)	0.0194 (16)	
B2	0.3980 (7)	0.4969 (3)	0.4840 (4)	0.0159 (15)	
Co2_5	1.2099 (16)	0.8480 (7)	0.6903 (8)	0.039 (3)	0.369 (17)
O1_5	1.310 (2)	0.7702 (8)	0.5926 (9)	0.048 (5)	0.369 (17)
O2_5	0.9259 (17)	0.8949 (10)	0.6339 (15)	0.066 (6)	0.369 (17)
O3_5	1.206 (3)	0.7871 (19)	0.8129 (15)	0.047 (6)	0.369 (17)
O4_5	1.408 (2)	0.9501 (9)	0.7151 (18)	0.032 (5)	0.369 (17)
C46_5	1.270 (2)	0.8005 (10)	0.6312 (12)	0.038 (4)	0.369 (17)
C47_5	1.037 (2)	0.8750 (11)	0.6579 (16)	0.044 (4)	0.369 (17)

C48_5	1.206 (4)	0.8097 (16)	0.7619 (14)	0.040 (4)	0.369 (17)
C49_5	1.328 (3)	0.9097 (10)	0.7049 (19)	0.034 (4)	0.369 (17)
Co2_6	1.2050 (8)	0.8440 (4)	0.7021 (3)	0.0239 (10)	0.631 (17)
O1_6	1.2172 (18)	0.7556 (5)	0.6000 (5)	0.064 (4)	0.631 (17)
O2_6	0.9458 (10)	0.9188 (5)	0.6774 (6)	0.042 (3)	0.631 (17)
O3_6	1.2367 (19)	0.7831 (10)	0.8280 (7)	0.039 (3)	0.631 (17)
O4_6	1.4403 (13)	0.9316 (6)	0.7139 (9)	0.036 (3)	0.631 (17)
C46_6	1.2139 (17)	0.7907 (6)	0.6405 (6)	0.037 (3)	0.631 (17)
C47_6	1.0446 (11)	0.8877 (6)	0.6873 (7)	0.025 (2)	0.631 (17)
C48_6	1.219 (2)	0.8073 (9)	0.7772 (7)	0.028 (2)	0.631 (17)
C49_6	1.3487 (14)	0.8959 (6)	0.7087 (9)	0.026 (3)	0.631 (17)
Cl1_1	1.0632 (14)	0.6501 (5)	0.4497 (7)	0.110 (4)	0.451 (6)
Cl2_1	0.9607 (6)	0.7228 (3)	0.5467 (3)	0.066 (2)	0.451 (6)
C1_1	0.904 (3)	0.6809 (17)	0.4782 (14)	0.087 (6)	0.451 (6)
H1A_1	0.850180	0.706542	0.444319	0.104*	0.451 (6)
H1B_1	0.838297	0.648450	0.488647	0.104*	0.451 (6)
Cl1_2	1.0929 (8)	0.6542 (3)	0.4223 (4)	0.0492 (15)	0.549 (6)
Cl2_2	0.9031 (7)	0.6191 (2)	0.5147 (3)	0.0768 (19)	0.549 (6)
C1_2	0.958 (2)	0.6787 (9)	0.4713 (9)	0.046 (4)	0.549 (6)
H1A_2	0.999634	0.710368	0.501401	0.056*	0.549 (6)
H1B_2	0.872815	0.695525	0.443254	0.056*	0.549 (6)
C1_3	0.5022 (16)	0.5381 (8)	0.5352 (9)	0.016 (3)	0.549 (6)
C2_3	0.4597 (18)	0.5972 (8)	0.5414 (9)	0.018 (3)	0.549 (6)
H2_3	0.378877	0.611885	0.512764	0.022*	0.549 (6)
C3_3	0.530 (2)	0.6357 (11)	0.5876 (13)	0.021 (3)	0.549 (6)
H3_3	0.493817	0.675021	0.591754	0.025*	0.549 (6)
C4_3	0.6538 (13)	0.6172 (5)	0.6276 (6)	0.022 (2)	0.549 (6)
H4_3	0.709056	0.644470	0.655940	0.027*	0.549 (6)
C5_3	0.6943 (12)	0.5583 (5)	0.6252 (6)	0.019 (2)	0.549 (6)
H5_3	0.775145	0.544146	0.654155	0.023*	0.549 (6)
C6_3	0.6188 (11)	0.5192 (5)	0.5810 (6)	0.018 (2)	0.549 (6)
H6_3	0.646932	0.478370	0.581782	0.022*	0.549 (6)
C1_4	0.506 (2)	0.5441 (10)	0.5268 (13)	0.024 (3)	0.451 (6)
C2_4	0.446 (2)	0.5951 (10)	0.5513 (12)	0.024 (3)	0.451 (6)
H2_4	0.342908	0.600432	0.543357	0.029*	0.451 (6)
C3_4	0.529 (3)	0.6385 (13)	0.5870 (18)	0.027 (3)	0.451 (6)
H3_4	0.483178	0.673616	0.600335	0.033*	0.451 (6)
C4_4	0.6780 (18)	0.6309 (7)	0.6029 (9)	0.030 (3)	0.451 (6)
H4_4	0.733622	0.657263	0.632241	0.036*	0.451 (6)
C5_4	0.7426 (16)	0.5845 (6)	0.5756 (8)	0.031 (3)	0.451 (6)
H5_4	0.845933	0.580670	0.582671	0.037*	0.451 (6)
C6_4	0.6590 (15)	0.5418 (6)	0.5367 (8)	0.028 (3)	0.451 (6)
H6_4	0.707624	0.510871	0.516811	0.033*	0.451 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0131 (4)	0.0176 (4)	0.0211 (5)	0.0003 (3)	-0.0035 (3)	-0.0019 (4)

N1	0.021 (3)	0.020 (3)	0.021 (3)	0.004 (2)	0.001 (2)	0.004 (2)
N2	0.016 (2)	0.017 (3)	0.023 (3)	0.001 (2)	-0.001 (2)	-0.002 (2)
N3	0.014 (2)	0.017 (3)	0.019 (3)	0.001 (2)	-0.004 (2)	0.000 (2)
N4	0.017 (3)	0.020 (3)	0.023 (3)	-0.001 (2)	-0.003 (2)	-0.005 (2)
N5	0.016 (2)	0.019 (3)	0.025 (3)	0.000 (2)	-0.001 (2)	0.000 (2)
N6	0.016 (3)	0.017 (3)	0.022 (3)	0.004 (2)	-0.003 (2)	0.000 (2)
C1	0.019 (3)	0.018 (3)	0.016 (4)	0.000 (2)	-0.002 (3)	0.004 (3)
C2	0.023 (3)	0.028 (4)	0.027 (4)	-0.004 (3)	0.003 (3)	-0.004 (3)
C3	0.021 (3)	0.035 (4)	0.037 (5)	-0.010 (3)	-0.002 (3)	-0.001 (4)
C4	0.031 (4)	0.028 (4)	0.036 (5)	-0.014 (3)	-0.006 (3)	-0.003 (3)
C5	0.033 (4)	0.018 (3)	0.025 (4)	-0.003 (3)	-0.003 (3)	0.000 (3)
C6	0.019 (3)	0.022 (3)	0.019 (4)	-0.001 (3)	0.001 (3)	0.002 (3)
C7	0.016 (3)	0.023 (3)	0.017 (4)	0.002 (3)	-0.002 (3)	-0.002 (3)
C8	0.029 (4)	0.025 (4)	0.033 (5)	-0.009 (3)	0.000 (3)	-0.004 (3)
C9	0.048 (5)	0.020 (4)	0.027 (5)	-0.013 (3)	-0.005 (4)	0.004 (3)
C10	0.041 (4)	0.030 (4)	0.026 (5)	-0.005 (3)	-0.009 (3)	0.008 (3)
C11	0.030 (4)	0.020 (3)	0.024 (4)	-0.002 (3)	-0.005 (3)	0.001 (3)
C12	0.018 (3)	0.021 (3)	0.026 (4)	-0.005 (3)	-0.001 (3)	-0.002 (3)
C13	0.019 (3)	0.023 (4)	0.041 (5)	0.001 (3)	-0.006 (3)	-0.007 (3)
C14	0.019 (3)	0.028 (4)	0.040 (5)	0.011 (3)	-0.007 (3)	0.002 (3)
C15	0.019 (3)	0.027 (4)	0.038 (5)	0.009 (3)	0.003 (3)	-0.004 (3)
C16	0.021 (3)	0.022 (4)	0.027 (4)	0.000 (3)	-0.006 (3)	0.000 (3)
C17	0.017 (3)	0.019 (3)	0.023 (4)	0.000 (2)	-0.004 (3)	0.004 (3)
C18	0.015 (3)	0.029 (4)	0.024 (4)	-0.002 (3)	-0.002 (3)	0.001 (3)
C19	0.018 (3)	0.036 (4)	0.022 (4)	-0.009 (3)	0.000 (3)	0.003 (3)
C20	0.030 (4)	0.041 (4)	0.015 (4)	-0.007 (3)	-0.003 (3)	0.005 (3)
C21	0.026 (3)	0.025 (3)	0.014 (4)	-0.008 (3)	-0.008 (3)	0.001 (3)
C22	0.020 (3)	0.023 (3)	0.026 (4)	0.006 (3)	-0.006 (3)	0.000 (3)
C23	0.032 (4)	0.022 (3)	0.023 (4)	0.003 (3)	-0.008 (3)	0.002 (3)
C24	0.029 (4)	0.022 (3)	0.031 (5)	-0.003 (3)	0.003 (3)	0.003 (3)
C25	0.017 (3)	0.017 (3)	0.023 (4)	-0.004 (2)	0.000 (3)	-0.006 (3)
C26	0.013 (3)	0.017 (3)	0.022 (4)	0.001 (2)	0.002 (3)	-0.002 (3)
C27	0.019 (3)	0.014 (3)	0.015 (4)	0.002 (2)	-0.003 (3)	-0.001 (3)
C28	0.017 (3)	0.029 (4)	0.020 (4)	-0.004 (3)	0.000 (3)	0.003 (3)
C29	0.022 (3)	0.044 (4)	0.020 (4)	-0.006 (3)	0.004 (3)	0.000 (3)
C30	0.019 (3)	0.036 (4)	0.027 (5)	-0.006 (3)	0.006 (3)	0.000 (3)
C31	0.015 (3)	0.025 (3)	0.026 (4)	-0.002 (3)	-0.001 (3)	-0.002 (3)
C32	0.011 (3)	0.021 (3)	0.015 (4)	-0.001 (2)	-0.001 (3)	0.004 (3)
C33	0.023 (4)	0.033 (4)	0.090 (8)	0.005 (3)	-0.028 (4)	-0.029 (5)
C34	0.022 (4)	0.037 (5)	0.109 (9)	0.008 (3)	-0.021 (5)	-0.028 (5)
C35	0.025 (3)	0.019 (3)	0.033 (4)	0.005 (3)	0.006 (3)	0.001 (3)
C36	0.025 (3)	0.018 (3)	0.020 (4)	0.001 (3)	0.001 (3)	-0.003 (3)
B1	0.013 (3)	0.018 (3)	0.027 (5)	-0.001 (3)	0.000 (3)	0.002 (3)
B2	0.014 (3)	0.017 (3)	0.016 (4)	-0.001 (3)	-0.003 (3)	-0.001 (3)
Co2_5	0.018 (3)	0.036 (3)	0.063 (6)	0.0030 (19)	0.008 (3)	0.009 (3)
O1_5	0.027 (8)	0.048 (9)	0.062 (10)	0.000 (7)	-0.014 (7)	-0.016 (7)
O2_5	0.025 (6)	0.068 (11)	0.104 (14)	0.006 (7)	0.008 (8)	0.051 (10)
O3_5	0.015 (10)	0.057 (11)	0.065 (12)	0.003 (9)	-0.008 (10)	0.018 (10)

O4_5	0.018 (8)	0.044 (9)	0.035 (9)	0.002 (6)	0.008 (8)	-0.007 (9)
C46_5	0.015 (6)	0.037 (6)	0.061 (8)	-0.002 (5)	0.003 (6)	0.004 (5)
C47_5	0.022 (5)	0.039 (7)	0.070 (9)	0.001 (5)	0.007 (6)	0.022 (6)
C48_5	0.018 (6)	0.039 (7)	0.064 (8)	0.003 (6)	0.006 (6)	0.011 (6)
C49_5	0.019 (6)	0.035 (6)	0.052 (8)	0.007 (5)	0.013 (6)	0.005 (6)
Co2_6	0.0159 (15)	0.0308 (17)	0.0237 (17)	-0.0011 (11)	-0.0021 (12)	0.0013 (13)
O1_6	0.090 (9)	0.057 (6)	0.041 (6)	0.011 (7)	-0.004 (6)	-0.015 (5)
O2_6	0.020 (4)	0.053 (6)	0.053 (7)	0.009 (4)	0.003 (5)	0.024 (5)
O3_6	0.026 (8)	0.056 (7)	0.031 (6)	0.005 (6)	-0.012 (5)	0.015 (5)
O4_6	0.023 (6)	0.056 (8)	0.028 (6)	-0.016 (5)	0.004 (5)	-0.001 (7)
C46_6	0.040 (5)	0.038 (5)	0.030 (5)	0.003 (4)	-0.006 (5)	-0.002 (4)
C47_6	0.016 (4)	0.034 (5)	0.024 (5)	-0.005 (3)	0.001 (4)	0.009 (4)
C48_6	0.019 (5)	0.035 (5)	0.027 (4)	-0.001 (4)	-0.006 (4)	0.005 (4)
C49_6	0.016 (4)	0.041 (5)	0.023 (5)	-0.002 (4)	0.005 (4)	-0.002 (5)
Cl1_1	0.085 (7)	0.058 (5)	0.180 (12)	0.005 (5)	-0.005 (7)	-0.050 (7)
Cl2_1	0.058 (3)	0.081 (4)	0.050 (4)	-0.028 (3)	-0.021 (3)	0.026 (3)
C1_1	0.074 (10)	0.067 (10)	0.113 (11)	-0.003 (9)	-0.012 (10)	-0.011 (10)
Cl1_2	0.055 (3)	0.024 (2)	0.074 (4)	0.0028 (19)	0.032 (3)	-0.003 (2)
Cl2_2	0.114 (4)	0.065 (3)	0.060 (3)	-0.024 (3)	0.040 (3)	0.001 (2)
C1_2	0.070 (8)	0.031 (6)	0.047 (7)	-0.004 (7)	0.040 (7)	0.000 (6)
C1_3	0.010 (4)	0.024 (5)	0.015 (5)	-0.002 (4)	0.004 (4)	0.001 (4)
C2_3	0.016 (5)	0.024 (5)	0.016 (5)	-0.001 (4)	0.003 (4)	0.004 (4)
C3_3	0.022 (5)	0.027 (5)	0.015 (5)	-0.003 (4)	0.005 (4)	0.001 (4)
C4_3	0.021 (4)	0.031 (4)	0.015 (5)	-0.009 (4)	0.002 (4)	0.000 (4)
C5_3	0.014 (4)	0.031 (4)	0.013 (5)	-0.004 (3)	0.000 (3)	-0.003 (4)
C6_3	0.014 (4)	0.027 (4)	0.014 (5)	0.000 (3)	0.003 (3)	-0.002 (4)
C1_4	0.024 (5)	0.018 (6)	0.029 (7)	-0.005 (5)	0.001 (5)	0.003 (5)
C2_4	0.026 (6)	0.018 (6)	0.029 (7)	-0.007 (5)	0.003 (6)	0.001 (6)
C3_4	0.030 (6)	0.020 (6)	0.030 (7)	-0.008 (5)	0.001 (6)	0.000 (5)
C4_4	0.031 (6)	0.023 (5)	0.033 (7)	-0.010 (5)	-0.006 (5)	0.001 (5)
C5_4	0.028 (5)	0.025 (5)	0.035 (6)	-0.004 (4)	-0.005 (5)	0.005 (5)
C6_4	0.025 (5)	0.024 (5)	0.033 (7)	-0.004 (4)	-0.002 (5)	0.004 (5)

Geometric parameters (Å, °)

Co1—N1	1.937 (5)	C27—C28	1.397 (9)
Co1—N5	1.939 (6)	C27—B2	1.623 (9)
Co1—N4	1.960 (5)	C28—C29	1.379 (9)
Co1—N3	1.968 (6)	C28—H28	0.9500
Co1—N2	1.972 (5)	C29—C30	1.383 (10)
Co1—N6	1.979 (5)	C29—H29	0.9500
N1—C7	1.344 (8)	C30—C31	1.348 (10)
N1—C11	1.363 (9)	C30—H30	0.9500
N2—C12	1.348 (8)	C31—H31	0.9500
N2—C16	1.349 (8)	C32—C33	1.391 (9)
N3—C18	1.354 (8)	C32—B2	1.624 (9)
N3—C17	1.368 (8)	C33—C34	1.382 (11)
N4—C26	1.356 (8)	C33—H33	0.9500

N4—C22	1.356 (9)	C34—C35	1.357 (11)
N5—C27	1.351 (8)	C34—H34	0.9500
N5—C31	1.371 (8)	C35—C36	1.359 (9)
N6—C32	1.351 (8)	C35—H35	0.9500
N6—C36	1.353 (8)	C36—H36	0.9500
C1—C6	1.403 (9)	B2—C1_3	1.625 (18)
C1—C2	1.404 (9)	B2—C1_4	1.63 (2)
C1—B1	1.625 (9)	Co2_5—C48_5	1.725 (19)
C2—C3	1.387 (10)	Co2_5—C47_5	1.752 (17)
C2—H2	0.9500	Co2_5—C49_5	1.762 (17)
C3—C4	1.371 (10)	Co2_5—C46_5	1.769 (18)
C3—H3	0.9500	O1_5—C46_5	1.147 (19)
C4—C5	1.379 (10)	O2_5—C47_5	1.172 (19)
C4—H4	0.9500	O3_5—C48_5	1.18 (2)
C5—C6	1.382 (9)	O4_5—C49_5	1.169 (19)
C5—H5	0.9500	Co2_6—C49_6	1.755 (11)
C6—H6	0.9500	Co2_6—C48_6	1.757 (12)
C7—C8	1.411 (9)	Co2_6—C46_6	1.760 (12)
C7—B1	1.633 (10)	Co2_6—C47_6	1.767 (11)
C8—C9	1.383 (11)	O1_6—C46_6	1.156 (13)
C8—H8	0.9500	O2_6—C47_6	1.145 (12)
C9—C10	1.383 (10)	O3_6—C48_6	1.179 (14)
C9—H9	0.9500	O4_6—C49_6	1.157 (13)
C10—C11	1.375 (10)	C11_1—C1_1	1.79 (2)
C10—H10	0.9500	C12_1—C1_1	1.73 (3)
C11—H11	0.9500	C1_1—H1A_1	0.9900
C12—C13	1.405 (9)	C1_1—H1B_1	0.9900
C12—B1	1.629 (9)	C11_2—C1_2	1.797 (15)
C13—C14	1.386 (9)	C12_2—C1_2	1.724 (18)
C13—H13	0.9500	C1_2—H1A_2	0.9900
C14—C15	1.370 (10)	C1_2—H1B_2	0.9900
C14—H14	0.9500	C1_3—C2_3	1.391 (16)
C15—C16	1.378 (9)	C1_3—C6_3	1.406 (16)
C15—H15	0.9500	C2_3—C3_3	1.388 (16)
C16—H16	0.9500	C2_3—H2_3	0.9500
C17—C21	1.395 (10)	C3_3—C4_3	1.383 (18)
C17—B1	1.644 (9)	C3_3—H3_3	0.9500
C18—C19	1.368 (10)	C4_3—C5_3	1.371 (15)
C18—H18	0.9500	C4_3—H4_3	0.9500
C19—C20	1.392 (10)	C5_3—C6_3	1.389 (15)
C19—H19	0.9500	C5_3—H5_3	0.9500
C20—C21	1.368 (10)	C6_3—H6_3	0.9500
C20—H20	0.9500	C1_4—C2_4	1.394 (19)
C21—H21	0.9500	C1_4—C6_4	1.41 (2)
C22—C23	1.375 (9)	C2_4—C3_4	1.391 (18)
C22—H22	0.9500	C2_4—H2_4	0.9500
C23—C24	1.383 (10)	C3_4—C4_4	1.38 (2)
C23—H23	0.9500	C3_4—H3_4	0.9500

C24—C25	1.378 (10)	C4_4—C5_4	1.359 (18)
C24—H24	0.9500	C4_4—H4_4	0.9500
C25—C26	1.402 (8)	C5_4—C6_4	1.413 (18)
C25—H25	0.9500	C5_4—H5_4	0.9500
C26—B2	1.629 (10)	C6_4—H6_4	0.9500
N1—Co1—N5	89.0 (2)	N5—C27—B2	118.4 (6)
N1—Co1—N4	179.1 (2)	C28—C27—B2	123.8 (6)
N5—Co1—N4	91.1 (2)	C29—C28—C27	122.1 (6)
N1—Co1—N3	90.9 (2)	C29—C28—H28	119.0
N5—Co1—N3	179.9 (2)	C27—C28—H28	119.0
N4—Co1—N3	89.0 (2)	C28—C29—C30	118.3 (7)
N1—Co1—N2	91.3 (2)	C28—C29—H29	120.9
N5—Co1—N2	89.5 (2)	C30—C29—H29	120.9
N4—Co1—N2	89.6 (2)	C31—C30—C29	119.2 (6)
N3—Co1—N2	90.5 (2)	C31—C30—H30	120.4
N1—Co1—N6	88.7 (2)	C29—C30—H30	120.4
N5—Co1—N6	91.1 (2)	C30—C31—N5	122.5 (6)
N4—Co1—N6	90.4 (2)	C30—C31—H31	118.8
N3—Co1—N6	88.9 (2)	N5—C31—H31	118.8
N2—Co1—N6	179.4 (3)	N6—C32—C33	117.1 (6)
C7—N1—C11	120.4 (5)	N6—C32—B2	117.1 (5)
C7—N1—Co1	119.6 (5)	C33—C32—B2	125.8 (6)
C11—N1—Co1	119.9 (5)	C34—C33—C32	121.4 (7)
C12—N2—C16	120.4 (6)	C34—C33—H33	119.3
C12—N2—Co1	120.5 (4)	C32—C33—H33	119.3
C16—N2—Co1	119.0 (4)	C35—C34—C33	119.5 (7)
C18—N3—C17	120.0 (6)	C35—C34—H34	120.3
C18—N3—Co1	119.9 (4)	C33—C34—H34	120.3
C17—N3—Co1	119.7 (4)	C34—C35—C36	118.7 (6)
C26—N4—C22	120.2 (6)	C34—C35—H35	120.6
C26—N4—Co1	119.2 (4)	C36—C35—H35	120.6
C22—N4—Co1	120.3 (4)	N6—C36—C35	122.0 (6)
C27—N5—C31	120.3 (6)	N6—C36—H36	119.0
C27—N5—Co1	119.8 (4)	C35—C36—H36	119.0
C31—N5—Co1	119.9 (5)	C1—B1—C12	116.4 (5)
C32—N6—C36	121.3 (6)	C1—B1—C7	108.4 (5)
C32—N6—Co1	120.1 (4)	C12—B1—C7	107.2 (6)
C36—N6—Co1	118.6 (5)	C1—B1—C17	114.7 (6)
C6—C1—C2	114.4 (6)	C12—B1—C17	101.1 (5)
C6—C1—B1	122.7 (5)	C7—B1—C17	108.6 (5)
C2—C1—B1	122.3 (6)	C27—B2—C32	105.0 (5)
C3—C2—C1	122.9 (7)	C27—B2—C1_3	106.8 (8)
C3—C2—H2	118.5	C32—B2—C1_3	118.1 (7)
C1—C2—H2	118.5	C27—B2—C26	108.4 (5)
C4—C3—C2	120.3 (7)	C32—B2—C26	103.8 (5)
C4—C3—H3	119.8	C1_3—B2—C26	114.1 (8)
C2—C3—H3	119.8	C27—B2—C1_4	112.3 (11)

C3—C4—C5	118.9 (7)	C32—B2—C1_4	120.3 (9)
C3—C4—H4	120.5	C26—B2—C1_4	106.4 (10)
C5—C4—H4	120.5	C48_5—Co2_5—C47_5	112.4 (14)
C4—C5—C6	120.4 (7)	C48_5—Co2_5—C49_5	108.8 (16)
C4—C5—H5	119.8	C47_5—Co2_5—C49_5	108.0 (13)
C6—C5—H5	119.8	C48_5—Co2_5—C46_5	110.3 (14)
C5—C6—C1	122.9 (6)	C47_5—Co2_5—C46_5	107.0 (13)
C5—C6—H6	118.6	C49_5—Co2_5—C46_5	110.3 (14)
C1—C6—H6	118.6	O1_5—C46_5—Co2_5	179 (2)
N1—C7—C8	118.7 (6)	O2_5—C47_5—Co2_5	176 (2)
N1—C7—B1	118.8 (5)	O3_5—C48_5—Co2_5	175 (4)
C8—C7—B1	122.5 (6)	O4_5—C49_5—Co2_5	179 (3)
C9—C8—C7	120.7 (7)	C49_6—Co2_6—C48_6	105.8 (8)
C9—C8—H8	119.6	C49_6—Co2_6—C46_6	113.5 (8)
C7—C8—H8	119.6	C48_6—Co2_6—C46_6	109.1 (8)
C8—C9—C10	119.4 (6)	C49_6—Co2_6—C47_6	104.8 (7)
C8—C9—H9	120.3	C48_6—Co2_6—C47_6	112.0 (8)
C10—C9—H9	120.3	C46_6—Co2_6—C47_6	111.5 (7)
C11—C10—C9	118.2 (7)	O1_6—C46_6—Co2_6	178.9 (14)
C11—C10—H10	120.9	O2_6—C47_6—Co2_6	176.0 (11)
C9—C10—H10	120.9	O3_6—C48_6—Co2_6	176.4 (15)
N1—C11—C10	122.5 (7)	O4_6—C49_6—Co2_6	177.6 (14)
N1—C11—H11	118.7	Cl2_1—C1_1—Cl1_1	108.0 (14)
C10—C11—H11	118.7	Cl2_1—C1_1—H1A_1	110.1
N2—C12—C13	118.0 (6)	Cl1_1—C1_1—H1A_1	110.1
N2—C12—B1	116.8 (6)	Cl2_1—C1_1—H1B_1	110.1
C13—C12—B1	125.1 (6)	Cl1_1—C1_1—H1B_1	110.1
C14—C13—C12	121.5 (7)	H1A_1—C1_1—H1B_1	108.4
C14—C13—H13	119.2	Cl2_2—C1_2—Cl1_2	109.7 (10)
C12—C13—H13	119.2	Cl2_2—C1_2—H1A_2	109.7
C15—C14—C13	118.5 (6)	Cl1_2—C1_2—H1A_2	109.7
C15—C14—H14	120.7	Cl2_2—C1_2—H1B_2	109.7
C13—C14—H14	120.7	Cl1_2—C1_2—H1B_2	109.7
C14—C15—C16	118.6 (6)	H1A_2—C1_2—H1B_2	108.2
C14—C15—H15	120.7	C2_3—C1_3—C6_3	115.0 (14)
C16—C15—H15	120.7	C2_3—C1_3—B2	116.8 (12)
N2—C16—C15	122.7 (6)	C6_3—C1_3—B2	127.5 (13)
N2—C16—H16	118.6	C3_3—C2_3—C1_3	122.8 (15)
C15—C16—H16	118.6	C3_3—C2_3—H2_3	118.6
N3—C17—C21	117.9 (6)	C1_3—C2_3—H2_3	118.6
N3—C17—B1	116.7 (6)	C4_3—C3_3—C2_3	120.4 (15)
C21—C17—B1	125.2 (6)	C4_3—C3_3—H3_3	119.8
N3—C18—C19	123.2 (6)	C2_3—C3_3—H3_3	119.8
N3—C18—H18	118.4	C5_3—C4_3—C3_3	118.3 (13)
C19—C18—H18	118.4	C5_3—C4_3—H4_3	120.9
C18—C19—C20	117.4 (6)	C3_3—C4_3—H4_3	120.9
C18—C19—H19	121.3	C4_3—C5_3—C6_3	120.9 (11)
C20—C19—H19	121.3	C4_3—C5_3—H5_3	119.6

C21—C20—C19	119.7 (7)	C6 ₃ —C5 ₃ —H5 ₃	119.6
C21—C20—H20	120.1	C5 ₃ —C6 ₃ —C1 ₃	122.2 (12)
C19—C20—H20	120.1	C5 ₃ —C6 ₃ —H6 ₃	118.9
C20—C21—C17	121.6 (6)	C1 ₃ —C6 ₃ —H6 ₃	118.9
C20—C21—H21	119.2	C2 ₄ —C1 ₄ —C6 ₄	114.5 (18)
C17—C21—H21	119.2	C2 ₄ —C1 ₄ —B2	119.3 (16)
N4—C22—C23	122.7 (7)	C6 ₄ —C1 ₄ —B2	125.9 (18)
N4—C22—H22	118.7	C3 ₄ —C2 ₄ —C1 ₄	123.4 (19)
C23—C22—H22	118.7	C3 ₄ —C2 ₄ —H2 ₄	118.3
C22—C23—C24	118.4 (7)	C1 ₄ —C2 ₄ —H2 ₄	118.3
C22—C23—H23	120.8	C4 ₄ —C3 ₄ —C2 ₄	120 (2)
C24—C23—H23	120.8	C4 ₄ —C3 ₄ —H3 ₄	119.9
C25—C24—C23	118.5 (6)	C2 ₄ —C3 ₄ —H3 ₄	119.9
C25—C24—H24	120.7	C5 ₄ —C4 ₄ —C3 ₄	118.2 (16)
C23—C24—H24	120.7	C5 ₄ —C4 ₄ —H4 ₄	120.9
C24—C25—C26	122.0 (6)	C3 ₄ —C4 ₄ —H4 ₄	120.9
C24—C25—H25	119.0	C4 ₄ —C5 ₄ —C6 ₄	121.2 (14)
C26—C25—H25	119.0	C4 ₄ —C5 ₄ —H5 ₄	119.4
N4—C26—C25	117.9 (6)	C6 ₄ —C5 ₄ —H5 ₄	119.4
N4—C26—B2	118.0 (5)	C1 ₄ —C6 ₄ —C5 ₄	121.6 (16)
C25—C26—B2	124.1 (6)	C1 ₄ —C6 ₄ —H6 ₄	119.2
N5—C27—C28	117.7 (5)	C5 ₄ —C6 ₄ —H6 ₄	119.2
C6—C1—C2—C3	-3.6 (10)	C2—C1—B1—C12	-36.4 (9)
B1—C1—C2—C3	-175.2 (7)	C6—C1—B1—C7	-86.5 (7)
C1—C2—C3—C4	1.1 (12)	C2—C1—B1—C7	84.4 (7)
C2—C3—C4—C5	1.3 (12)	C6—C1—B1—C17	35.1 (9)
C3—C4—C5—C6	-1.0 (11)	C2—C1—B1—C17	-154.0 (6)
C4—C5—C6—C1	-1.8 (11)	N2—C12—B1—C1	171.1 (6)
C2—C1—C6—C5	3.9 (10)	C13—C12—B1—C1	-12.3 (10)
B1—C1—C6—C5	175.5 (6)	N2—C12—B1—C7	49.6 (7)
C11—N1—C7—C8	0.5 (9)	C13—C12—B1—C7	-133.8 (7)
Co1—N1—C7—C8	-175.6 (5)	N2—C12—B1—C17	-64.0 (8)
C11—N1—C7—B1	179.9 (6)	C13—C12—B1—C17	112.6 (7)
Co1—N1—C7—B1	3.8 (8)	N1—C7—B1—C1	176.6 (5)
N1—C7—C8—C9	0.4 (10)	C8—C7—B1—C1	-4.0 (8)
B1—C7—C8—C9	-179.0 (7)	N1—C7—B1—C12	-57.0 (7)
C7—C8—C9—C10	-1.2 (11)	C8—C7—B1—C12	122.4 (6)
C8—C9—C10—C11	1.1 (12)	N1—C7—B1—C17	51.4 (8)
C7—N1—C11—C10	-0.6 (10)	C8—C7—B1—C17	-129.2 (6)
Co1—N1—C11—C10	175.6 (6)	N3—C17—B1—C1	-169.7 (5)
C9—C10—C11—N1	-0.3 (11)	C21—C17—B1—C1	15.1 (9)
C16—N2—C12—C13	5.0 (10)	N3—C17—B1—C12	64.3 (7)
Co1—N2—C12—C13	-169.8 (5)	C21—C17—B1—C12	-110.9 (7)
C16—N2—C12—B1	-178.2 (6)	N3—C17—B1—C7	-48.2 (7)
Co1—N2—C12—B1	7.0 (8)	C21—C17—B1—C7	136.6 (6)
N2—C12—C13—C14	-4.6 (11)	N5—C27—B2—C32	-58.4 (7)
B1—C12—C13—C14	178.9 (7)	C28—C27—B2—C32	117.3 (6)

C12—C13—C14—C15	0.8 (12)	N5—C27—B2—C1_3	175.5 (8)
C13—C14—C15—C16	2.4 (11)	C28—C27—B2—C1_3	-8.9 (10)
C12—N2—C16—C15	-1.9 (10)	N5—C27—B2—C26	52.0 (7)
Co1—N2—C16—C15	173.0 (6)	C28—C27—B2—C26	-132.3 (6)
C14—C15—C16—N2	-2.0 (11)	N5—C27—B2—C1_4	169.2 (9)
C18—N3—C17—C21	-5.0 (9)	C28—C27—B2—C1_4	-15.1 (12)
Co1—N3—C17—C21	168.1 (5)	N6—C32—B2—C27	57.3 (7)
C18—N3—C17—B1	179.5 (5)	C33—C32—B2—C27	-124.6 (8)
Co1—N3—C17—B1	-7.5 (7)	N6—C32—B2—C1_3	176.1 (9)
C17—N3—C18—C19	1.5 (10)	C33—C32—B2—C1_3	-5.8 (13)
Co1—N3—C18—C19	-171.6 (5)	N6—C32—B2—C26	-56.4 (7)
N3—C18—C19—C20	2.4 (10)	C33—C32—B2—C26	121.7 (8)
C18—C19—C20—C21	-2.7 (11)	N6—C32—B2—C1_4	-175.1 (12)
C19—C20—C21—C17	-0.8 (11)	C33—C32—B2—C1_4	3.0 (16)
N3—C17—C21—C20	4.7 (10)	N4—C26—B2—C27	-48.5 (7)
B1—C17—C21—C20	179.8 (6)	C25—C26—B2—C27	134.6 (6)
C26—N4—C22—C23	3.4 (10)	N4—C26—B2—C32	62.7 (6)
Co1—N4—C22—C23	-171.2 (5)	C25—C26—B2—C32	-114.2 (6)
N4—C22—C23—C24	0.7 (10)	N4—C26—B2—C1_3	-167.5 (8)
C22—C23—C24—C25	-2.9 (10)	C25—C26—B2—C1_3	15.6 (10)
C23—C24—C25—C26	1.2 (10)	N4—C26—B2—C1_4	-169.5 (10)
C22—N4—C26—C25	-5.0 (9)	C25—C26—B2—C1_4	13.6 (12)
Co1—N4—C26—C25	169.6 (4)	C27—B2—C1_3—C2_3	-73.5 (17)
C22—N4—C26—B2	177.9 (5)	C32—B2—C1_3—C2_3	168.7 (13)
Co1—N4—C26—B2	-7.5 (7)	C26—B2—C1_3—C2_3	46.3 (18)
C24—C25—C26—N4	2.8 (9)	C27—B2—C1_3—C6_3	96.5 (16)
C24—C25—C26—B2	179.7 (6)	C32—B2—C1_3—C6_3	-21 (2)
C31—N5—C27—C28	3.5 (9)	C26—B2—C1_3—C6_3	-143.7 (15)
Co1—N5—C27—C28	-173.8 (4)	C6_3—C1_3—C2_3—C3_3	2.4 (18)
C31—N5—C27—B2	179.4 (5)	B2—C1_3—C2_3—C3_3	173.7 (17)
Co1—N5—C27—B2	2.2 (7)	C1_3—C2_3—C3_3—C4_3	4 (2)
N5—C27—C28—C29	-2.5 (9)	C2_3—C3_3—C4_3—C5_3	-7 (3)
B2—C27—C28—C29	-178.2 (6)	C3_3—C4_3—C5_3—C6_3	4 (2)
C27—C28—C29—C30	0.2 (10)	C4_3—C5_3—C6_3—C1_3	2.6 (19)
C28—C29—C30—C31	1.1 (11)	C2_3—C1_3—C6_3—C5_3	-6 (2)
C29—C30—C31—N5	-0.1 (11)	B2—C1_3—C6_3—C5_3	-175.8 (13)
C27—N5—C31—C30	-2.3 (10)	C27—B2—C1_4—C2_4	-45 (2)
Co1—N5—C31—C30	174.9 (5)	C32—B2—C1_4—C2_4	-169.3 (17)
C36—N6—C32—C33	0.4 (10)	C26—B2—C1_4—C2_4	73 (2)
Co1—N6—C32—C33	179.8 (6)	C27—B2—C1_4—C6_4	142 (2)
C36—N6—C32—B2	178.6 (6)	C32—B2—C1_4—C6_4	17 (3)
Co1—N6—C32—B2	-1.9 (8)	C26—B2—C1_4—C6_4	-100 (2)
N6—C32—C33—C34	-0.3 (14)	C6_4—C1_4—C2_4—C3_4	-4 (2)
B2—C32—C33—C34	-178.4 (9)	B2—C1_4—C2_4—C3_4	-178 (2)
C32—C33—C34—C35	-0.1 (16)	C1_4—C2_4—C3_4—C4_4	-4 (3)
C33—C34—C35—C36	0.4 (15)	C2_4—C3_4—C4_4—C5_4	9 (4)
C32—N6—C36—C35	-0.1 (10)	C3_4—C4_4—C5_4—C6_4	-6 (3)
Co1—N6—C36—C35	-179.6 (5)	C2_4—C1_4—C6_4—C5_4	8 (3)

C34—C35—C36—N6	-0.3 (12)	B2—C1_4—C6_4—C5_4	-179.0 (17)
C6—C1—B1—C12	152.7 (6)	C4_4—C5_4—C6_4—C1_4	-3 (3)
