Electronic Supplementary Information for

Cobalt Analogs of Ru-Based Water Oxidation Catalysts: Overcoming Instability and Lability to Achieve Electrocatalytic O_2 Evolution

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General Procedures

The Hbpp ligand was obtained from TCI America and used without further purification. Except where noted, all other chemicals were obtained from Sigma-Aldrich and used without further purification. Except where otherwise noted, electrochemical experiments were performed using a BASinc Potentiostat with a glass slide coated with fluorine-doped tin oxide (FTO, obtained from Hartford Glass, 1 cm^2) as the working electrode, a Ag/AgCl reference electrode, and a platinum counter-electrode. All CVs were performed at a scan rate of 100 mV/s. Electrolysis experiments were conducted in a divided cell, and O_2 detection experiments were performed in a custom-built H-cell. O_2 detection was carried out using an Ocean Optics NeoFox FOSPOR fluorescence-quench O_2 probe. All electrochemical experiments were performed with 0.1 M supporting electrolyte.

Aqueous Electrochemical and Spectroscopic Data

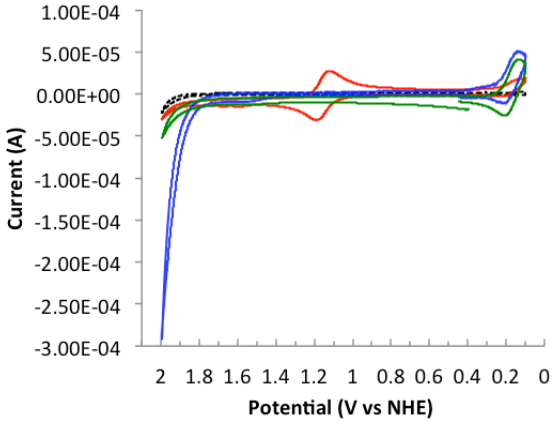


Figure S1. CVs of FTO background (black dashed), complex **1**-initial (red), complex **1**-stirred 5 h (blue), and $Co(tpy)_2[ClO_4]_2$ (green) in 0.1 M pH 2.1 phosphate; [complex] = 0.25 mM.

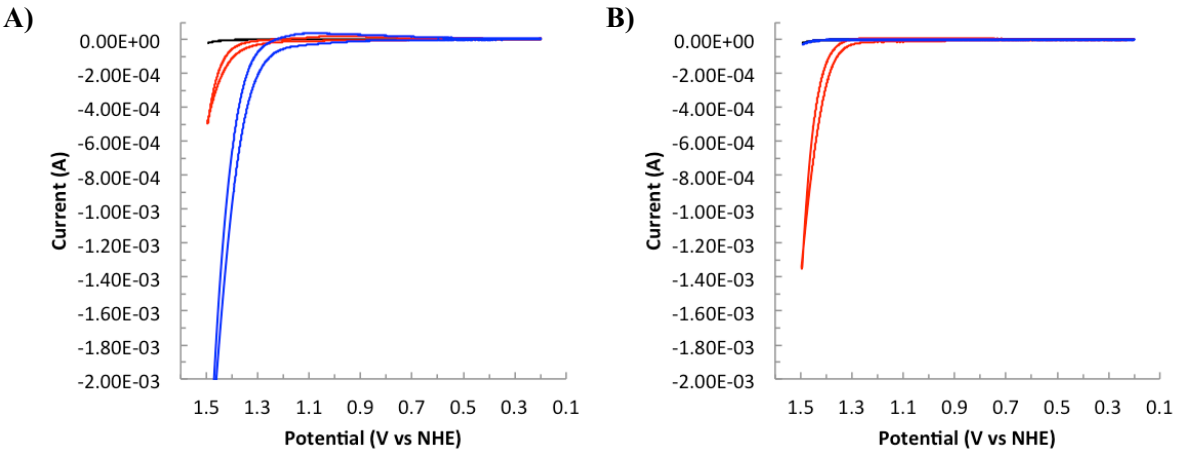


Figure S2. A) CVs of FTO background (black), complex **1** (red), solution of complex **1** after 1 h CPE at 1.5 V vs NHE (blue) in pH 7 0.1 M phosphate. **B**) CVs of FTO background (black) and the electrode after CPE of **1** and rinsing with DI water (red), the same electrode after CPE of **1** and rinsing with 5% HCl (blue) in fresh Co-free 0.1 M pH 7 phosphate; [complex] = 0.25 mM. These experiments suggest the formation of heterogeneous deposits at neutral pH, precluding further electrolysis studies under these conditions (similar observations for complexes **2** and **5** can be found in Figures S6 and S10, respectively)

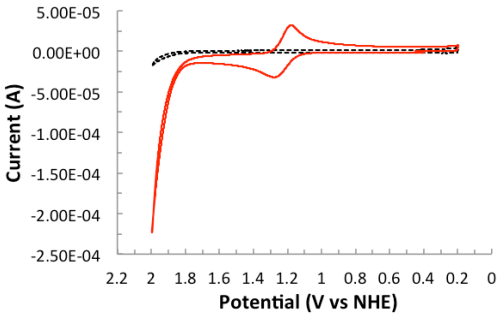


Figure S3. CVs of FTO background (black) and initial CV of **2** (red) in 0.1 M pH 2.1 phosphate.

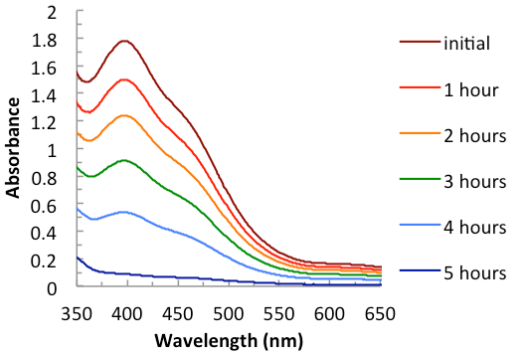


Figure S4. UV-visible spectra of complex **2** (0.25 mM) acquired over the course of several hours after dissolution in 0.1 M pH 2.1 phosphate.

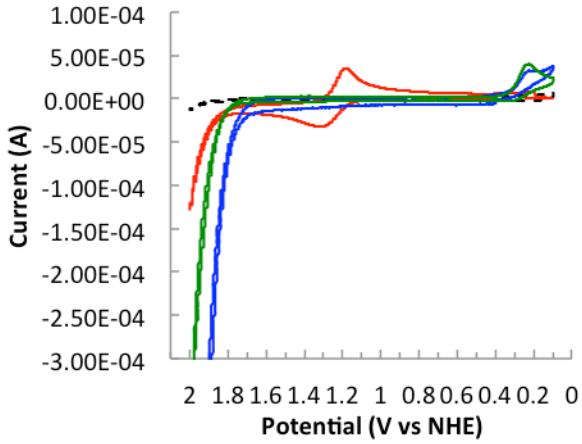


Figure S5. CVs of FTO background (black dashed), complex **2**-initial (red), complex **2**-stirred 5 hours (blue), $Co(bpy)_3[ClO_4]_2$ (green) in 0.1 M pH 2.1 phosphate; [complex] = 0.25 mM.

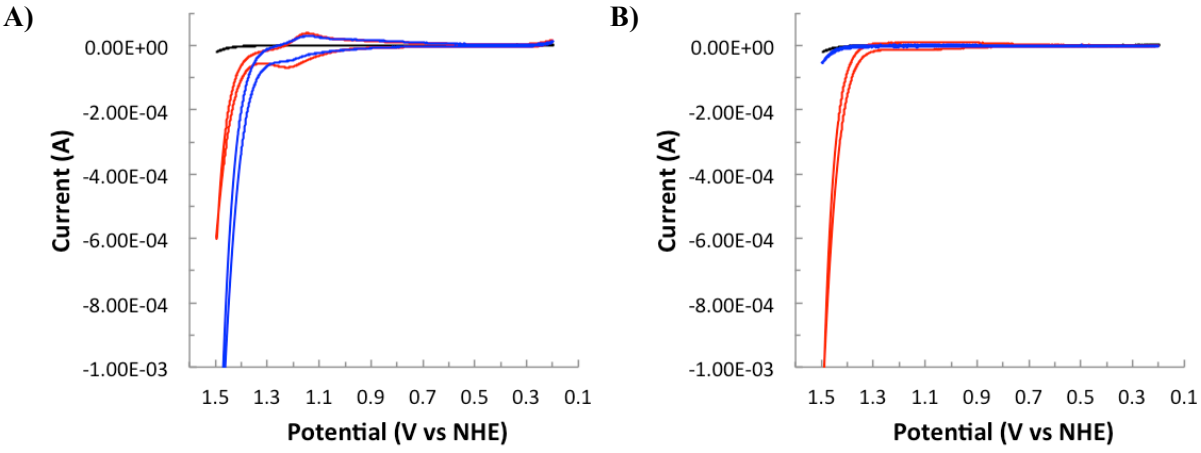


Figure S6. A) CVs of FTO background (black), complex **2** (red), and solution of complex **2** after 1 h CPE at 1.5 V vs NHE (blue). in pH 7 0.1 M phosphate. **B**) CVs of FTO background (black), electrode from CPE of **2** after rinse with DI water (red), and electrode from CPE of **2** after rinse with 5% HCl (blue) fresh Co-free 0.1 M pH 7 phosphate; [complex] = 0.25 mM.

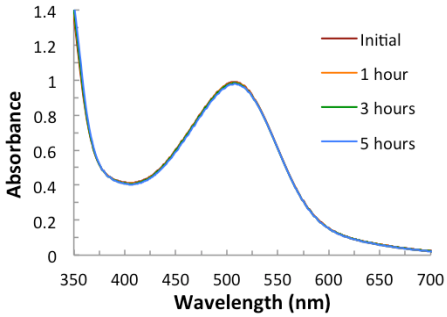


Figure S7. UV-vis spectra of 0.1 mM **5** in 0.1 M pH 2.1 phosphate over several hours.

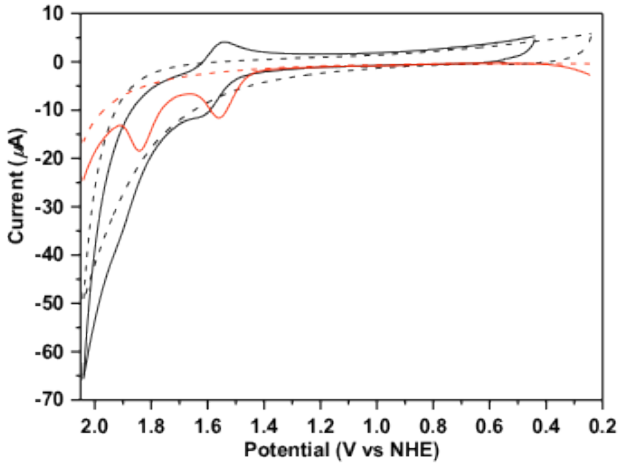


Figure S8: Complex **5** in 0.1 M pH 2.1 phosphate buffer on glassy carbon working electrode. CV: complex (black solid line), conditions: [**5**] = 0.5 mM, scan rate = 100 $mV \cdot s^{-1}$; blank with no complex (black dashed line). DPV: complex (red solid line), conditions: [**5**] = 0.5 mM, amplitude = 50 mV, pulse period = 0.3 s; blank with no complex (red dashed line). [Note: The CV/DPV experiments in Figures S8 and S11 were carried out with CH Instruments 630B potentiostat, with glassy carbon electrode (3 mm diameter) as working electrode, Pt as auxiliary and measured versus SCE reference electrodes.]

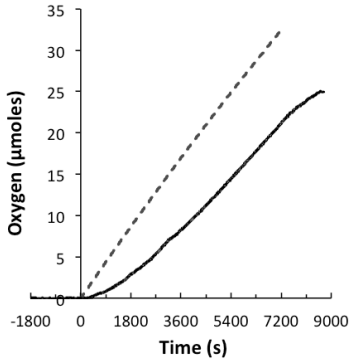


Figure S9. O_2 production measured using a fluorescence quench sensor during electrolysis at 2.0 V in a stirred 0.10 mM solution of **5** with a 12.5 cm^2 FTO working electrode (40 mL, 4 μmoles complex). Theoretical O_2 yield assuming 100% Faradaic efficiency (dashed); experimental O_2 yield (solid).

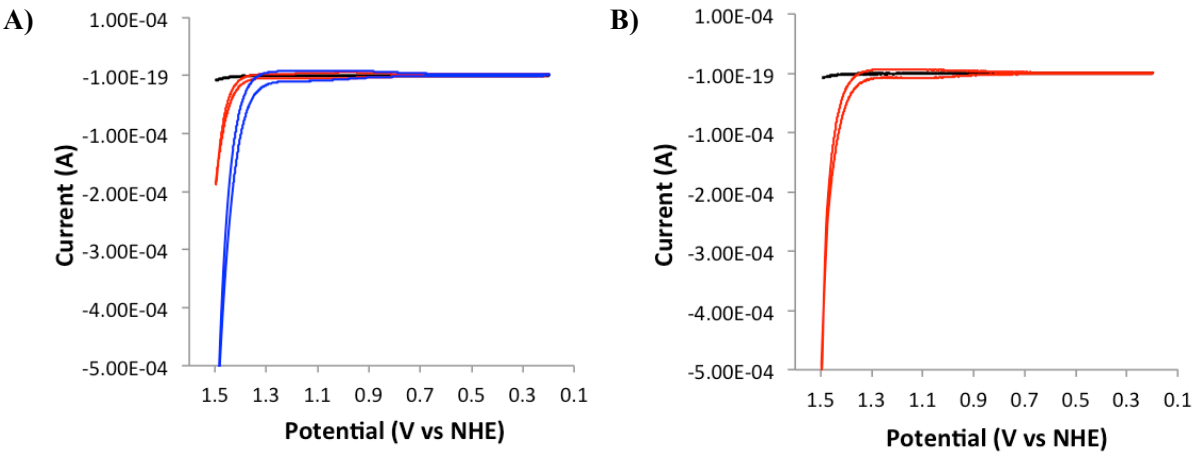


Figure S10. A) CVs of FTO background (black), complex **5** (red), and solution of complex **5** after 1 h CPE at 1.5 V vs NHE (blue) in pH 7 0.1 M phosphate. **B**) CVs of fresh Co-free 0.1 M pH 7 phosphate; FTO background (black), electrode from CPE of **5** after rinse with DI water; [complex] = 0.25 mM

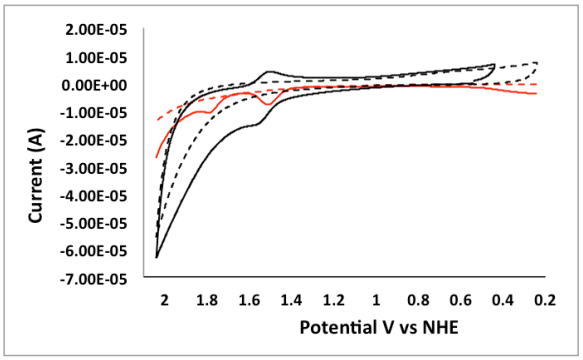


Figure S11: (**5**) in 0.1 M triflic acid on glassy carbon working electrode. CV: complex (black solid line), conditions: [complex] = 0.5 mM, scan rate = 100 $mV \cdot s^{-1}$; blank with no complex (black dashed line). DPV: complex (red solid line), conditions: [complex] = 0.5 mM, amplitude = 50 mV, pulse period = 0.3 s; blank with no complex (red dashed line).

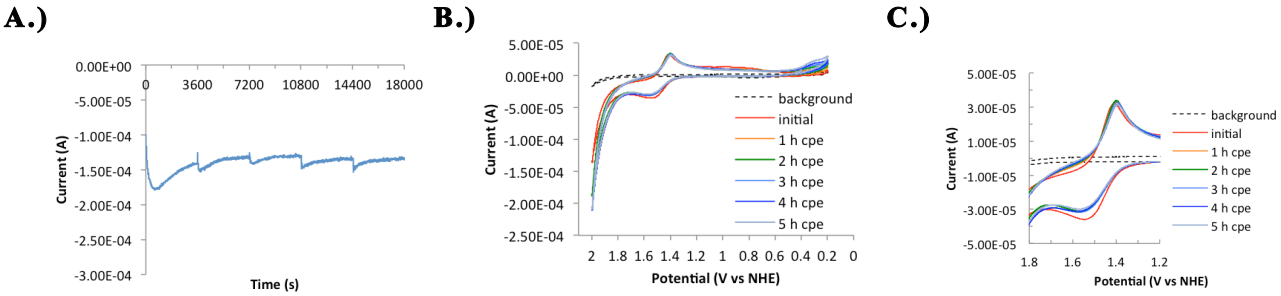


Figure S12. A.) Successive 1 hour controlled potential electrolyses of stirred solutions of **5** in 0.1 M pH 2.1 phosphate (approximately 1.5 equivalents of electrons passed during each electrolysis period); B.) CVs of **5** in 0.1 M pH 2.1 phosphate following electrolyses at 2.0 V; 1 cm^2 FTO working electrode, C.) Same CVs, reversible region enhanced for clarity; [complex] = 0.25 mM

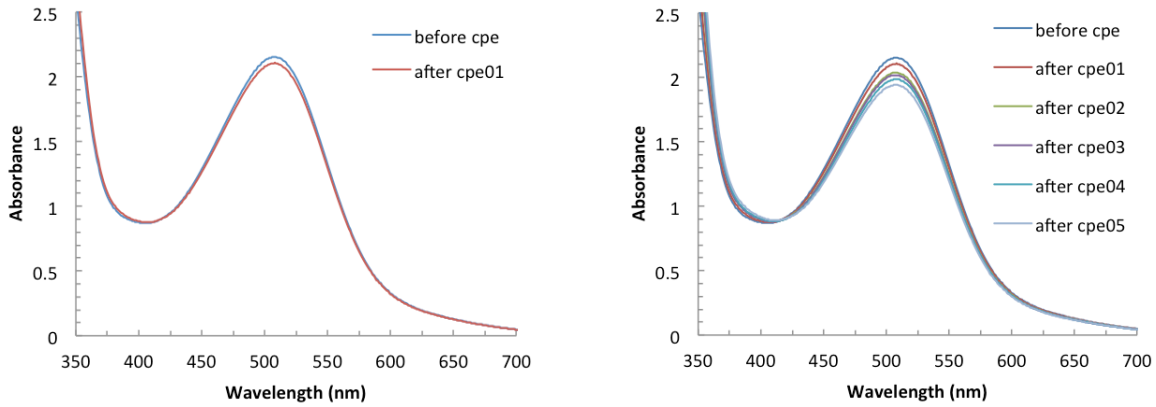


Figure S13. Absorbance spectra of **5** in 0.1 M pH 2.1 phosphate following electrolyses at 2.0 V shown in Figure S12; [complex] = 0.25 mM

Table S1: Summary of data from Figures S12 and S13. Though some bleaching is observed in the absorbance spectrum (1.31% bleaching per equivalent of electrons passed), the bleaching is not associated with an increase in the steady state catalytic currents, suggesting the complex is not decomposing into the more active simple Co salts. Instead, bleaching may be attributable to build-up of some intermediate during homogeneous electrolysis.

Electrolysis time	Current (uA)	Electron equiv. passed	A @ 508 nm	% bleaching
1	-140	1.68	2.11	2.21
2	-133	3.14	2.03	5.49
3	-131	4.57	2.01	6.27
4	-134	6.03	1.98	7.89
5	-134	7.51	1.94	9.90

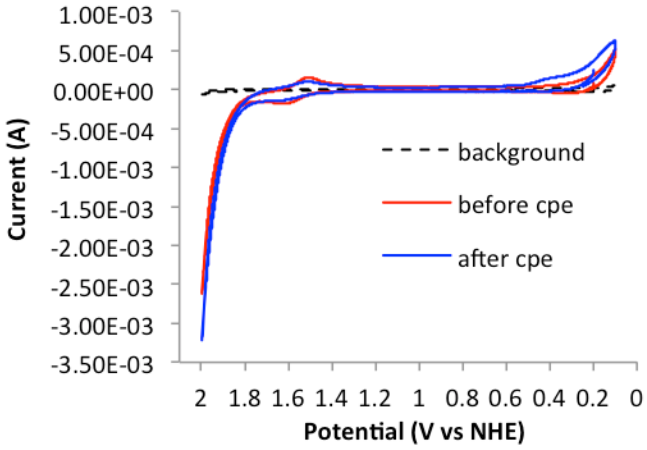


Figure S14. CVs of **5** in 0.1 M pH 2.1 phosphate before and after 2 hour electrolysis at 2.0 V used for O_2 detection in Figure S9; 12.5 cm^2 FTO working electrode, [complex] = 0.1 mM

EPR Spectroscopy Study

The X-band EPR spectra were recorded at 5 K using X-band Bruker EMX-plus spectrometer equipped with a dual mode cavity (ER 4116DM). Low temperature was achieved and controlled with an Oxford Instruments ESR900 liquid He quartz cryostat with an Oxford instruments ITC503 temperature and gas flow controller. The experimental parameters for EPR spectra were as follows: Microwave frequency = 9.646 GHz, microwave power = 1.017 mW, modulation amplitude = 10 G, gain = 5 x 10^3, modulation frequency = 100 kHz, time constant = 40.96 ms, and conversion time = 81.00 ms.

The $1e^-$ oxidized species of **5** was generated by treating complex **5** with one equivalent of cerium(IV) ammonium nitrate in an aqueous solution of pH 1 triflic acid at room temperature. After a few minutes stirring at room temperature (~3 mins) the reaction mixture was transferred to an EPR tube and frozen in liquid N_2. The spectra were recorded at 5 K.

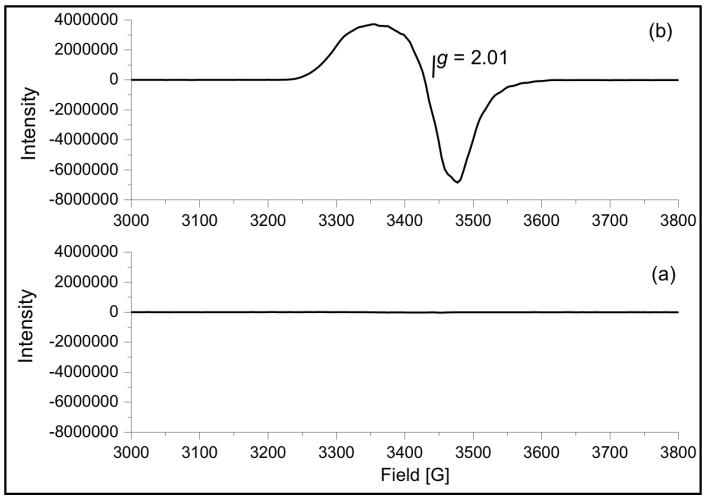


Figure S15: X-band EPR spectra of (a) $[Co^{III}\text{-O-O-}Co^{III}]^{3+}$ (**5**) and (b) $1e^-$ oxidized $[Co^{III}\text{-O-O-}Co^{IV}]^{4+}$ species in frozen aqueous pH1 triflic acid at 5K. [complex] = 0.5 mM.

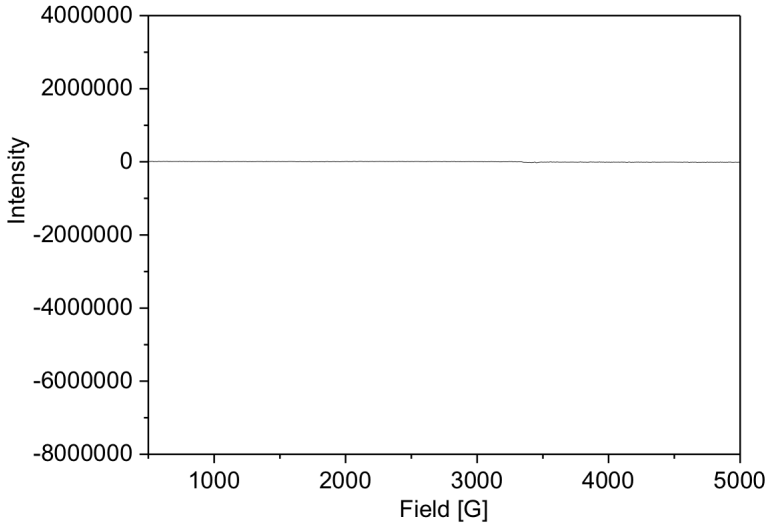
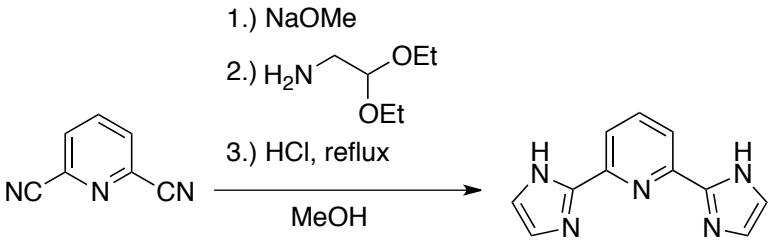


Figure S16: X-band EPR spectrum of ammonium cerium(III) nitrate in frozen aqueous pH1 triflic acid at 5K. [Ce(III)] = 0.5 mM.

Synthetic Protocols

Complexes **1**[1] and **2**[2] were prepared according to literature procedures.

2,6-bis(imidazol-2-yl)pyridine (bimpy):

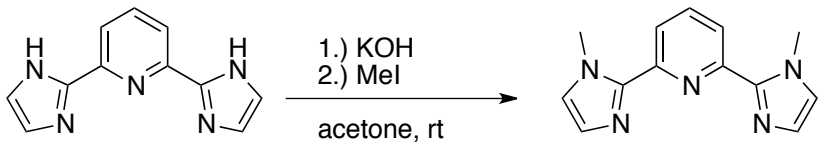


This compound was prepared following a modification of a literature procedure.[3] 2,6-Pyridinedicarbonitrile (510 mg, 4 mmol) was dissolved in MeOH (5 mL). NaOMe (45 mg, 0.8 mmol) was added, and the mixture was stirred for two h at room temperature. Aminoacetaldehyde diethylacetal (1.1 mL, 8 mmol) was added to the reaction mixture, followed by 500 µL of acetic acid, and the reaction was stirred at 50 °C for 1 h. The reaction mixture was allowed cool to room temperature and 2 mL of 6 N aqueous HCl was added. The mixture was heated to reflux and stirred for 8 h.

The reaction mixture was allowed to cool to room temperature and the solvent was removed by rotary evaporation. The remaining oil was reconstituted in 10 mL H_2O. The aqueous phase was extracted with Et_2O (3 x 10 mL) and the organic layer was discarded. The pH of the aqueous layer was adjusted with 2 M NaOH to pH 8-9, resulting in precipitation of a solid. Solid material was collected by filtration and dried under vacuum, and the product was recovered as a fluffy white solid in 87% yield.

^{1}H-NMR (300 MHz, DMSO-d_6): δ 7.83-7.95 (m, 3H), 7.28 (br s, 4H); ^{13}C NMR (75 MHz, DMSO-d6): δ 148.4, 146.3, 139.2, 118.1; HRMS (ESI) (M+H) $[C_{11}H_{10}N_5]^+$ *m/z* calc'd: 212.2, found 212.1.

2,6-bis((N-methyl)imidazol-2-yl)pyridine (Me_2bimpy):



This ligand was prepared following a modification of a literature procedure.[4] KOH (290, 5 mmol) was added to a stirring suspension of bimpy (210, 1 mmol) in 25 mL of acetone. The mixture was stirred at room temperature for 15 minutes. Methyl iodide (330 µL, 5 mmol) was added and the mixture was stirred for 8 h. Then, 2 M NaOH (20 mL) was added and the mixture was extracted with CH_2Cl_2 (3 x 30 mL). The combined organic layers were dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation, and the residue was dried under vacuum in a desiccator. The product was recovered as a yellow solid in 73% yield.

^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.98 (d, 2H, J=7.8 Hz), 7.75 (t, 2H, 7.8 Hz), 7.04 (s, 2H), 6.90 (s, 2H), 3.97 (s, 6H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ 149.9, 145.4, 137.7, 128.9, 124.3, 122.5, 35.9; HRMS (ESI) (M+H) $[C_{13}H_{14}N_5]^+$ *m/z* calc'd: 240.3, found 240.1.

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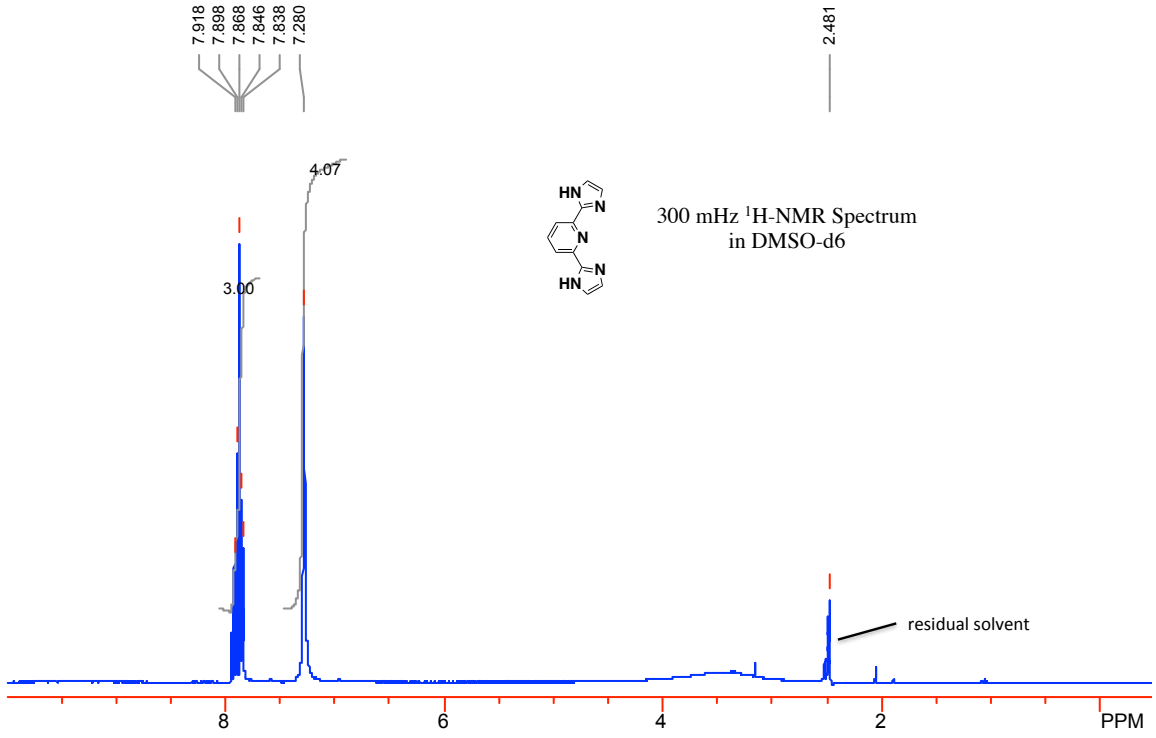
[1] Ramprasad, D.; Gilicinski, A. G.; Markley, T. J.; Pez, G. P. *Inorg. Chem.* **1994**, *33*, 2841.
[2] Bogucki, R. F.; McLendon, G.; Martell, A. E. *J. Am. Chem. Soc.* **1976**, *98*, 3202.
[3] Voss, M. E.; Beer, C. M.; Mitchell, S. A.; Blomgren, P. A.; Zhichkin, P. E. *Tetrahedron* **2008**, *64*, 645.
[4] Zhang, W.; Sun, W.-H.; Zhang, S.; Hou, J.; Wedeking, K.' Schultz, S.; Fröhlich, R.; Song, H. *Organometallics*, **2006**, *25*, 1961.

General procedure for 5 and 6: NaOH (1 equiv) was added to a stirring suspension of the Hbpp ligand in MeOH. The mixture was stirred for 10 minutes at room temperature, followed by addition of 2 equiv $CoCl_2$•$6H_2O$. This red solution was stirred for an additional 30 min. The tridentate ligand (tpy or Me_2bimpy, 2 equiv) was added, and the mixture was heated at reflux under air for 3 h. The deep purple reaction mixture was cooled to room temperature. Addition of 3-4 mL of 1M $NaPF_6$ in MeOH to this solution led to precipitation of a purple solid, which was collected by filtration and washed with cold MeOH and ether (2-3 mL each). A ^{1}H-NMR spectrum of the crude solid displays some line-broadening, together with peaks associated with multiple diamagnetic species. The crude material can be purified on an alumina column, eluted with 50 mM $NaPF_6$ in 5% MeOH/MeCN, redissolved in MeCN/MeOH mixtures, and precipitated by addition of excess $NaPF_6$. Yields of 25-30% have been consistently obtained for analytically pure **5** and **6**. Crystals for X-ray analysis were grown by vapor diffusion of pentanes into solutions of purple solids in acetone.

Elemental Analysis for **5** indicates the complex is hydrated with two water molecules. Anal. Calcd. for **5•2H$_2$O**: C, 39.47; H, 2.70; N, 10.70. Found: C, 39.24; H, 2.64; N, 10.64.

Elemental Analysis for **6**: Anal Calcd. For **6**: C, 36.47; H, 2.75; N, 15.27. Found: C, 36.20; H, 2.90; N, 15.14.

NMR Spectra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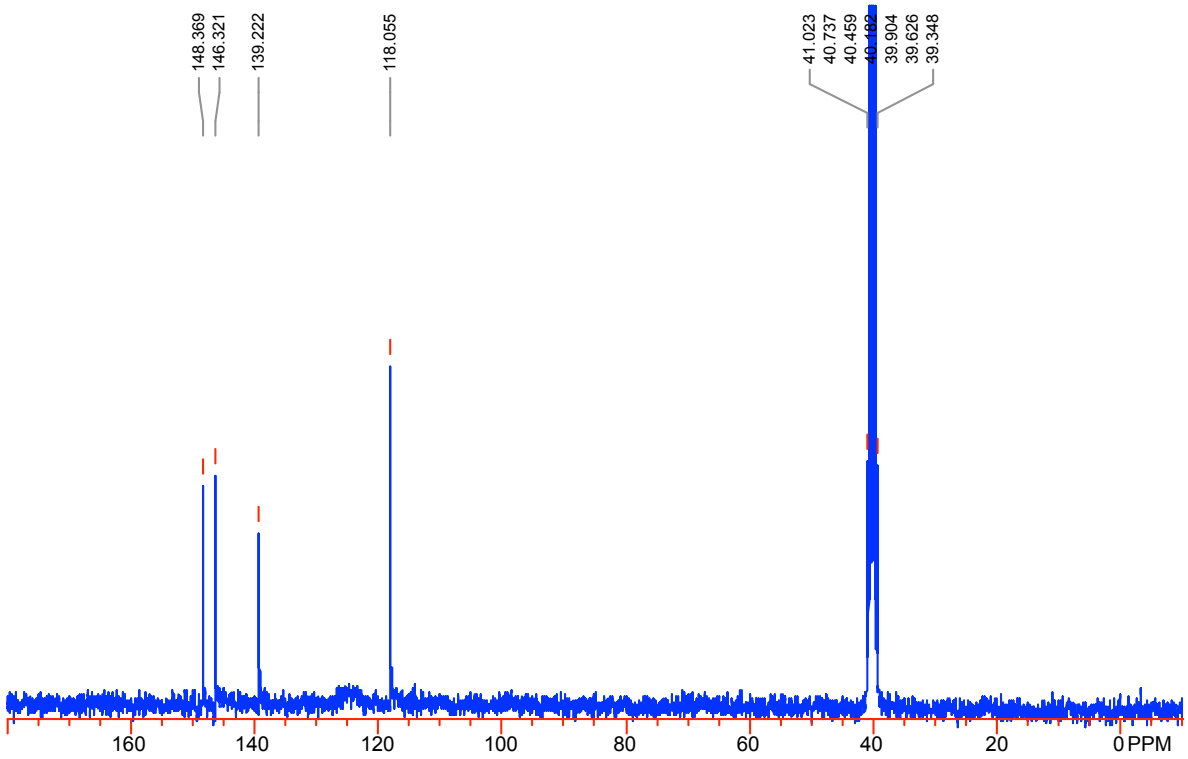
7.898
7.868
7.846
7.838
7.280
2.481
4.07
3.00
HN
N
N
N
HN
300 mHz ¹H-NMR Spectrum
in DMSO-d6
residual solvent
8
6
4
2
PPM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100
80
60
40
20
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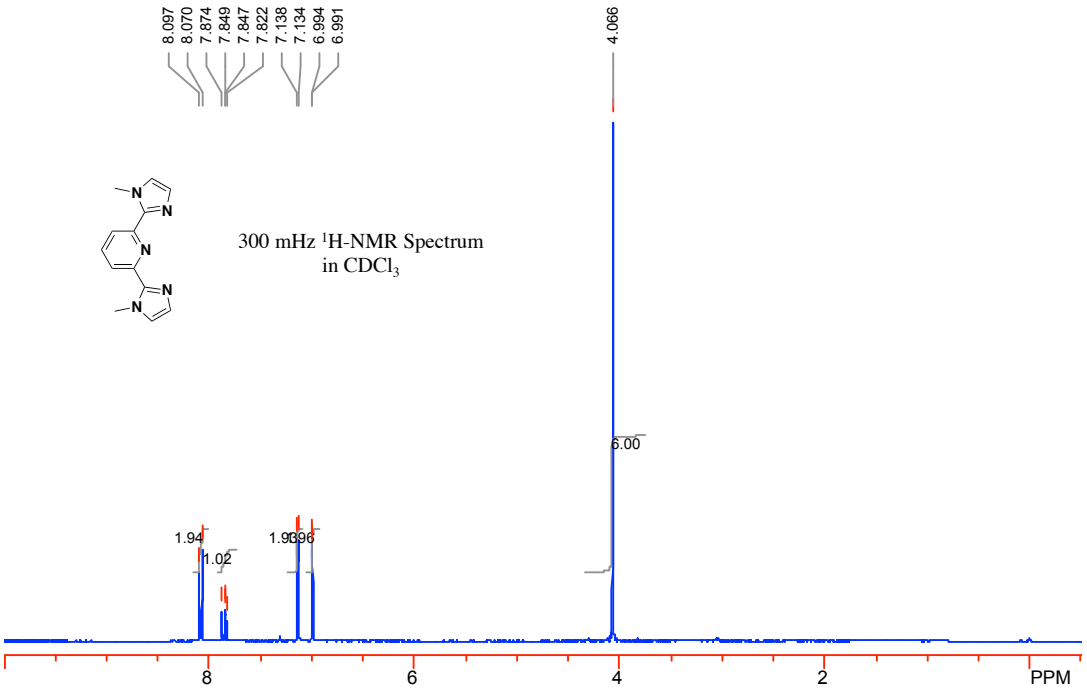
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8.070
7.874
7.849
7.847
7.822
7.138
7.134
6.994
6.991
4.066
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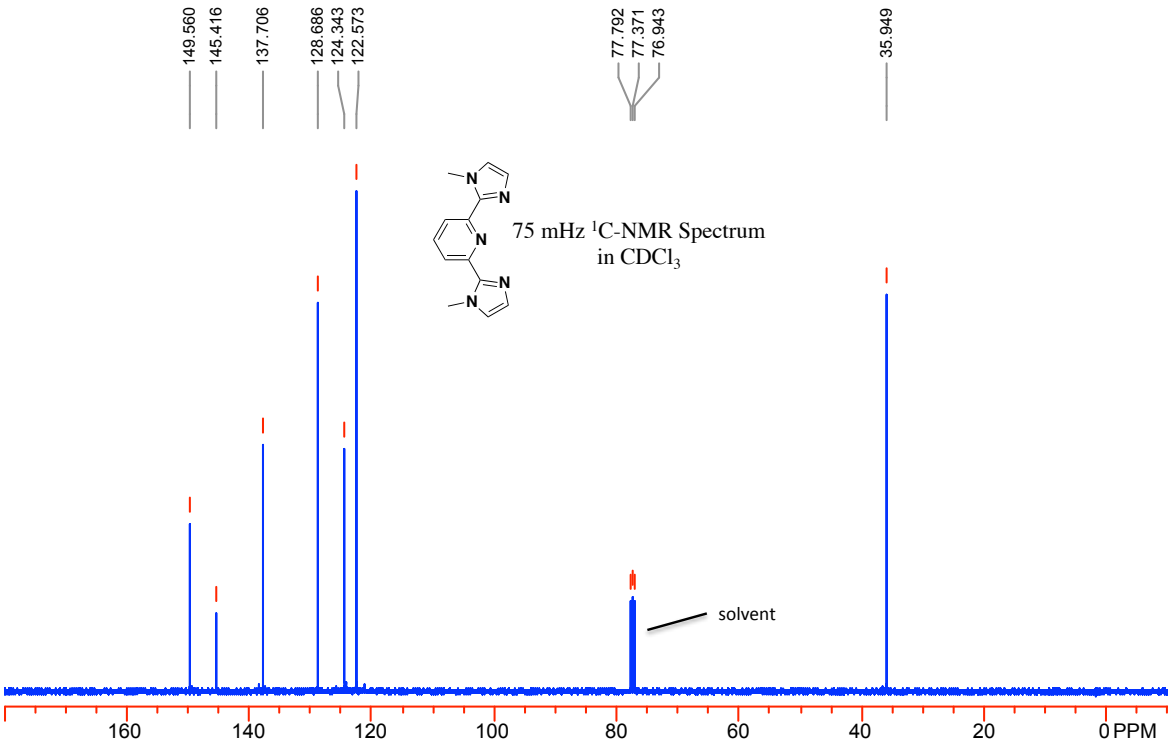
in CDCl3
6.00
1.94
1.02
1.9396
8
6
4
2
PPM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solvent
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140
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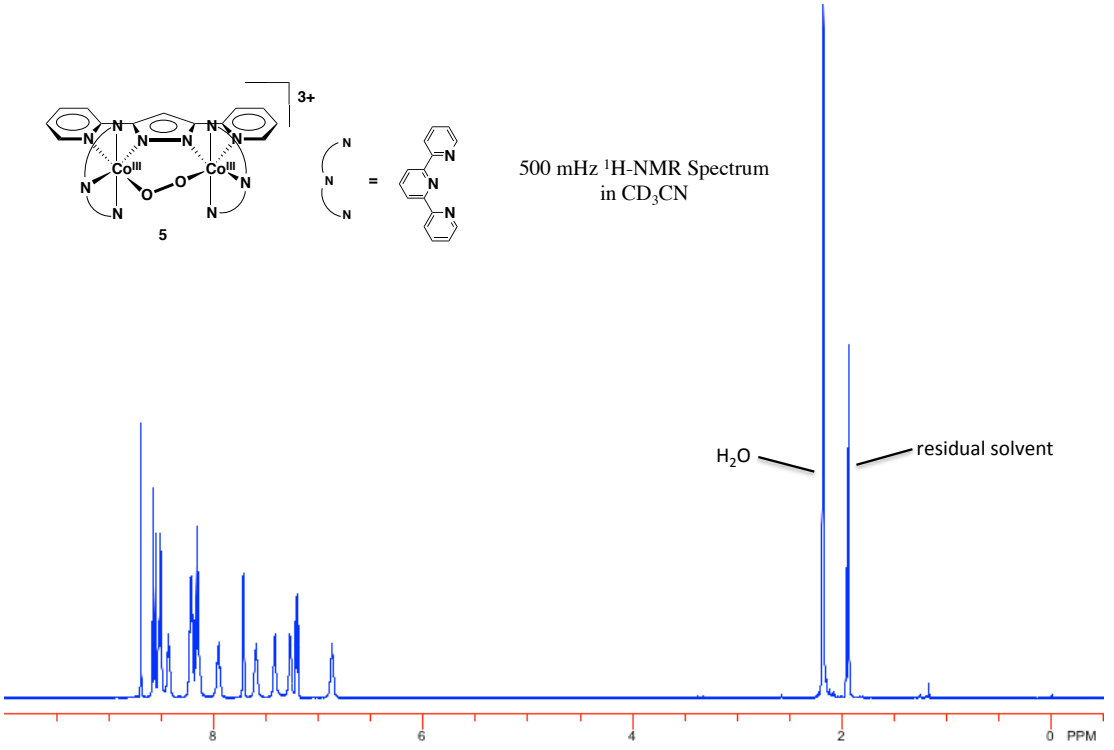
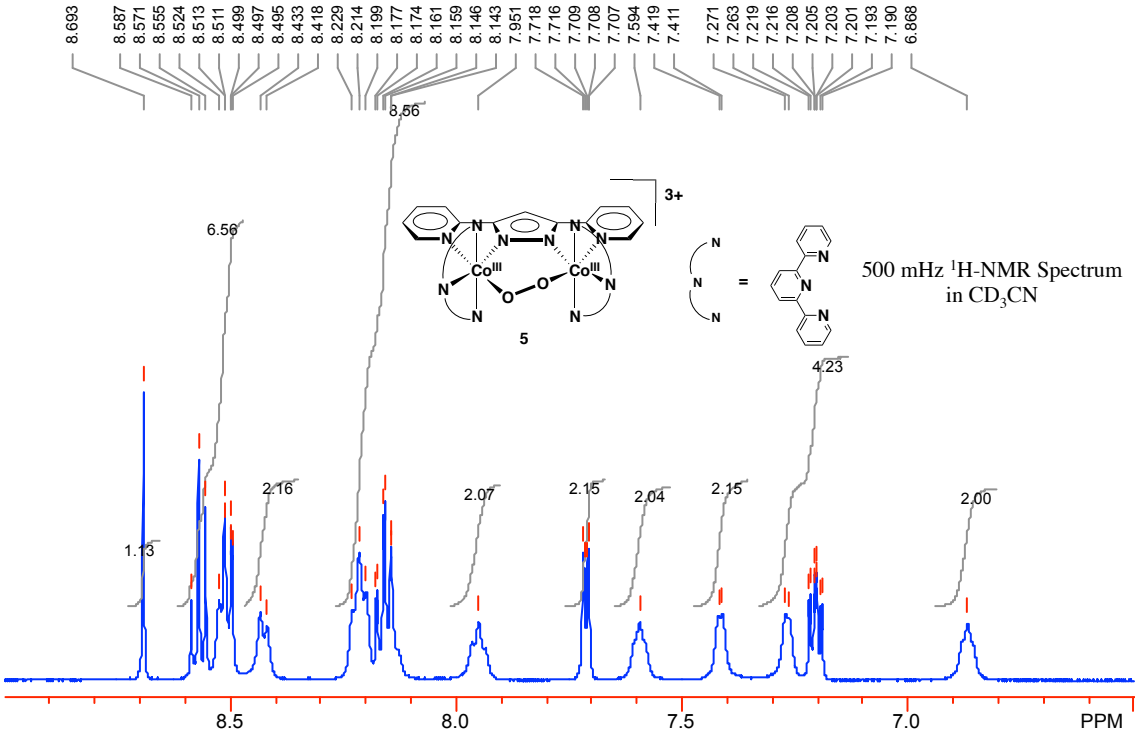
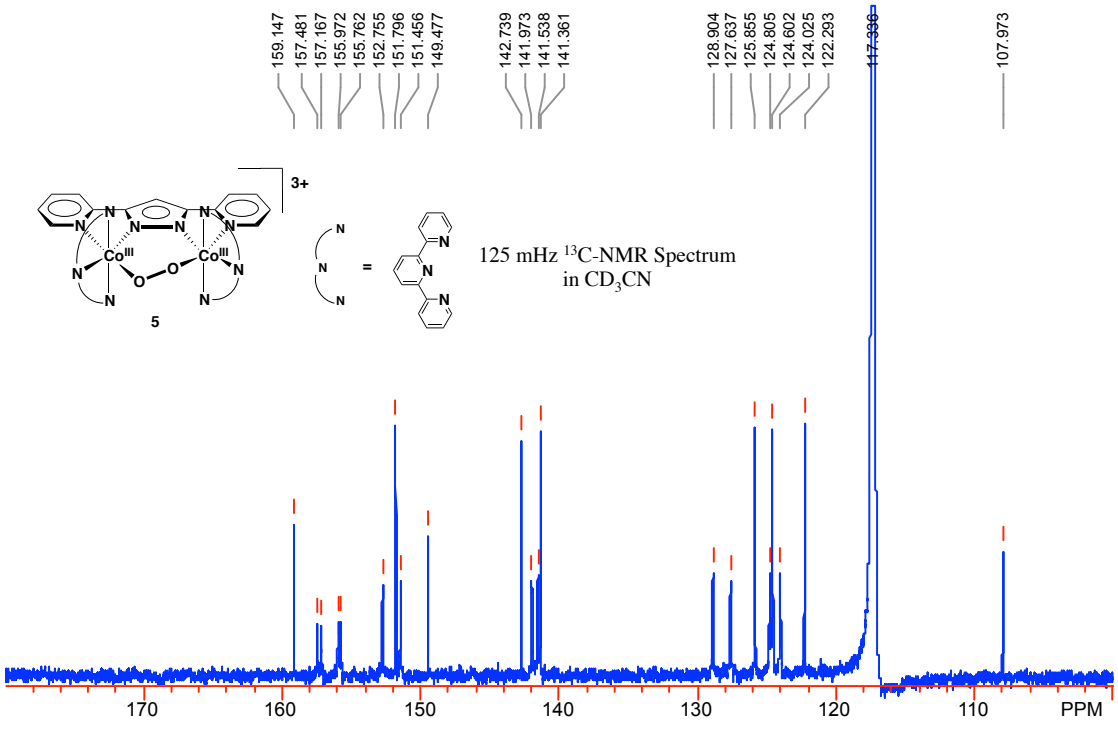
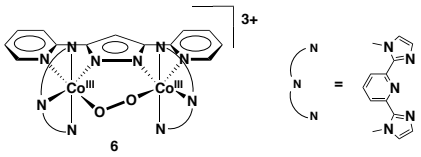
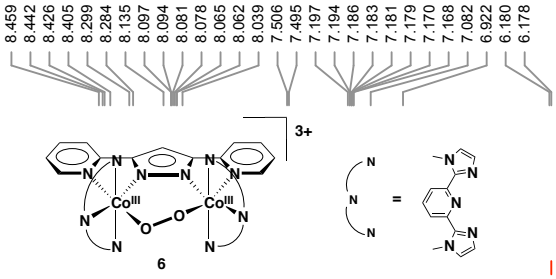




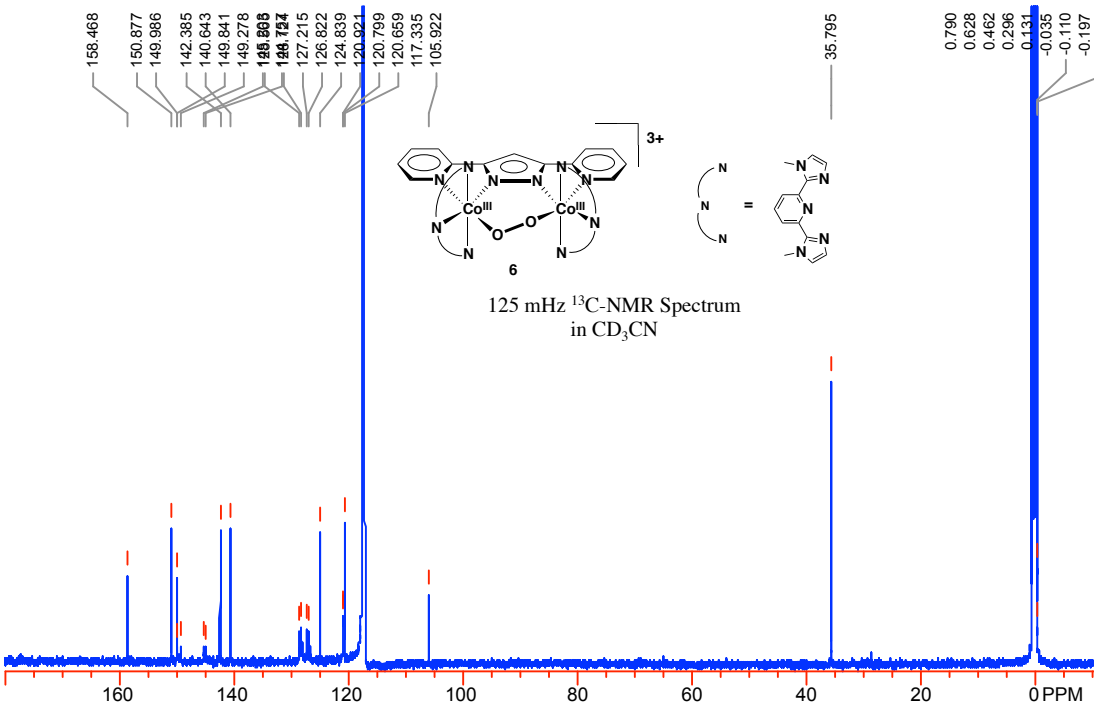




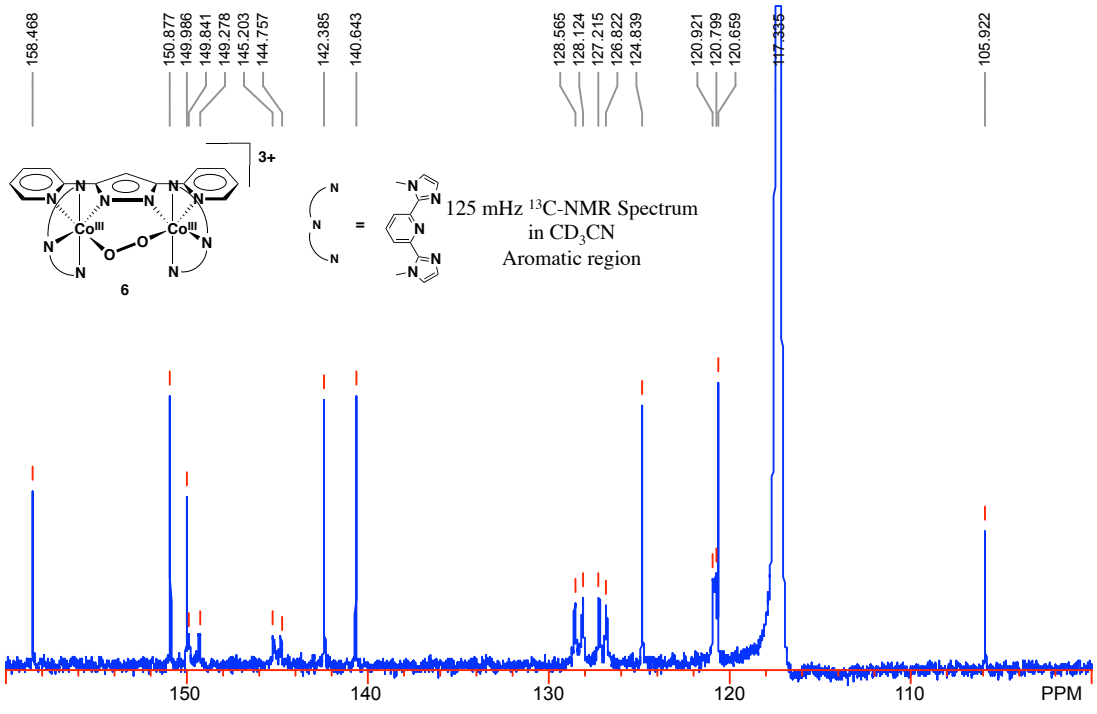
500 mHz ^{1}H-NMR Spectrum
in CD_3CN



500 mHz ^{1}H-NMR Spectrum
in CD_3CN



125 mHz ^{13}C-NMR Spectrum
in CD_3CN



125 mHz ^{13}C-NMR Spectrum
in CD_3CN
Aromatic region

Single crystal X-ray crystallography for [(μ-bpp)(μ-O_2)(Co(tpy))$_2$][PF_6]$_3$ (5)

Data Collection

A red crystal with approximate dimensions 0.26 x 0.18 x 0.14 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker Quazar SMART APEXII diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.97 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5º in a 10º range about ω with the exposure time of 10 second per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program suite. The final cell constants were calculated from a set of 9887 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.82 Å. A total of 64546 data were harvested by collecting 5 sets of frames with 0.4º scans in ω and ϕ with exposure times of 50 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent for the space group $P2_1/c$ that yielded chemically reasonable and computationally stable results of refinement [2-3].

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculations at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. The asymmetric unit contains one dicobalt complex, three PF_6 anions, and 3.5 molecules of dichloromethane (only 2 could be confidently refined). The C45 dichloromethane molecule is disordered over two positions with a major component contribution of 84.1(4)%. In the F3 anion, atoms F13-F16 are also disordered over two positions with an 88.8(4)% major component contribution. These disordered moieties were refined with restraints and constraints.

There were also several partially occupied solvate molecules of dichloromethane (DCM) present in the asymmetric unit in addition to the two well-behaved DCM molecules. A significant amount of time was invested in identifying and refining the disordered molecules. Bond length restraints were applied to model the molecules but the resulting isotropic displacement coefficients suggested the molecules were mobile. In addition, the refinement was computationally unstable. Option SQUEEZE of program PLATON [4] was used to correct the diffraction data for diffuse scattering effects and to identify the solvate molecules. PLATON calculated the upper limit of volume that can be occupied by the solvent to be 1059.5 Å^3, or 17.2% of the unit cell volume. The program calculated 249 electrons in the unit cell for the

diffuse species. This approximately corresponds to 6 molecules of DCM in the asymmetric unit (252 electrons). It is very likely that these solvate molecules are disordered over several positions. Please note that all derived results in the following tables are based on the known contents. No data are given for the diffusely scattering species.

The final least-squares refinement of 780 parameters against 10763 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0668 and 0.1915, respectively.

The molecular diagrams are drawn with 40% probability ellipsoids.

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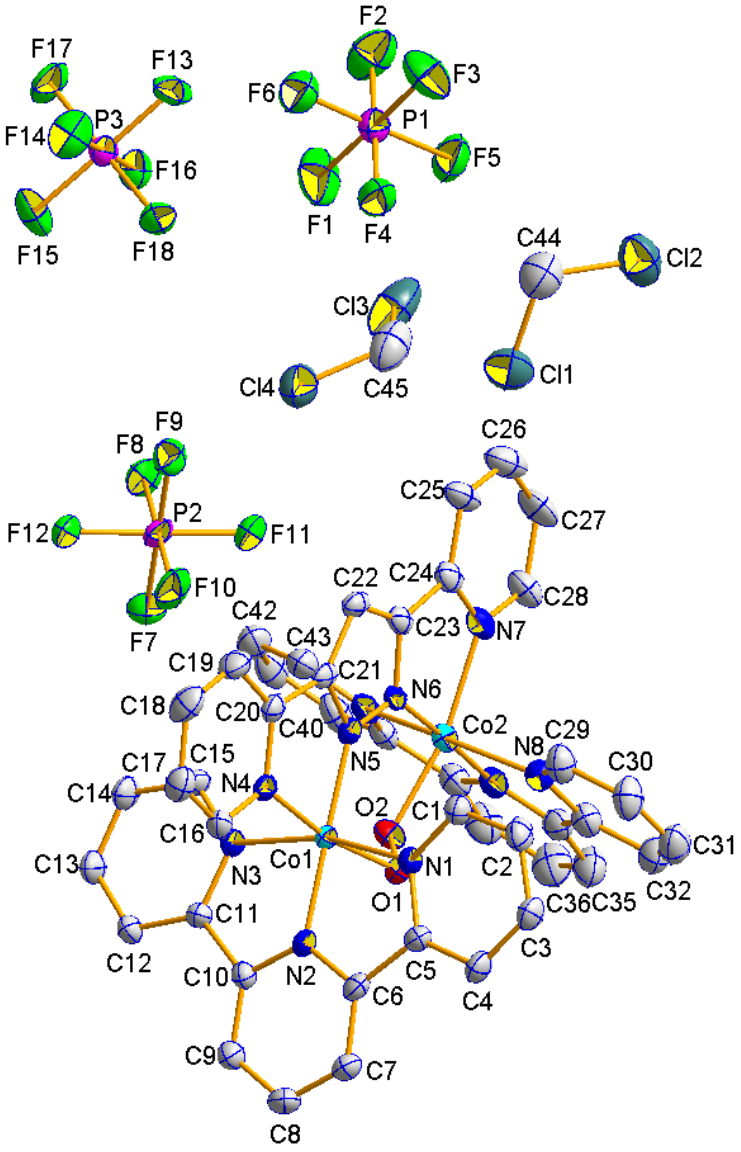

Figure S17. A molecular drawing of the asymmetric unit of **5**. All minor components of disordered atoms and hydrogen atoms were omitted for clarity.

Table S2. Crystal data and structure refinement for **5**.

Identification code	stahl108	
Empirical formula	$[C_{43}H_{31}Co_2N_{10}O_2]^{3+}$ $[PF_6]_3^-$ x 3.5(CH_2Cl_2)	
Formula weight	1442.40	
Temperature	100(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.6543(6) Å	a= 90°.
	b = 24.2520(10) Å	b= 94.437(2)°.
	c = 18.6535(8) Å	g = 90°.
Volume	6158.5(5) $Å^3$	
Z	4	
Density (calculated)	1.556 Mg/m^3	

Absorption coefficient	0.889 mm^{-1}
F(000)	2880
Crystal size	0.26 x 0.18 x 0.14 mm^3
Theta range for data collection	2.25 to 25.00°.
Index ranges	-16<=h<=16, -28<=k<=28, -22<=l<=21
Reflections collected	83280
Independent reflections	10763 [R(int) = 0.0676]
Completeness to theta = 25.00°	99.2 %
Absorption correction	Analytical with SADBS
Max. and min. transmission	0.8856 and 0.8017
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10763 / 13 / 780
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0668, wR2 = 0.1823
R indices (all data)	R1 = 0.0793, wR2 = 0.1915
Largest diff. peak and hole	1.217 and -0.905 e.$Å^{-3}$

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	9011(1)	846(1)	8440(1)	20(1)
Co(2)	7991(1)	-451(1)	7474(1)	25(1)
O(1)	9510(2)	136(1)	8197(2)	27(1)
O(2)	8893(2)	-297(1)	8280(2)	30(1)
N(1)	9818(3)	1142(2)	7710(2)	26(1)
N(2)	10168(2)	938(1)	9021(2)	22(1)
N(3)	8521(3)	628(2)	9344(2)	24(1)
N(4)	8384(2)	1595(1)	8510(2)	22(1)
N(5)	7849(2)	725(1)	7856(2)	22(1)
N(6)	7532(2)	289(2)	7483(2)	22(1)
N(7)	6823(3)	-491(2)	6723(2)	31(1)
N(8)	8954(3)	-347(2)	6772(2)	32(1)
N(9)	8508(3)	-1172(2)	7482(2)	28(1)
N(10)	7125(3)	-788(2)	8155(2)	29(1)
C(1)	9522(3)	1302(2)	7039(2)	29(1)
C(2)	10186(4)	1472(2)	6552(2)	33(1)
C(3)	11172(3)	1478(2)	6772(3)	32(1)
C(4)	11481(3)	1346(2)	7476(2)	31(1)
C(5)	10785(3)	1192(2)	7940(2)	26(1)
C(6)	10989(3)	1070(2)	8703(2)	25(1)
C(7)	11884(3)	1082(2)	9102(2)	29(1)
C(8)	11911(3)	943(2)	9823(3)	32(1)
C(9)	11058(3)	804(2)	10143(2)	28(1)
C(10)	10182(3)	799(2)	9716(2)	24(1)
C(11)	9200(3)	646(2)	9915(2)	23(1)
C(12)	8968(3)	527(2)	10607(2)	27(1)
C(13)	8007(3)	397(2)	10722(2)	32(1)
C(14)	7307(3)	389(2)	10146(2)	33(1)
C(15)	7584(3)	512(2)	9460(2)	29(1)
C(16)	8734(3)	2022(2)	8901(2)	28(1)
C(17)	8235(4)	2524(2)	8906(3)	34(1)
C(18)	7354(4)	2578(2)	8509(3)	40(1)
C(19)	6984(3)	2133(2)	8095(3)	35(1)
C(20)	7512(3)	1650(2)	8103(2)	26(1)
C(21)	7223(3)	1150(2)	7703(2)	22(1)
C(22)	6482(3)	975(2)	7214(2)	25(1)
C(23)	6702(3)	428(2)	7084(2)	26(1)
C(24)	6287(3)	-20(2)	6647(2)	30(1)
C(25)	5421(4)	9(2)	6203(3)	36(1)
C(26)	5084(4)	-444(3)	5845(3)	49(1)
C(27)	5609(4)	-931(2)	5922(3)	47(1)
C(28)	6487(4)	-942(2)	6360(3)	39(1)
C(29)	9086(4)	101(2)	6385(3)	38(1)
C(30)	9847(4)	140(2)	5931(3)	45(1)
C(31)	10465(4)	-299(2)	5871(3)	45(1)
C(32)	10320(4)	-774(2)	6252(3)	44(1)
C(33)	9555(4)	-794(2)	6701(3)	35(1)
C(34)	9295(4)	-1266(2)	7130(3)	33(1)
C(35)	9776(4)	-1763(2)	7198(3)	45(1)
C(36)	9419(5)	-2155(2)	7649(3)	52(2)
C(37)	8623(5)	-2050(2)	8032(3)	47(1)

C(38)	8153(4)	-1544(2)	7934(2)	34(1)
C(39)	7315(4)	-1334(2)	8291(2)	32(1)
C(40)	6733(4)	-1641(2)	8722(3)	41(1)
C(41)	5957(4)	-1392(2)	9013(3)	44(1)
C(42)	5755(4)	-853(2)	8871(3)	41(1)
C(43)	6361(3)	-553(2)	8437(2)	35(1)
P(1)	1478(1)	2365(1)	4662(1)	39(1)
F(1)	1701(4)	2110(2)	5430(2)	84(1)
F(2)	505(3)	2011(2)	4523(3)	73(1)
F(3)	1255(3)	2661(2)	3904(2)	68(1)
F(4)	2457(2)	2730(2)	4798(2)	60(1)
F(5)	2085(3)	1905(2)	4291(2)	64(1)
F(6)	872(3)	2851(2)	5009(2)	60(1)
P(2)	4553(1)	741(1)	8707(1)	33(1)
F(7)	5242(2)	364(2)	9240(2)	56(1)
F(8)	3678(2)	310(1)	8760(2)	44(1)
F(9)	3863(2)	1118(1)	8177(2)	45(1)
F(10)	5431(2)	1165(2)	8660(2)	58(1)
F(11)	4905(2)	406(1)	8031(2)	42(1)
F(12)	4185(2)	1072(1)	9378(2)	42(1)
P(3)	2673(1)	8792(1)	4868(1)	30(1)
F(13)	2299(2)	8759(2)	4048(2)	46(1)
F(14)	2544(3)	9452(2)	4858(2)	57(1)
F(15)	3042(3)	8831(2)	5699(2)	57(1)
F(16)	2821(3)	8142(1)	4897(2)	42(1)
F(13A)	2078(18)	9273(7)	4464(11)	46(1)
F(14A)	2790(20)	9141(9)	5601(8)	57(1)
F(15A)	3200(20)	8281(8)	5273(11)	57(1)
F(16A)	2490(20)	8420(8)	4164(8)	42(1)
F(17)	1568(2)	8716(2)	5087(2)	55(1)
F(18)	3765(2)	8872(1)	4643(2)	45(1)
C(44)	4167(5)	2607(3)	3743(4)	64(2)
Cl(1)	5031(1)	2424(1)	4454(1)	65(1)
Cl(2)	4357(2)	2230(1)	2962(1)	70(1)
C(45)	3814(8)	1470(4)	5711(4)	68(2)
Cl(3)	3158(2)	839(1)	5745(2)	89(1)
Cl(4)	3926(2)	1792(1)	6548(1)	80(1)
C(45A)	3590(50)	1242(13)	5593(8)	68(2)
Cl(3A)	3077(11)	575(6)	5421(9)	89(1)
Cl(4A)	3836(9)	1341(8)	6513(6)	80(1)

Table S4. Bond lengths [Å] and angles [°] for **5**.

Co(1)-N(2)	1.859(3)	C(14)-C(15)	1.393(6)
Co(1)-N(5)	1.877(3)	C(14)-H(14)	0.9500
Co(1)-O(1)	1.918(3)	C(15)-H(15)	0.9500
Co(1)-N(3)	1.934(3)	C(16)-C(17)	1.395(7)
Co(1)-N(1)	1.955(4)	C(16)-H(16)	0.9500
Co(1)-N(4)	2.017(4)	C(17)-C(18)	1.369(7)
Co(2)-N(9)	1.887(4)	C(17)-H(17)	0.9500
Co(2)-N(6)	1.900(4)	C(18)-C(19)	1.399(7)
Co(2)-O(2)	1.905(3)	C(18)-H(18)	0.9500
Co(2)-N(8)	1.942(4)	C(19)-C(20)	1.375(6)
Co(2)-N(10)	1.979(4)	C(19)-H(19)	0.9500
Co(2)-N(7)	2.042(4)	C(20)-C(21)	1.462(6)
O(1)-O(2)	1.363(4)	C(21)-C(22)	1.376(6)
N(1)-C(1)	1.342(6)	C(22)-C(23)	1.386(6)
N(1)-C(5)	1.362(6)	C(22)-H(22)	0.9500
N(2)-C(10)	1.337(5)	C(23)-C(24)	1.447(6)
N(2)-C(6)	1.347(5)	C(24)-C(25)	1.393(7)
N(3)-C(15)	1.344(6)	C(25)-C(26)	1.347(8)
N(3)-C(11)	1.358(5)	C(25)-H(25)	0.9500
N(4)-C(16)	1.335(6)	C(26)-C(27)	1.382(9)
N(4)-C(20)	1.369(6)	C(26)-H(26)	0.9500
N(5)-N(6)	1.321(5)	C(27)-C(28)	1.397(8)
N(5)-C(21)	1.354(5)	C(27)-H(27)	0.9500
N(6)-C(23)	1.351(6)	C(28)-H(28)	0.9500
N(7)-C(28)	1.348(6)	C(29)-C(30)	1.394(7)
N(7)-C(24)	1.358(6)	C(29)-H(29)	0.9500
N(8)-C(29)	1.324(6)	C(30)-C(31)	1.369(8)
N(8)-C(33)	1.373(6)	C(30)-H(30)	0.9500
N(9)-C(34)	1.321(6)	C(31)-C(32)	1.375(8)
N(9)-C(38)	1.350(6)	C(31)-H(31)	0.9500
N(10)-C(43)	1.332(6)	C(32)-C(33)	1.390(7)
N(10)-C(39)	1.369(6)	C(32)-H(32)	0.9500
C(1)-C(2)	1.394(6)	C(33)-C(34)	1.457(7)
C(1)-H(1)	0.9500	C(34)-C(35)	1.374(7)
C(2)-C(3)	1.377(7)	C(35)-C(36)	1.383(8)
C(2)-H(2)	0.9500	C(35)-H(35)	0.9500
C(3)-C(4)	1.385(7)	C(36)-C(37)	1.370(9)
C(3)-H(3)	0.9500	C(36)-H(36)	0.9500
C(4)-C(5)	1.386(6)	C(37)-C(38)	1.389(7)
C(4)-H(4)	0.9500	C(37)-H(37)	0.9500
C(5)-C(6)	1.459(6)	C(38)-C(39)	1.459(7)
C(6)-C(7)	1.381(6)	C(39)-C(40)	1.389(7)
C(7)-C(8)	1.384(7)	C(40)-C(41)	1.368(8)
C(7)-H(7)	0.9500	C(40)-H(40)	0.9500
C(8)-C(9)	1.392(6)	C(41)-C(42)	1.359(8)
C(8)-H(8)	0.9500	C(41)-H(41)	0.9500
C(9)-C(10)	1.385(6)	C(42)-C(43)	1.405(7)
C(9)-H(9)	0.9500	C(42)-H(42)	0.9500
C(10)-C(11)	1.467(6)	C(43)-H(43)	0.9500
C(11)-C(12)	1.383(6)	P(1)-F(1)	1.568(4)
C(12)-C(13)	1.382(7)	P(1)-F(5)	1.581(4)
C(12)-H(12)	0.9500	P(1)-F(2)	1.585(4)
C(13)-C(14)	1.382(7)	P(1)-F(3)	1.595(4)
C(13)-H(13)	0.9500	P(1)-F(6)	1.604(4)

P(1)-F(4)	1.607(4)	P(3)-F(14A)	1.605(6)
P(2)-F(10)	1.587(3)	P(3)-F(14)	1.608(4)
P(2)-F(8)	1.597(3)	C(44)-Cl(2)	1.756(7)
P(2)-F(9)	1.598(3)	C(44)-Cl(1)	1.763(7)
P(2)-F(12)	1.601(3)	C(44)-H(44A)	0.9900
P(2)-F(7)	1.603(3)	C(44)-H(44B)	0.9900
P(2)-F(11)	1.606(3)	C(45)-Cl(4)	1.741(9)
P(3)-F(13)	1.578(3)	C(45)-Cl(3)	1.778(10)
P(3)-F(13A)	1.579(6)	C(45)-H(45A)	0.9900
P(3)-F(16)	1.590(3)	C(45)-H(45B)	0.9900
P(3)-F(18)	1.592(3)	C(45A)-Cl(4A)	1.741(10)
P(3)-F(15A)	1.594(6)	C(45A)-Cl(3A)	1.779(11)
P(3)-F(15)	1.594(4)	C(45A)-H(45C)	0.9900
P(3)-F(16A)	1.597(6)	C(45A)-H(45D)	0.9900
P(3)-F(17)	1.603(3)		

N(2)-Co(1)-N(5)	177.99(15)	C(11)-N(3)-Co(1)	114.5(3)
N(2)-Co(1)-O(1)	86.84(14)	C(16)-N(4)-C(20)	119.1(4)
N(5)-Co(1)-O(1)	91.31(14)	C(16)-N(4)-Co(1)	126.8(3)
N(2)-Co(1)-N(3)	81.99(15)	C(20)-N(4)-Co(1)	114.0(3)
N(5)-Co(1)-N(3)	97.47(15)	N(6)-N(5)-C(21)	108.8(3)
O(1)-Co(1)-N(3)	96.58(14)	N(6)-N(5)-Co(1)	131.2(3)
N(2)-Co(1)-N(1)	82.07(15)	C(21)-N(5)-Co(1)	119.7(3)
N(5)-Co(1)-N(1)	98.58(15)	N(5)-N(6)-C(23)	108.5(4)
O(1)-Co(1)-N(1)	86.28(14)	N(5)-N(6)-Co(2)	131.8(3)
N(3)-Co(1)-N(1)	163.62(15)	C(23)-N(6)-Co(2)	119.6(3)
N(2)-Co(1)-N(4)	101.48(14)	C(28)-N(7)-C(24)	118.0(4)
N(5)-Co(1)-N(4)	80.45(14)	C(28)-N(7)-Co(2)	127.0(4)
O(1)-Co(1)-N(4)	169.65(13)	C(24)-N(7)-Co(2)	114.6(3)
N(3)-Co(1)-N(4)	90.73(14)	C(29)-N(8)-C(33)	119.2(4)
N(1)-Co(1)-N(4)	88.76(14)	C(29)-N(8)-Co(2)	127.0(3)
N(9)-Co(2)-N(6)	177.19(16)	C(33)-N(8)-Co(2)	113.8(3)
N(9)-Co(2)-O(2)	87.50(15)	C(34)-N(9)-C(38)	122.7(4)
N(6)-Co(2)-O(2)	90.10(14)	C(34)-N(9)-Co(2)	118.3(3)
N(9)-Co(2)-N(8)	81.60(17)	C(38)-N(9)-Co(2)	118.2(3)
N(6)-Co(2)-N(8)	97.14(16)	C(43)-N(10)-C(39)	119.0(4)
O(2)-Co(2)-N(8)	94.40(15)	C(43)-N(10)-Co(2)	126.9(3)
N(9)-Co(2)-N(10)	81.51(16)	C(39)-N(10)-Co(2)	113.9(3)
N(6)-Co(2)-N(10)	99.84(15)	N(1)-C(1)-C(2)	122.0(4)
O(2)-Co(2)-N(10)	87.46(14)	N(1)-C(1)-H(1)	119.0
N(8)-Co(2)-N(10)	162.91(17)	C(2)-C(1)-H(1)	119.0
N(9)-Co(2)-N(7)	103.45(16)	C(3)-C(2)-C(1)	118.7(4)
N(6)-Co(2)-N(7)	79.13(15)	C(3)-C(2)-H(2)	120.7
O(2)-Co(2)-N(7)	166.83(15)	C(1)-C(2)-H(2)	120.7
N(8)-Co(2)-N(7)	94.44(16)	C(2)-C(3)-C(4)	119.9(4)
N(10)-Co(2)-N(7)	86.95(15)	C(2)-C(3)-H(3)	120.1
O(2)-O(1)-Co(1)	115.5(2)	C(4)-C(3)-H(3)	120.1
O(1)-O(2)-Co(2)	115.4(2)	C(3)-C(4)-C(5)	118.7(4)
C(1)-N(1)-C(5)	118.8(4)	C(3)-C(4)-H(4)	120.6
C(1)-N(1)-Co(1)	127.7(3)	C(5)-C(4)-H(4)	120.6
C(5)-N(1)-Co(1)	113.5(3)	N(1)-C(5)-C(4)	121.5(4)
C(10)-N(2)-C(6)	122.4(4)	N(1)-C(5)-C(6)	113.3(4)
C(10)-N(2)-Co(1)	118.8(3)	C(4)-C(5)-C(6)	125.1(4)
C(6)-N(2)-Co(1)	118.1(3)	N(2)-C(6)-C(7)	120.0(4)
C(15)-N(3)-C(11)	118.8(4)	N(2)-C(6)-C(5)	112.0(4)
C(15)-N(3)-Co(1)	126.5(3)	C(7)-C(6)-C(5)	128.0(4)

C(6)-C(7)-C(8)	118.3(4)	C(24)-C(25)-H(25)	120.1
C(6)-C(7)-H(7)	120.8	C(25)-C(26)-C(27)	119.3(5)
C(8)-C(7)-H(7)	120.8	C(25)-C(26)-H(26)	120.3
C(7)-C(8)-C(9)	121.0(4)	C(27)-C(26)-H(26)	120.3
C(7)-C(8)-H(8)	119.5	C(26)-C(27)-C(28)	119.5(5)
C(9)-C(8)-H(8)	119.5	C(26)-C(27)-H(27)	120.3
C(10)-C(9)-C(8)	118.0(4)	C(28)-C(27)-H(27)	120.3
C(10)-C(9)-H(9)	121.0	N(7)-C(28)-C(27)	121.4(5)
C(8)-C(9)-H(9)	121.0	N(7)-C(28)-H(28)	119.3
N(2)-C(10)-C(9)	120.2(4)	C(27)-C(28)-H(28)	119.3
N(2)-C(10)-C(11)	111.4(4)	N(8)-C(29)-C(30)	121.8(5)
C(9)-C(10)-C(11)	128.4(4)	N(8)-C(29)-H(29)	119.1
N(3)-C(11)-C(12)	122.2(4)	C(30)-C(29)-H(29)	119.1
N(3)-C(11)-C(10)	113.0(4)	C(31)-C(30)-C(29)	119.4(5)
C(12)-C(11)-C(10)	124.8(4)	C(31)-C(30)-H(30)	120.3
C(13)-C(12)-C(11)	118.8(4)	C(29)-C(30)-H(30)	120.3
C(13)-C(12)-H(12)	120.6	C(30)-C(31)-C(32)	119.7(5)
C(11)-C(12)-H(12)	120.6	C(30)-C(31)-H(31)	120.2
C(14)-C(13)-C(12)	119.4(4)	C(32)-C(31)-H(31)	120.2
C(14)-C(13)-H(13)	120.3	C(31)-C(32)-C(33)	119.0(5)
C(12)-C(13)-H(13)	120.3	C(31)-C(32)-H(32)	120.5
C(13)-C(14)-C(15)	119.3(4)	C(33)-C(32)-H(32)	120.5
C(13)-C(14)-H(14)	120.3	N(8)-C(33)-C(32)	120.9(5)
C(15)-C(14)-H(14)	120.3	N(8)-C(33)-C(34)	113.3(4)
N(3)-C(15)-C(14)	121.5(4)	C(32)-C(33)-C(34)	125.8(5)
N(3)-C(15)-H(15)	119.3	N(9)-C(34)-C(35)	120.4(5)
C(14)-C(15)-H(15)	119.3	N(9)-C(34)-C(33)	112.3(4)
N(4)-C(16)-C(17)	121.8(4)	C(35)-C(34)-C(33)	127.2(5)
N(4)-C(16)-H(16)	119.1	C(34)-C(35)-C(36)	118.1(5)
C(17)-C(16)-H(16)	119.1	C(34)-C(35)-H(35)	121.0
C(18)-C(17)-C(16)	119.3(4)	C(36)-C(35)-H(35)	121.0
C(18)-C(17)-H(17)	120.4	C(35)-C(36)-C(37)	121.3(5)
C(16)-C(17)-H(17)	120.4	C(35)-C(36)-H(36)	119.3
C(17)-C(18)-C(19)	119.3(4)	C(37)-C(36)-H(36)	119.3
C(17)-C(18)-H(18)	120.3	C(36)-C(37)-C(38)	118.2(5)
C(19)-C(18)-H(18)	120.3	C(36)-C(37)-H(37)	120.9
C(20)-C(19)-C(18)	119.0(4)	C(38)-C(37)-H(37)	120.9
C(20)-C(19)-H(19)	120.5	N(9)-C(38)-C(37)	119.2(5)
C(18)-C(19)-H(19)	120.5	N(9)-C(38)-C(39)	112.6(4)
N(4)-C(20)-C(19)	121.4(4)	C(37)-C(38)-C(39)	128.2(5)
N(4)-C(20)-C(21)	113.0(4)	N(10)-C(39)-C(40)	121.0(5)
C(19)-C(20)-C(21)	125.5(4)	N(10)-C(39)-C(38)	113.4(4)
N(5)-C(21)-C(22)	109.0(4)	C(40)-C(39)-C(38)	125.6(5)
N(5)-C(21)-C(20)	112.5(4)	C(41)-C(40)-C(39)	119.3(5)
C(22)-C(21)-C(20)	138.5(4)	C(41)-C(40)-H(40)	120.3
C(21)-C(22)-C(23)	104.6(4)	C(39)-C(40)-H(40)	120.3
C(21)-C(22)-H(22)	127.7	C(42)-C(41)-C(40)	119.9(5)
C(23)-C(22)-H(22)	127.7	C(42)-C(41)-H(41)	120.1
N(6)-C(23)-C(22)	109.1(4)	C(40)-C(41)-H(41)	120.1
N(6)-C(23)-C(24)	113.4(4)	C(41)-C(42)-C(43)	119.5(5)
C(22)-C(23)-C(24)	137.5(4)	C(41)-C(42)-H(42)	120.3
N(7)-C(24)-C(25)	122.0(4)	C(43)-C(42)-H(42)	120.3
N(7)-C(24)-C(23)	113.0(4)	N(10)-C(43)-C(42)	121.3(5)
C(25)-C(24)-C(23)	125.0(5)	N(10)-C(43)-H(43)	119.3
C(26)-C(25)-C(24)	119.7(5)	C(42)-C(43)-H(43)	119.3
C(26)-C(25)-H(25)	120.1	F(1)-P(1)-F(5)	92.9(2)

F(1)-P(1)-F(2)	92.2(3)
F(5)-P(1)-F(2)	90.4(2)
F(1)-P(1)-F(3)	176.4(2)
F(5)-P(1)-F(3)	89.9(2)
F(2)-P(1)-F(3)	89.9(2)
F(1)-P(1)-F(6)	89.5(2)
F(5)-P(1)-F(6)	177.2(2)
F(2)-P(1)-F(6)	90.7(2)
F(3)-P(1)-F(6)	87.6(2)
F(1)-P(1)-F(4)	88.4(3)
F(5)-P(1)-F(4)	89.9(2)
F(2)-P(1)-F(4)	179.3(3)
F(3)-P(1)-F(4)	89.5(2)
F(6)-P(1)-F(4)	88.9(2)
F(10)-P(2)-F(8)	179.3(2)
F(10)-P(2)-F(9)	90.4(2)
F(8)-P(2)-F(9)	90.30(17)
F(10)-P(2)-F(12)	90.08(17)
F(8)-P(2)-F(12)	89.94(16)
F(9)-P(2)-F(12)	89.49(17)
F(10)-P(2)-F(7)	89.7(2)
F(8)-P(2)-F(7)	89.65(19)
F(9)-P(2)-F(7)	179.8(2)
F(12)-P(2)-F(7)	90.34(17)
F(10)-P(2)-F(11)	90.67(17)
F(8)-P(2)-F(11)	89.32(17)
F(9)-P(2)-F(11)	90.11(17)
F(12)-P(2)-F(11)	179.16(17)
F(7)-P(2)-F(11)	90.06(17)
F(13)-P(3)-F(13A)	57.2(8)
F(13)-P(3)-F(16)	90.8(2)
F(13A)-P(3)-F(16)	143.9(9)
F(13)-P(3)-F(18)	89.36(17)
F(13A)-P(3)-F(18)	104.0(10)
F(16)-P(3)-F(18)	90.57(18)
F(13)-P(3)-F(15A)	121.4(8)
F(13A)-P(3)-F(15A)	175.8(15)
F(16)-P(3)-F(15A)	33.0(9)
F(18)-P(3)-F(15A)	79.7(12)
F(13)-P(3)-F(15)	179.4(2)
F(13A)-P(3)-F(15)	122.2(8)
F(16)-P(3)-F(15)	89.7(2)
F(18)-P(3)-F(15)	91.0(2)
F(15A)-P(3)-F(15)	59.2(8)
F(13)-P(3)-F(16A)	32.3(8)
F(13A)-P(3)-F(16A)	89.0(8)
F(16)-P(3)-F(16A)	58.6(8)
F(18)-P(3)-F(16A)	86.6(10)
F(15A)-P(3)-F(16A)	89.2(8)
F(15)-P(3)-F(16A)	148.2(8)
F(13)-P(3)-F(17)	90.11(19)
F(13A)-P(3)-F(17)	75.4(10)
F(16)-P(3)-F(17)	89.82(19)
F(18)-P(3)-F(17)	179.3(2)
F(15A)-P(3)-F(17)	100.9(12)
F(15)-P(3)-F(17)	89.5(2)
F(16A)-P(3)-F(17)	93.2(10)
F(13)-P(3)-F(14A)	149.0(9)
F(13A)-P(3)-F(14A)	91.8(8)
F(16)-P(3)-F(14A)	119.3(9)
F(18)-P(3)-F(14A)	97.3(12)
F(15A)-P(3)-F(14A)	89.7(8)
F(15)-P(3)-F(14A)	30.5(8)
F(16A)-P(3)-F(14A)	175.7(16)
F(17)-P(3)-F(14A)	82.9(12)
F(13)-P(3)-F(14)	90.7(2)
F(13A)-P(3)-F(14)	37.7(9)
F(16)-P(3)-F(14)	178.4(2)
F(18)-P(3)-F(14)	88.9(2)
F(15A)-P(3)-F(14)	145.4(10)
F(15)-P(3)-F(14)	88.8(2)
F(16A)-P(3)-F(14)	122.8(9)
F(17)-P(3)-F(14)	90.8(2)
F(14A)-P(3)-F(14)	59.3(9)
Cl(2)-C(44)-Cl(1)	111.1(4)
Cl(2)-C(44)-H(44A)	109.4
Cl(1)-C(44)-H(44A)	109.4
Cl(2)-C(44)-H(44B)	109.4
Cl(1)-C(44)-H(44B)	109.4
H(44A)-C(44)-H(44B)	108.0
Cl(4)-C(45)-Cl(3)	111.3(4)
Cl(4)-C(45)-H(45A)	109.4
Cl(3)-C(45)-H(45A)	109.4
Cl(4)-C(45)-H(45B)	109.4
Cl(3)-C(45)-H(45B)	109.4
H(45A)-C(45)-H(45B)	108.0
Cl(4A)-C(45A)-Cl(3A)	110.4(10)
Cl(4A)-C(45A)-H(45C)	109.6
Cl(3A)-C(45A)-H(45C)	109.6
Cl(4A)-C(45A)-H(45D)	109.6
Cl(3A)-C(45A)-H(45D)	109.6
H(45C)-C(45A)-H(45D)	108.1

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	15(1)	29(1)	17(1)	0(1)	2(1)	1(1)
Co(2)	26(1)	29(1)	20(1)	-1(1)	1(1)	0(1)
O(1)	21(2)	35(2)	26(2)	-2(1)	4(1)	5(1)
O(2)	33(2)	32(2)	25(2)	3(1)	-2(1)	0(1)
N(1)	21(2)	37(2)	19(2)	-2(2)	3(1)	3(2)
N(2)	19(2)	27(2)	21(2)	-1(1)	5(1)	1(1)
N(3)	21(2)	29(2)	21(2)	1(1)	3(1)	0(1)
N(4)	18(2)	30(2)	20(2)	3(1)	5(1)	1(1)
N(5)	19(2)	27(2)	21(2)	0(1)	5(1)	0(1)
N(6)	20(2)	35(2)	13(2)	2(1)	1(1)	-1(2)
N(7)	36(2)	36(2)	21(2)	-3(2)	1(2)	-7(2)
N(8)	29(2)	39(2)	27(2)	-4(2)	2(2)	2(2)
N(9)	33(2)	27(2)	24(2)	0(2)	-2(2)	2(2)
N(10)	33(2)	35(2)	20(2)	1(2)	-1(2)	-2(2)
C(1)	27(2)	34(2)	26(2)	1(2)	5(2)	2(2)
C(2)	37(3)	38(3)	23(2)	4(2)	7(2)	4(2)
C(3)	28(2)	42(3)	29(2)	0(2)	11(2)	-2(2)
C(4)	23(2)	40(3)	30(2)	1(2)	10(2)	1(2)
C(5)	19(2)	33(2)	25(2)	-3(2)	2(2)	2(2)
C(6)	19(2)	28(2)	29(2)	-1(2)	6(2)	4(2)
C(7)	19(2)	38(3)	29(2)	0(2)	2(2)	1(2)
C(8)	21(2)	43(3)	32(2)	-3(2)	-3(2)	0(2)
C(9)	26(2)	33(2)	24(2)	2(2)	2(2)	2(2)
C(10)	24(2)	28(2)	20(2)	1(2)	3(2)	2(2)
C(11)	20(2)	27(2)	20(2)	0(2)	0(2)	0(2)
C(12)	26(2)	36(2)	18(2)	0(2)	1(2)	0(2)
C(13)	31(2)	44(3)	22(2)	4(2)	8(2)	0(2)
C(14)	28(2)	46(3)	26(2)	6(2)	11(2)	-2(2)
C(15)	19(2)	41(3)	26(2)	0(2)	2(2)	-4(2)
C(16)	24(2)	39(3)	22(2)	-5(2)	4(2)	-3(2)
C(17)	35(3)	31(2)	36(3)	-4(2)	9(2)	0(2)
C(18)	35(3)	30(3)	54(3)	-3(2)	12(2)	6(2)
C(19)	26(2)	42(3)	37(3)	4(2)	3(2)	10(2)
C(20)	22(2)	36(2)	21(2)	3(2)	8(2)	4(2)
C(21)	16(2)	33(2)	18(2)	8(2)	6(2)	1(2)
C(22)	18(2)	34(2)	23(2)	7(2)	4(2)	0(2)
C(23)	23(2)	40(3)	16(2)	4(2)	2(2)	-4(2)
C(24)	31(2)	40(3)	20(2)	3(2)	3(2)	-4(2)
C(25)	30(2)	50(3)	28(2)	7(2)	-6(2)	-14(2)
C(26)	39(3)	70(4)	37(3)	11(3)	-10(2)	-16(3)
C(27)	58(4)	46(3)	35(3)	-9(2)	-13(3)	-14(3)
C(28)	49(3)	41(3)	27(2)	-4(2)	-4(2)	-6(2)
C(29)	44(3)	40(3)	32(3)	-1(2)	11(2)	-4(2)
C(30)	55(3)	51(3)	33(3)	3(2)	15(2)	0(3)
C(31)	43(3)	55(3)	38(3)	-7(2)	13(2)	-7(3)
C(32)	44(3)	49(3)	38(3)	-6(2)	5(2)	11(2)
C(33)	38(3)	40(3)	26(2)	-3(2)	2(2)	0(2)
C(34)	34(3)	34(3)	31(2)	-7(2)	-2(2)	3(2)
C(35)	53(3)	45(3)	39(3)	-2(2)	8(2)	11(3)

C(36)	66(4)	40(3)	50(3)	3(3)	4(3)	16(3)
C(37)	60(4)	40(3)	41(3)	6(2)	4(3)	3(3)
C(38)	42(3)	31(2)	27(2)	-1(2)	-4(2)	1(2)
C(39)	38(3)	38(3)	19(2)	-3(2)	-2(2)	-5(2)
C(40)	57(3)	41(3)	25(2)	1(2)	2(2)	-13(2)
C(41)	49(3)	55(3)	28(3)	5(2)	6(2)	-18(3)
C(42)	32(3)	52(3)	38(3)	-4(2)	6(2)	-8(2)
C(43)	30(2)	46(3)	28(2)	-2(2)	-1(2)	-1(2)
P(1)	37(1)	50(1)	32(1)	2(1)	6(1)	4(1)
F(1)	119(4)	88(3)	45(2)	24(2)	17(2)	32(3)
F(2)	59(2)	61(2)	102(3)	-5(2)	24(2)	-14(2)
F(3)	96(3)	58(2)	48(2)	6(2)	-13(2)	-5(2)
F(4)	41(2)	81(3)	58(2)	-20(2)	6(2)	-4(2)
F(5)	60(2)	66(2)	70(2)	-17(2)	22(2)	8(2)
F(6)	53(2)	63(2)	64(2)	-8(2)	10(2)	6(2)
P(2)	19(1)	48(1)	32(1)	4(1)	9(1)	2(1)
F(7)	43(2)	79(2)	44(2)	-1(2)	-6(1)	21(2)
F(8)	35(2)	53(2)	45(2)	4(1)	13(1)	-10(1)
F(9)	45(2)	57(2)	33(2)	10(1)	8(1)	10(1)
F(10)	33(2)	80(2)	63(2)	-16(2)	24(2)	-17(2)
F(11)	30(2)	57(2)	40(2)	-4(1)	13(1)	3(1)
F(12)	28(1)	65(2)	32(2)	-5(1)	8(1)	1(1)
P(3)	27(1)	39(1)	26(1)	3(1)	4(1)	-2(1)
F(13)	35(2)	74(3)	28(2)	16(2)	-6(1)	-7(2)
F(14)	61(3)	42(2)	71(3)	7(2)	18(2)	0(2)
F(15)	80(3)	62(3)	28(2)	-6(2)	2(2)	-17(2)
F(16)	47(2)	37(2)	41(2)	0(1)	9(2)	-1(2)
F(13A)	35(2)	74(3)	28(2)	16(2)	-6(1)	-7(2)
F(14A)	61(3)	42(2)	71(3)	7(2)	18(2)	0(2)
F(15A)	80(3)	62(3)	28(2)	-6(2)	2(2)	-17(2)
F(16A)	47(2)	37(2)	41(2)	0(1)	9(2)	-1(2)
F(17)	33(2)	73(2)	61(2)	4(2)	24(2)	-3(2)
F(18)	27(1)	64(2)	44(2)	-5(2)	5(1)	-12(1)
C(44)	63(4)	64(4)	67(4)	1(3)	11(3)	5(3)
Cl(1)	60(1)	64(1)	70(1)	0(1)	-4(1)	-8(1)
Cl(2)	80(1)	76(1)	56(1)	-4(1)	13(1)	-22(1)
C(45)	73(7)	70(6)	64(5)	17(4)	27(4)	21(5)
Cl(3)	78(2)	72(2)	122(3)	27(2)	45(2)	27(1)
Cl(4)	66(1)	130(3)	46(1)	5(1)	9(1)	34(2)
C(45A)	73(7)	70(6)	64(5)	17(4)	27(4)	21(5)
Cl(3A)	78(2)	72(2)	122(3)	27(2)	45(2)	27(1)
Cl(4A)	66(1)	130(3)	46(1)	5(1)	9(1)	34(2)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **5**.

	x	y	z	U(eq)
H(1)	8841	1300	6892	34
H(2)	9962	1581	6078	39
H(3)	11640	1573	6441	39
H(4)	12158	1361	7637	37
H(7)	12466	1184	8887	34
H(8)	12522	943	10103	39
H(9)	11075	716	10640	33
H(12)	9459	535	10996	32
H(13)	7829	314	11192	38
H(14)	6644	300	10216	40
H(15)	7100	513	9066	35
H(16)	9339	1984	9184	34
H(17)	8504	2825	9182	40
H(18)	6998	2914	8515	47
H(19)	6377	2164	7812	42
H(22)	5940	1184	7010	30
H(25)	5070	346	6151	44
H(26)	4492	-429	5543	59
H(27)	5374	-1255	5679	57
H(28)	6854	-1275	6402	47
H(29)	8651	404	6418	46
H(30)	9936	468	5666	54
H(31)	10991	-276	5567	54
H(32)	10738	-1084	6209	52
H(35)	10338	-1835	6943	54
H(36)	9731	-2505	7694	63
H(37)	8399	-2315	8357	56
H(40)	6873	-2019	8814	49
H(41)	5559	-1596	9314	53
H(42)	5209	-680	9064	49
H(43)	6223	-175	8342	42
H(44A)	3496	2536	3886	77
H(44B)	4224	3006	3642	77
H(45A)	4477	1398	5551	82
H(45B)	3466	1719	5356	82
H(45C)	4198	1281	5347	82
H(45D)	3116	1526	5399	82

Table S7. Torsion angles [°] for **5**.

N(2)-Co(1)-O(1)-O(2)	128.1(3)	N(1)-Co(1)-N(5)-N(6)	90.6(4)
N(5)-Co(1)-O(1)-O(2)	-51.1(3)	N(4)-Co(1)-N(5)-N(6)	177.9(4)
N(3)-Co(1)-O(1)-O(2)	46.6(3)	N(2)-Co(1)-N(5)-C(21)	169(4)
N(1)-Co(1)-O(1)-O(2)	-149.6(3)	O(1)-Co(1)-N(5)-C(21)	-168.4(3)
N(4)-Co(1)-O(1)-O(2)	-88.1(8)	N(3)-Co(1)-N(5)-C(21)	94.8(3)
Co(1)-O(1)-O(2)-Co(2)	87.0(3)	N(1)-Co(1)-N(5)-C(21)	-82.0(3)
N(9)-Co(2)-O(2)-O(1)	123.7(3)	N(4)-Co(1)-N(5)-C(21)	5.3(3)
N(6)-Co(2)-O(2)-O(1)	-54.8(3)	C(21)-N(5)-N(6)-C(23)	0.2(4)
N(8)-Co(2)-O(2)-O(1)	42.4(3)	Co(1)-N(5)-N(6)-C(23)	-172.9(3)
N(10)-Co(2)-O(2)-O(1)	-154.7(3)	C(21)-N(5)-N(6)-Co(2)	-175.6(3)
N(7)-Co(2)-O(2)-O(1)	-89.7(7)	Co(1)-N(5)-N(6)-Co(2)	11.2(5)
N(2)-Co(1)-N(1)-C(1)	-170.6(4)	N(9)-Co(2)-N(6)-N(5)	-23(3)
N(5)-Co(1)-N(1)-C(1)	11.3(4)	O(2)-Co(2)-N(6)-N(5)	7.7(4)
O(1)-Co(1)-N(1)-C(1)	102.1(4)	N(8)-Co(2)-N(6)-N(5)	-86.7(4)
N(3)-Co(1)-N(1)-C(1)	-157.2(5)	N(10)-Co(2)-N(6)-N(5)	95.2(4)
N(4)-Co(1)-N(1)-C(1)	-68.8(4)	N(7)-Co(2)-N(6)-N(5)	-179.9(4)
N(2)-Co(1)-N(1)-C(5)	8.2(3)	N(9)-Co(2)-N(6)-C(23)	161(3)
N(5)-Co(1)-N(1)-C(5)	-169.9(3)	O(2)-Co(2)-N(6)-C(23)	-167.7(3)
O(1)-Co(1)-N(1)-C(5)	-79.1(3)	N(8)-Co(2)-N(6)-C(23)	97.8(3)
N(3)-Co(1)-N(1)-C(5)	21.6(7)	N(10)-Co(2)-N(6)-C(23)	-80.3(3)
N(4)-Co(1)-N(1)-C(5)	110.0(3)	N(7)-Co(2)-N(6)-C(23)	4.6(3)
N(5)-Co(1)-N(2)-C(10)	-71(4)	N(9)-Co(2)-N(7)-C(28)	3.4(4)
O(1)-Co(1)-N(2)-C(10)	-93.3(3)	N(6)-Co(2)-N(7)-C(28)	-177.7(4)
N(3)-Co(1)-N(2)-C(10)	3.8(3)	O(2)-Co(2)-N(7)-C(28)	-142.1(6)
N(1)-Co(1)-N(2)-C(10)	-180.0(3)	N(8)-Co(2)-N(7)-C(28)	85.9(4)
N(4)-Co(1)-N(2)-C(10)	92.9(3)	N(10)-Co(2)-N(7)-C(28)	-77.1(4)
N(5)-Co(1)-N(2)-C(6)	100(4)	N(9)-Co(2)-N(7)-C(24)	176.4(3)
O(1)-Co(1)-N(2)-C(6)	77.6(3)	N(6)-Co(2)-N(7)-C(24)	-4.8(3)
N(3)-Co(1)-N(2)-C(6)	174.7(3)	O(2)-Co(2)-N(7)-C(24)	30.8(8)
N(1)-Co(1)-N(2)-C(6)	-9.1(3)	N(8)-Co(2)-N(7)-C(24)	-101.2(3)
N(4)-Co(1)-N(2)-C(6)	-96.2(3)	N(10)-Co(2)-N(7)-C(24)	95.9(3)
N(2)-Co(1)-N(3)-C(15)	173.9(4)	N(9)-Co(2)-N(8)-C(29)	174.8(4)
N(5)-Co(1)-N(3)-C(15)	-8.0(4)	N(6)-Co(2)-N(8)-C(29)	-7.7(4)
O(1)-Co(1)-N(3)-C(15)	-100.2(4)	O(2)-Co(2)-N(8)-C(29)	-98.4(4)
N(1)-Co(1)-N(3)-C(15)	160.5(5)	N(10)-Co(2)-N(8)-C(29)	165.9(5)
N(4)-Co(1)-N(3)-C(15)	72.4(4)	N(7)-Co(2)-N(8)-C(29)	71.8(4)
N(2)-Co(1)-N(3)-C(11)	0.0(3)	N(9)-Co(2)-N(8)-C(33)	-6.6(3)
N(5)-Co(1)-N(3)-C(11)	178.0(3)	N(6)-Co(2)-N(8)-C(33)	170.9(3)
O(1)-Co(1)-N(3)-C(11)	85.8(3)	O(2)-Co(2)-N(8)-C(33)	80.2(3)
N(1)-Co(1)-N(3)-C(11)	-13.4(7)	N(10)-Co(2)-N(8)-C(33)	-15.5(7)
N(4)-Co(1)-N(3)-C(11)	-101.5(3)	N(7)-Co(2)-N(8)-C(33)	-109.6(3)
N(2)-Co(1)-N(4)-C(16)	-2.0(4)	N(6)-Co(2)-N(9)-C(34)	-55(3)
N(5)-Co(1)-N(4)-C(16)	177.5(4)	O(2)-Co(2)-N(9)-C(34)	-86.4(3)
O(1)-Co(1)-N(4)-C(16)	-145.0(7)	N(8)-Co(2)-N(9)-C(34)	8.4(3)
N(3)-Co(1)-N(4)-C(16)	80.0(4)	N(10)-Co(2)-N(9)-C(34)	-174.2(4)
N(1)-Co(1)-N(4)-C(16)	-83.6(4)	N(7)-Co(2)-N(9)-C(34)	101.0(3)
N(2)-Co(1)-N(4)-C(20)	177.9(3)	N(6)-Co(2)-N(9)-C(38)	115(3)
N(5)-Co(1)-N(4)-C(20)	-2.7(3)	O(2)-Co(2)-N(9)-C(38)	83.5(3)
O(1)-Co(1)-N(4)-C(20)	34.9(9)	N(8)-Co(2)-N(9)-C(38)	178.3(4)
N(3)-Co(1)-N(4)-C(20)	-100.1(3)	N(10)-Co(2)-N(9)-C(38)	-4.3(3)
N(1)-Co(1)-N(4)-C(20)	96.2(3)	N(7)-Co(2)-N(9)-C(38)	-89.1(3)
N(2)-Co(1)-N(5)-N(6)	-18(4)	N(9)-Co(2)-N(10)-C(43)	-174.3(4)
O(1)-Co(1)-N(5)-N(6)	4.2(4)	N(6)-Co(2)-N(10)-C(43)	8.2(4)
N(3)-Co(1)-N(5)-N(6)	-92.7(4)	O(2)-Co(2)-N(10)-C(43)	97.9(4)

N(8)-Co(2)-N(10)-C(43)	-165.4(5)	C(16)-N(4)-C(20)-C(19)	-0.8(6)
N(7)-Co(2)-N(10)-C(43)	-70.2(4)	Co(1)-N(4)-C(20)-C(19)	179.4(3)
N(9)-Co(2)-N(10)-C(39)	0.4(3)	C(16)-N(4)-C(20)-C(21)	179.9(3)
N(6)-Co(2)-N(10)-C(39)	-177.1(3)	Co(1)-N(4)-C(20)-C(21)	0.0(4)
O(2)-Co(2)-N(10)-C(39)	-87.5(3)	C(18)-C(19)-C(20)-N(4)	0.5(7)
N(8)-Co(2)-N(10)-C(39)	9.3(7)	C(18)-C(19)-C(20)-C(21)	179.8(4)
N(7)-Co(2)-N(10)-C(39)	104.5(3)	N(6)-N(5)-C(21)-C(22)	0.0(4)
C(5)-N(1)-C(1)-C(2)	5.8(7)	Co(1)-N(5)-C(21)-C(22)	174.1(3)
Co(1)-N(1)-C(1)-C(2)	-175.5(3)	N(6)-N(5)-C(21)-C(20)	179.2(3)
N(1)-C(1)-C(2)-C(3)	-0.5(7)	Co(1)-N(5)-C(21)-C(20)	-6.7(4)
C(1)-C(2)-C(3)-C(4)	-3.5(7)	N(4)-C(20)-C(21)-N(5)	4.0(5)
C(2)-C(3)-C(4)-C(5)	2.1(7)	C(19)-C(20)-C(21)-N(5)	-175.3(4)
C(1)-N(1)-C(5)-C(4)	-7.2(6)	N(4)-C(20)-C(21)-C(22)	-177.1(5)
Co(1)-N(1)-C(5)-C(4)	173.9(3)	C(19)-C(20)-C(21)-C(22)	3.6(8)
C(1)-N(1)-C(5)-C(6)	172.8(4)	N(5)-C(21)-C(22)-C(23)	-0.2(4)
Co(1)-N(1)-C(5)-C(6)	-6.1(5)	C(20)-C(21)-C(22)-C(23)	-179.1(5)
C(3)-C(4)-C(5)-N(1)	3.3(7)	N(5)-N(6)-C(23)-C(22)	-0.3(4)
C(3)-C(4)-C(5)-C(6)	-176.6(4)	Co(2)-N(6)-C(23)-C(22)	176.1(3)
C(10)-N(2)-C(6)-C(7)	-2.2(6)	N(5)-N(6)-C(23)-C(24)	179.9(3)
Co(1)-N(2)-C(6)-C(7)	-172.8(3)	Co(2)-N(6)-C(23)-C(24)	-3.7(5)
C(10)-N(2)-C(6)-C(5)	178.5(4)	C(21)-C(22)-C(23)-N(6)	0.3(4)
Co(1)-N(2)-C(6)-C(5)	8.0(5)	C(21)-C(22)-C(23)-C(24)	-179.9(5)
N(1)-C(5)-C(6)-N(2)	-0.8(5)	C(28)-N(7)-C(24)-C(25)	-1.0(7)
C(4)-C(5)-C(6)-N(2)	179.2(4)	Co(2)-N(7)-C(24)-C(25)	-174.6(3)
N(1)-C(5)-C(6)-C(7)	-179.9(4)	C(28)-N(7)-C(24)-C(23)	177.8(4)
C(4)-C(5)-C(6)-C(7)	0.0(8)	Co(2)-N(7)-C(24)-C(23)	4.2(5)
N(2)-C(6)-C(7)-C(8)	1.6(7)	N(6)-C(23)-C(24)-N(7)	-0.6(5)
C(5)-C(6)-C(7)-C(8)	-179.2(4)	C(22)-C(23)-C(24)-N(7)	179.7(5)
C(6)-C(7)-C(8)-C(9)	-1.2(7)	N(6)-C(23)-C(24)-C(25)	178.2(4)
C(7)-C(8)-C(9)-C(10)	1.2(7)	C(22)-C(23)-C(24)-C(25)	-1.6(8)
C(6)-N(2)-C(10)-C(9)	2.3(6)	N(7)-C(24)-C(25)-C(26)	1.5(7)
Co(1)-N(2)-C(10)-C(9)	172.7(3)	C(23)-C(24)-C(25)-C(26)	-177.1(5)
C(6)-N(2)-C(10)-C(11)	-176.9(4)	C(24)-C(25)-C(26)-C(27)	-0.4(8)
Co(1)-N(2)-C(10)-C(11)	-6.4(5)	C(25)-C(26)-C(27)-C(28)	-1.0(9)
C(8)-C(9)-C(10)-N(2)	-1.7(6)	C(24)-N(7)-C(28)-C(27)	-0.5(7)
C(8)-C(9)-C(10)-C(11)	177.3(4)	Co(2)-N(7)-C(28)-C(27)	172.2(4)
C(15)-N(3)-C(11)-C(12)	2.7(6)	C(26)-C(27)-C(28)-N(7)	1.6(8)
Co(1)-N(3)-C(11)-C(12)	177.2(3)	C(33)-N(8)-C(29)-C(30)	-2.9(7)
C(15)-N(3)-C(11)-C(10)	-177.7(4)	Co(2)-N(8)-C(29)-C(30)	175.7(4)
Co(1)-N(3)-C(11)-C(10)	-3.3(5)	N(8)-C(29)-C(30)-C(31)	1.3(8)
N(2)-C(10)-C(11)-N(3)	6.0(5)	C(29)-C(30)-C(31)-C(32)	0.7(9)
C(9)-C(10)-C(11)-N(3)	-173.0(4)	C(30)-C(31)-C(32)-C(33)	-1.0(8)
N(2)-C(10)-C(11)-C(12)	-174.4(4)	C(29)-N(8)-C(33)-C(32)	2.6(7)
C(9)-C(10)-C(11)-C(12)	6.5(7)	Co(2)-N(8)-C(33)-C(32)	-176.1(4)
N(3)-C(11)-C(12)-C(13)	-1.5(7)	C(29)-N(8)-C(33)-C(34)	-177.1(4)
C(10)-C(11)-C(12)-C(13)	179.0(4)	Co(2)-N(8)-C(33)-C(34)	4.2(5)
C(11)-C(12)-C(13)-C(14)	0.1(7)	C(31)-C(32)-C(33)-N(8)	-0.7(8)
C(12)-C(13)-C(14)-C(15)	0.0(7)	C(31)-C(32)-C(33)-C(34)	179.0(5)
C(11)-N(3)-C(15)-C(14)	-2.6(7)	C(38)-N(9)-C(34)-C(35)	1.8(7)
Co(1)-N(3)-C(15)-C(14)	-176.3(3)	Co(2)-N(9)-C(34)-C(35)	171.2(4)
C(13)-C(14)-C(15)-N(3)	1.3(7)	C(38)-N(9)-C(34)-C(33)	-177.6(4)
C(20)-N(4)-C(16)-C(17)	0.0(6)	Co(2)-N(9)-C(34)-C(33)	-8.1(5)
Co(1)-N(4)-C(16)-C(17)	179.8(3)	N(8)-C(33)-C(34)-N(9)	2.3(6)
N(4)-C(16)-C(17)-C(18)	1.1(7)	C(32)-C(33)-C(34)-N(9)	-177.4(5)
C(16)-C(17)-C(18)-C(19)	-1.4(7)	N(8)-C(33)-C(34)-C(35)	-177.1(5)
C(17)-C(18)-C(19)-C(20)	0.6(7)	C(32)-C(33)-C(34)-C(35)	3.3(8)

N(9)-C(34)-C(35)-C(36)	-0.7(8)	Co(2)-N(10)-C(39)-C(38)	3.2(5)
C(33)-C(34)-C(35)-C(36)	178.6(5)	N(9)-C(38)-C(39)-N(10)	-6.5(6)
C(34)-C(35)-C(36)-C(37)	-1.6(9)	C(37)-C(38)-C(39)-N(10)	170.3(5)
C(35)-C(36)-C(37)-C(38)	2.7(9)	N(9)-C(38)-C(39)-C(40)	172.6(4)
C(34)-N(9)-C(38)-C(37)	-0.6(7)	C(37)-C(38)-C(39)-C(40)	-10.6(8)
Co(2)-N(9)-C(38)-C(37)	-170.0(4)	N(10)-C(39)-C(40)-C(41)	0.2(7)
C(34)-N(9)-C(38)-C(39)	176.6(4)	C(38)-C(39)-C(40)-C(41)	-178.8(5)
Co(2)-N(9)-C(38)-C(39)	7.1(5)	C(39)-C(40)-C(41)-C(42)	0.9(8)
C(36)-C(37)-C(38)-N(9)	-1.7(8)	C(40)-C(41)-C(42)-C(43)	-1.3(8)
C(36)-C(37)-C(38)-C(39)	-178.3(5)	C(39)-N(10)-C(43)-C(42)	0.4(7)
C(43)-N(10)-C(39)-C(40)	-0.8(7)	Co(2)-N(10)-C(43)-C(42)	174.8(4)
Co(2)-N(10)-C(39)-C(40)	-175.9(4)	C(41)-C(42)-C(43)-N(10)	0.6(8)
C(43)-N(10)-C(39)-C(38)	178.3(4)		

Symmetry transformations used to generate equivalent atoms:

Single crystal X-ray crystallography for [(μ-bpp)(μ-O_2)(Co(Me_2bimpy))$_2$][PF_6]$_3$ (6)

Data Collection

A colorless crystal with approximate dimensions 0.26 x 0.25 x 0.20 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker Quazar SMART APEXII diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.96 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5º in a 6º range about ω with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program suite. The final cell constants were calculated from a set of 9874 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.83 Å. A total of 29785 data were harvested by collecting 4 sets of frames with 0.5º scans in ω and ϕ with exposure times of 40 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups $P\bar{1}$ and $P1$. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$ that yielded chemically reasonable and computationally stable results of refinement [2-4].

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients unless otherwise specified. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The asymmetric unit contains the dinuclear Co complex, three hexafluorophosphate anions, one molecule of solvent acetone, and one molecule of solvent pentane. The latter is disordered over two positions over a crystallographic inversion center and was refined with an idealized geometry and thermal displacement parameter constraints.

The final least-squares refinement of 756 parameters against 9227 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0384 and 0.1132, respectively. The final difference Fourier map was featureless.

The molecular diagrams are drawn with 50% probability ellipsoids.

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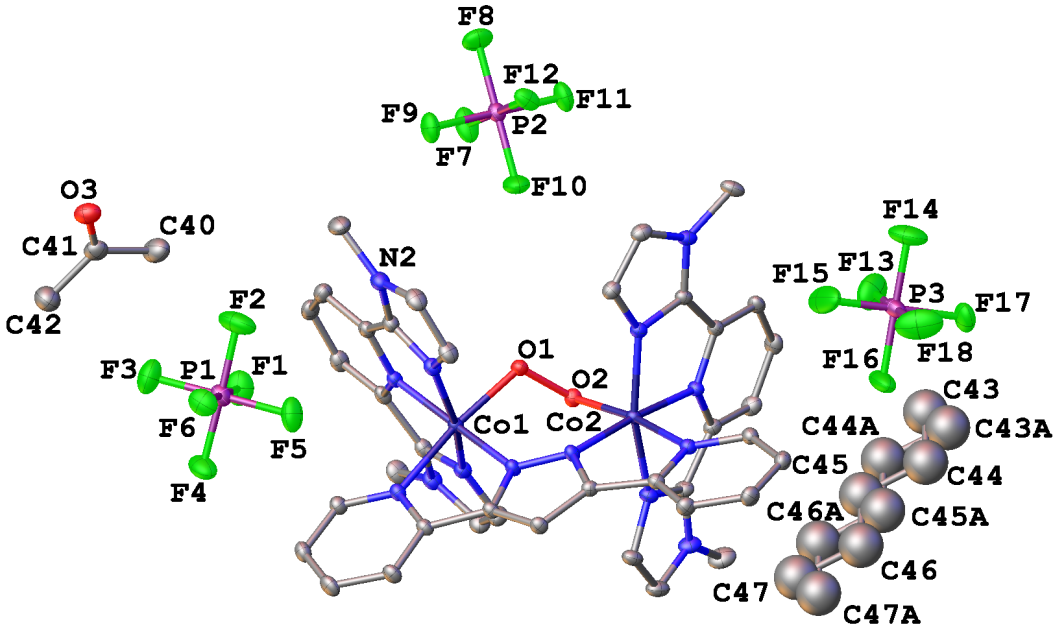

Figure S18. A molecular drawing of the content of the asymmetric unit of **6**. Both positions of the disordered pentane molecule are shown. All H atoms are omitted.

Table S8. Crystal data and structure refinement for **6**.

Identification code	stahl125	
Empirical formula	$C_{47}\ H_{53}\ Co_2\ F_{18}\ N_{14}\ O_3\ P_3$	
Formula weight	1414.80	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.150(4) Å	a= 95.70(2)°.
	b = 13.310(4) Å	b= 96.001(19)°.
	c = 17.433(5) Å	g = 107.53(3)°.
Volume	2648.0(13) $Å^3$	
Z	2	
Density (calculated)	1.774 Mg/m^3	
Absorption coefficient	0.840 mm^{-1}	
F(000)	1436	
Crystal size	0.26 x 0.25 x 0.20 mm^3	
Theta range for data collection	2.81 to 25.00°.	
Index ranges	-14<=h<=14, -15<=k<=15, -20<=l<=20	

Reflections collected	29785
Independent reflections	9227 [R(int) = 0.0246]
Completeness to theta = 25.00°	99.0 %
Absorption correction	Numerical with SADABS
Max. and min. transmission	0.8500 and 0.8112
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9227 / 0 / 746
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.1095
R indices (all data)	R1 = 0.0438, wR2 = 0.1132
Largest diff. peak and hole	0.871 and -1.132 e.$Å^{-3}$

Table S9. Bond lengths [Å] and angles [°] for **6**.

Co(1)-N(7)	1.869(2)	N(13)-C(38)	1.375(3)
Co(1)-O(1)	1.8853(18)	N(13)-C(37)	1.472(3)
Co(1)-N(3)	1.893(2)	N(14)-C(36)	1.347(3)
Co(1)-N(1)	1.913(2)	N(14)-C(39)	1.361(3)
Co(1)-N(5)	1.925(2)	C(1)-C(2)	1.359(4)
Co(1)-N(6)	2.031(2)	C(1)-H(1)	0.9500
Co(2)-N(8)	1.871(2)	C(2)-H(2)	0.9500
Co(2)-O(2)	1.8951(18)	C(3)-H(3A)	0.9800
Co(2)-N(12)	1.897(2)	C(3)-H(3B)	0.9800
Co(2)-N(10)	1.920(2)	C(3)-H(3C)	0.9800
Co(2)-N(14)	1.937(2)	C(4)-C(5)	1.458(4)
Co(2)-N(9)	2.044(2)	C(5)-C(6)	1.391(4)
O(1)-O(2)	1.391(3)	C(6)-C(7)	1.388(4)
N(1)-C(4)	1.335(3)	C(6)-H(6)	0.9500
N(1)-C(1)	1.370(3)	C(7)-C(8)	1.383(4)
N(2)-C(4)	1.347(4)	C(7)-H(7)	0.9500
N(2)-C(2)	1.379(4)	C(8)-C(9)	1.391(4)
N(2)-C(3)	1.463(4)	C(8)-H(8)	0.9500
N(3)-C(9)	1.348(3)	C(9)-C(10)	1.454(4)
N(3)-C(5)	1.350(3)	C(11)-H(11A)	0.9800
N(4)-C(10)	1.348(4)	C(11)-H(11B)	0.9800
N(4)-C(12)	1.370(4)	C(11)-H(11C)	0.9800
N(4)-C(11)	1.464(3)	C(12)-C(13)	1.364(4)
N(5)-C(10)	1.337(3)	C(12)-H(12)	0.9500
N(5)-C(13)	1.360(4)	C(13)-H(13)	0.9500
N(6)-C(14)	1.341(3)	C(14)-C(15)	1.378(4)
N(6)-C(18)	1.362(3)	C(14)-H(14)	0.9500
N(7)-N(8)	1.325(3)	C(15)-C(16)	1.384(4)
N(7)-C(19)	1.353(3)	C(15)-H(15)	0.9500
N(8)-C(21)	1.350(3)	C(16)-C(17)	1.389(4)
N(9)-C(26)	1.340(3)	C(16)-H(16)	0.9500
N(9)-C(22)	1.362(3)	C(17)-C(18)	1.381(4)
N(10)-C(30)	1.334(3)	C(17)-H(17)	0.9500
N(10)-C(27)	1.372(3)	C(18)-C(19)	1.466(4)
N(11)-C(30)	1.348(3)	C(19)-C(20)	1.391(4)
N(11)-C(28)	1.371(4)	C(20)-C(21)	1.392(4)
N(11)-C(29)	1.463(4)	C(20)-H(20)	0.9500
N(12)-C(31)	1.349(3)	C(21)-C(22)	1.459(4)
N(12)-C(35)	1.349(3)	C(22)-C(23)	1.385(4)
N(13)-C(36)	1.346(3)	C(23)-C(24)	1.386(4)

C(23)-H(23)	0.9500	P(3)-F(16)	1.593(2)
C(24)-C(25)	1.387(4)	P(3)-F(18)	1.602(2)
C(24)-H(24)	0.9500	O(3)-C(41)	1.206(4)
C(25)-C(26)	1.386(4)	C(40)-C(41)	1.504(4)
C(25)-H(25)	0.9500	C(40)-H(40A)	0.9800
C(26)-H(26)	0.9500	C(40)-H(40B)	0.9800
C(27)-C(28)	1.363(4)	C(40)-H(40C)	0.9800
C(27)-H(27)	0.9500	C(41)-C(42)	1.500(4)
C(28)-H(28)	0.9500	C(42)-H(42A)	0.9800
C(29)-H(29A)	0.9800	C(42)-H(42B)	0.9800
C(29)-H(29B)	0.9800	C(42)-H(42C)	0.9800
C(29)-H(29C)	0.9800	C(43)-C(44)	1.5314(17)
C(30)-C(31)	1.457(4)	C(43)-H(43D)	0.9800
C(31)-C(32)	1.388(4)	C(43)-H(43E)	0.9800
C(32)-C(33)	1.387(4)	C(43)-H(43F)	0.9800
C(32)-H(32)	0.9500	C(44)-C(45)	1.5328
C(33)-C(34)	1.389(4)	C(44)-H(44C)	0.9900
C(33)-H(33)	0.9500	C(44)-H(44D)	0.9900
C(34)-C(35)	1.388(4)	C(45)-C(46)	1.534(2)
C(34)-H(34)	0.9500	C(45)-H(45C)	0.9900
C(35)-C(36)	1.450(4)	C(45)-H(45D)	0.9900
C(37)-H(37A)	0.9800	C(46)-C(47)	1.5310
C(37)-H(37B)	0.9800	C(46)-H(46C)	0.9900
C(37)-H(37C)	0.9800	C(46)-H(46D)	0.9900
C(38)-C(39)	1.370(4)	C(47)-H(47D)	0.9800
C(38)-H(38)	0.9500	C(47)-H(47E)	0.9800
C(39)-H(39)	0.9500	C(47)-H(47F)	0.9800
P(1)-F(4)	1.592(2)	C(43A)-C(44A)	1.5310
P(1)-F(2)	1.591(2)	C(43A)-H(43A)	0.9800
P(1)-F(5)	1.592(2)	C(43A)-H(43B)	0.9800
P(1)-F(6)	1.5965(18)	C(43A)-H(43C)	0.9800
P(1)-F(3)	1.597(2)	C(44A)-C(45A)	1.5331(18)
P(1)-F(1)	1.6028(19)	C(44A)-H(44A)	0.9900
P(2)-F(10)	1.588(2)	C(44A)-H(44B)	0.9900
P(2)-F(8)	1.5967(19)	C(45A)-C(46A)	1.5328
P(2)-F(11)	1.5969(18)	C(45A)-H(45A)	0.9900
P(2)-F(7)	1.5994(18)	C(45A)-H(45B)	0.9900
P(2)-F(9)	1.5999(17)	C(46A)-C(47A)	1.531(2)
P(2)-F(12)	1.6069(17)	C(46A)-H(46A)	0.9900
P(3)-F(13)	1.585(2)	C(46A)-H(46B)	0.9900
P(3)-F(15)	1.588(2)	C(47A)-H(47A)	0.9800
P(3)-F(14)	1.589(2)	C(47A)-H(47B)	0.9800
P(3)-F(17)	1.5908(19)	C(47A)-H(47C)	0.9800

N(7)-Co(1)-O(1)	90.48(9)	N(3)-Co(1)-N(6)	98.27(9)
N(7)-Co(1)-N(3)	174.79(9)	N(1)-Co(1)-N(6)	91.42(9)
O(1)-Co(1)-N(3)	90.93(8)	N(5)-Co(1)-N(6)	91.79(9)
N(7)-Co(1)-N(1)	93.07(10)	N(8)-Co(2)-O(2)	91.48(8)
O(1)-Co(1)-N(1)	87.77(9)	N(8)-Co(2)-N(12)	173.67(9)
N(3)-Co(1)-N(1)	81.98(10)	O(2)-Co(2)-N(12)	87.00(8)
N(7)-Co(1)-N(5)	103.42(10)	N(8)-Co(2)-N(10)	92.46(9)
O(1)-Co(1)-N(5)	91.64(9)	O(2)-Co(2)-N(10)	87.94(9)
N(3)-Co(1)-N(5)	81.55(10)	N(12)-Co(2)-N(10)	81.35(9)
N(1)-Co(1)-N(5)	163.51(9)	N(8)-Co(2)-N(14)	104.50(9)
N(7)-Co(1)-N(6)	80.17(9)	O(2)-Co(2)-N(14)	92.36(9)
O(1)-Co(1)-N(6)	170.56(8)	N(12)-Co(2)-N(14)	81.71(9)

N(10)-Co(2)-N(14)	163.02(9)	N(2)-C(3)-H(3A)	109.5
N(8)-Co(2)-N(9)	79.63(9)	N(2)-C(3)-H(3B)	109.5
O(2)-Co(2)-N(9)	170.92(8)	H(3A)-C(3)-H(3B)	109.5
N(12)-Co(2)-N(9)	101.64(9)	N(2)-C(3)-H(3C)	109.5
N(10)-Co(2)-N(9)	90.59(9)	H(3A)-C(3)-H(3C)	109.5
N(14)-Co(2)-N(9)	91.66(9)	H(3B)-C(3)-H(3C)	109.5
O(2)-O(1)-Co(1)	112.61(13)	N(1)-C(4)-N(2)	110.4(2)
O(1)-O(2)-Co(2)	113.67(13)	N(1)-C(4)-C(5)	116.8(2)
C(4)-N(1)-C(1)	107.0(2)	N(2)-C(4)-C(5)	132.8(2)
C(4)-N(1)-Co(1)	113.75(18)	N(3)-C(5)-C(6)	120.1(2)
C(1)-N(1)-Co(1)	139.1(2)	N(3)-C(5)-C(4)	108.8(2)
C(4)-N(2)-C(2)	106.9(2)	C(6)-C(5)-C(4)	131.1(3)
C(4)-N(2)-C(3)	127.7(2)	C(7)-C(6)-C(5)	118.1(3)
C(2)-N(2)-C(3)	125.4(2)	C(7)-C(6)-H(6)	121.0
C(9)-N(3)-C(5)	122.1(2)	C(5)-C(6)-H(6)	121.0
C(9)-N(3)-Co(1)	119.31(18)	C(8)-C(7)-C(6)	121.5(3)
C(5)-N(3)-Co(1)	118.51(18)	C(8)-C(7)-H(7)	119.2
C(10)-N(4)-C(12)	107.0(2)	C(6)-C(7)-H(7)	119.2
C(10)-N(4)-C(11)	127.5(2)	C(7)-C(8)-C(9)	118.1(3)
C(12)-N(4)-C(11)	125.5(2)	C(7)-C(8)-H(8)	121.0
C(10)-N(5)-C(13)	106.8(2)	C(9)-C(8)-H(8)	121.0
C(10)-N(5)-Co(1)	113.46(18)	N(3)-C(9)-C(8)	120.2(2)
C(13)-N(5)-Co(1)	139.60(19)	N(3)-C(9)-C(10)	108.4(2)
C(14)-N(6)-C(18)	118.6(2)	C(8)-C(9)-C(10)	131.4(2)
C(14)-N(6)-Co(1)	127.70(18)	N(5)-C(10)-N(4)	110.4(2)
C(18)-N(6)-Co(1)	113.74(17)	N(5)-C(10)-C(9)	117.3(2)
N(8)-N(7)-C(19)	108.7(2)	N(4)-C(10)-C(9)	132.3(2)
N(8)-N(7)-Co(1)	129.85(17)	N(4)-C(11)-H(11A)	109.5
C(19)-N(7)-Co(1)	119.43(17)	N(4)-C(11)-H(11B)	109.5
N(7)-N(8)-C(21)	108.6(2)	H(11A)-C(11)-H(11B)	109.5
N(7)-N(8)-Co(2)	128.03(17)	N(4)-C(11)-H(11C)	109.5
C(21)-N(8)-Co(2)	119.73(17)	H(11A)-C(11)-H(11C)	109.5
C(26)-N(9)-C(22)	118.6(2)	H(11B)-C(11)-H(11C)	109.5
C(26)-N(9)-Co(2)	127.56(17)	C(13)-C(12)-N(4)	107.1(2)
C(22)-N(9)-Co(2)	113.81(17)	C(13)-C(12)-H(12)	126.4
C(30)-N(10)-C(27)	106.9(2)	N(4)-C(12)-H(12)	126.4
C(30)-N(10)-Co(2)	113.59(17)	N(5)-C(13)-C(12)	108.7(2)
C(27)-N(10)-Co(2)	139.43(19)	N(5)-C(13)-H(13)	125.7
C(30)-N(11)-C(28)	107.1(2)	C(12)-C(13)-H(13)	125.7
C(30)-N(11)-C(29)	127.7(2)	N(6)-C(14)-C(15)	122.2(2)
C(28)-N(11)-C(29)	125.2(2)	N(6)-C(14)-H(14)	118.9
C(31)-N(12)-C(35)	122.0(2)	C(15)-C(14)-H(14)	118.9
C(31)-N(12)-Co(2)	118.28(17)	C(14)-C(15)-C(16)	119.4(2)
C(35)-N(12)-Co(2)	119.09(17)	C(14)-C(15)-H(15)	120.3
C(36)-N(13)-C(38)	107.1(2)	C(16)-C(15)-H(15)	120.3
C(36)-N(13)-C(37)	127.6(2)	C(15)-C(16)-C(17)	119.1(2)
C(38)-N(13)-C(37)	125.3(2)	C(15)-C(16)-H(16)	120.4
C(36)-N(14)-C(39)	106.9(2)	C(17)-C(16)-H(16)	120.4
C(36)-N(14)-Co(2)	112.66(17)	C(18)-C(17)-C(16)	118.7(2)
C(39)-N(14)-Co(2)	140.42(18)	C(18)-C(17)-H(17)	120.7
C(2)-C(1)-N(1)	108.4(2)	C(16)-C(17)-H(17)	120.7
C(2)-C(1)-H(1)	125.8	N(6)-C(18)-C(17)	122.1(2)
N(1)-C(1)-H(1)	125.8	N(6)-C(18)-C(19)	112.7(2)
C(1)-C(2)-N(2)	107.3(2)	C(17)-C(18)-C(19)	125.2(2)
C(1)-C(2)-H(2)	126.4	N(7)-C(19)-C(20)	109.3(2)
N(2)-C(2)-H(2)	126.4	N(7)-C(19)-C(18)	112.6(2)

C(20)-C(19)-C(18)	138.1(2)	N(13)-C(37)-H(37A)	109.5
C(19)-C(20)-C(21)	103.8(2)	N(13)-C(37)-H(37B)	109.5
C(19)-C(20)-H(20)	128.1	H(37A)-C(37)-H(37B)	109.5
C(21)-C(20)-H(20)	128.1	N(13)-C(37)-H(37C)	109.5
N(8)-C(21)-C(20)	109.5(2)	H(37A)-C(37)-H(37C)	109.5
N(8)-C(21)-C(22)	112.8(2)	H(37B)-C(37)-H(37C)	109.5
C(20)-C(21)-C(22)	137.5(2)	C(39)-C(38)-N(13)	107.2(2)
N(9)-C(22)-C(23)	122.0(2)	C(39)-C(38)-H(38)	126.4
N(9)-C(22)-C(21)	112.6(2)	N(13)-C(38)-H(38)	126.4
C(23)-C(22)-C(21)	125.4(2)	N(14)-C(39)-C(38)	108.6(2)
C(24)-C(23)-C(22)	118.8(2)	N(14)-C(39)-H(39)	125.7
C(24)-C(23)-H(23)	120.6	C(38)-C(39)-H(39)	125.7
C(22)-C(23)-H(23)	120.6	F(4)-P(1)-F(2)	178.43(13)
C(23)-C(24)-C(25)	119.2(2)	F(4)-P(1)-F(5)	90.91(12)
C(23)-C(24)-H(24)	120.4	F(2)-P(1)-F(5)	90.61(13)
C(25)-C(24)-H(24)	120.4	F(4)-P(1)-F(6)	90.45(11)
C(24)-C(25)-C(26)	119.1(2)	F(2)-P(1)-F(6)	89.94(11)
C(24)-C(25)-H(25)	120.4	F(5)-P(1)-F(6)	90.37(11)
C(26)-C(25)-H(25)	120.4	F(4)-P(1)-F(3)	88.68(12)
N(9)-C(26)-C(25)	122.2(2)	F(2)-P(1)-F(3)	89.80(13)
N(9)-C(26)-H(26)	118.9	F(5)-P(1)-F(3)	179.47(12)
C(25)-C(26)-H(26)	118.9	F(6)-P(1)-F(3)	89.97(11)
C(28)-C(27)-N(10)	108.2(2)	F(4)-P(1)-F(1)	89.87(12)
C(28)-C(27)-H(27)	125.9	F(2)-P(1)-F(1)	89.75(12)
N(10)-C(27)-H(27)	125.9	F(5)-P(1)-F(1)	89.15(11)
C(27)-C(28)-N(11)	107.4(2)	F(6)-P(1)-F(1)	179.43(11)
C(27)-C(28)-H(28)	126.3	F(3)-P(1)-F(1)	90.51(11)
N(11)-C(28)-H(28)	126.3	F(10)-P(2)-F(8)	179.48(12)
N(11)-C(29)-H(29A)	109.5	F(10)-P(2)-F(11)	90.22(11)
N(11)-C(29)-H(29B)	109.5	F(8)-P(2)-F(11)	89.93(11)
H(29A)-C(29)-H(29B)	109.5	F(10)-P(2)-F(7)	90.85(12)
N(11)-C(29)-H(29C)	109.5	F(8)-P(2)-F(7)	89.65(11)
H(29A)-C(29)-H(29C)	109.5	F(11)-P(2)-F(7)	90.37(10)
H(29B)-C(29)-H(29C)	109.5	F(10)-P(2)-F(9)	89.76(11)
N(10)-C(30)-N(11)	110.3(2)	F(8)-P(2)-F(9)	90.09(11)
N(10)-C(30)-C(31)	116.6(2)	F(11)-P(2)-F(9)	179.56(10)
N(11)-C(30)-C(31)	132.8(2)	F(7)-P(2)-F(9)	90.07(10)
N(12)-C(31)-C(32)	120.4(2)	F(10)-P(2)-F(12)	89.34(11)
N(12)-C(31)-C(30)	108.7(2)	F(8)-P(2)-F(12)	90.16(10)
C(32)-C(31)-C(30)	130.9(3)	F(11)-P(2)-F(12)	89.65(10)
C(31)-C(32)-C(33)	117.8(2)	F(7)-P(2)-F(12)	179.81(12)
C(31)-C(32)-H(32)	121.1	F(9)-P(2)-F(12)	89.90(9)
C(33)-C(32)-H(32)	121.1	F(13)-P(3)-F(15)	90.44(16)
C(32)-C(33)-C(34)	121.5(2)	F(13)-P(3)-F(14)	89.36(13)
C(32)-C(33)-H(33)	119.3	F(15)-P(3)-F(14)	90.02(13)
C(34)-C(33)-H(33)	119.3	F(13)-P(3)-F(17)	89.48(12)
C(33)-C(34)-C(35)	118.1(2)	F(15)-P(3)-F(17)	179.34(14)
C(33)-C(34)-H(34)	120.9	F(14)-P(3)-F(17)	90.64(12)
C(35)-C(34)-H(34)	120.9	F(13)-P(3)-F(16)	91.75(14)
N(12)-C(35)-C(34)	120.0(2)	F(15)-P(3)-F(16)	90.31(12)
N(12)-C(35)-C(36)	108.7(2)	F(14)-P(3)-F(16)	178.85(14)
C(34)-C(35)-C(36)	131.1(2)	F(17)-P(3)-F(16)	89.03(11)
N(13)-C(36)-N(14)	110.3(2)	F(13)-P(3)-F(18)	179.17(15)
N(13)-C(36)-C(35)	132.1(2)	F(15)-P(3)-F(18)	90.30(17)
N(14)-C(36)-C(35)	117.5(2)	F(14)-P(3)-F(18)	90.26(13)
F(17)-P(3)-F(18)	89.79(13)	F(16)-P(3)-F(18)	88.63(14)

C(41)-C(40)-H(40A)	109.5
C(41)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(41)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(3)-C(41)-C(42)	121.7(3)
O(3)-C(41)-C(40)	121.6(3)
C(42)-C(41)-C(40)	116.7(3)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-H(43D)	109.5
C(44)-C(43)-H(43E)	109.5
H(43D)-C(43)-H(43E)	109.5
C(44)-C(43)-H(43F)	109.5
H(43D)-C(43)-H(43F)	109.5
H(43E)-C(43)-H(43F)	109.5
C(43)-C(44)-C(45)	113.3
C(43)-C(44)-H(44C)	108.9
C(45)-C(44)-H(44C)	108.9
C(43)-C(44)-H(44D)	108.9
C(45)-C(44)-H(44D)	108.9
H(44C)-C(44)-H(44D)	107.7
C(44)-C(45)-C(46)	113.8
C(44)-C(45)-H(45C)	108.8
C(46)-C(45)-H(45C)	108.8
C(44)-C(45)-H(45D)	108.8
C(46)-C(45)-H(45D)	108.8
H(45C)-C(45)-H(45D)	107.7
C(47)-C(46)-C(45)	113.3
C(47)-C(46)-H(46C)	108.9
C(45)-C(46)-H(46C)	108.9
C(47)-C(46)-H(46D)	108.9
C(45)-C(46)-H(46D)	108.9
H(46C)-C(46)-H(46D)	107.7
C(46)-C(47)-H(47D)	109.5
C(46)-C(47)-H(47E)	109.5
H(47D)-C(47)-H(47E)	109.5
C(46)-C(47)-H(47F)	109.5
H(47D)-C(47)-H(47F)	109.5
H(47E)-C(47)-H(47F)	109.5
C(44A)-C(43A)-H(43A)	109.5
C(44A)-C(43A)-H(43B)	109.5
H(43A)-C(43A)-H(43B)	109.5
C(44A)-C(43A)-H(43C)	109.5
H(43A)-C(43A)-H(43C)	109.5
H(43B)-C(43A)-H(43C)	109.5
C(43A)-C(44A)-C(45A)	113.3
C(43A)-C(44A)-H(44A)	108.9
C(45A)-C(44A)-H(44A)	108.9
C(43A)-C(44A)-H(44B)	108.9
C(45A)-C(44A)-H(44B)	108.9
H(44A)-C(44A)-H(44B)	107.7
C(46A)-C(45A)-C(44A)	113.8
C(46A)-C(45A)-H(45A)	108.8
C(44A)-C(45A)-H(45A)	108.8
C(46A)-C(45A)-H(45B)	108.8
C(44A)-C(45A)-H(45B)	108.8
H(45A)-C(45A)-H(45B)	107.7
C(47A)-C(46A)-C(45A)	113.3
C(47A)-C(46A)-H(46A)	108.9
C(45A)-C(46A)-H(46A)	108.9
C(47A)-C(46A)-H(46B)	108.9
C(45A)-C(46A)-H(46B)	108.9
H(46A)-C(46A)-H(46B)	107.7
C(46A)-C(47A)-H(47A)	109.5
C(46A)-C(47A)-H(47B)	109.5
H(47A)-C(47A)-H(47B)	109.5
C(46A)-C(47A)-H(47C)	109.5
H(47A)-C(47A)-H(47C)	109.5
H(47B)-C(47A)-H(47C)	109.5

Symmetry transformations used to generate equivalent atoms.

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	11(1)	14(1)	11(1)	0(1)	2(1)	5(1)
Co(2)	11(1)	12(1)	9(1)	0(1)	2(1)	2(1)
O(1)	17(1)	14(1)	14(1)	1(1)	0(1)	5(1)
O(2)	16(1)	17(1)	14(1)	4(1)	5(1)	7(1)
N(1)	14(1)	20(1)	13(1)	1(1)	2(1)	6(1)
N(2)	16(1)	21(1)	18(1)	4(1)	2(1)	2(1)
N(3)	12(1)	17(1)	10(1)	-1(1)	-1(1)	5(1)
N(4)	13(1)	24(1)	16(1)	2(1)	4(1)	6(1)
N(5)	14(1)	17(1)	13(1)	1(1)	1(1)	5(1)
N(6)	13(1)	17(1)	11(1)	3(1)	4(1)	4(1)
N(7)	13(1)	17(1)	11(1)	0(1)	1(1)	5(1)
N(8)	10(1)	15(1)	14(1)	2(1)	2(1)	5(1)
N(9)	12(1)	13(1)	14(1)	1(1)	2(1)	2(1)
N(10)	13(1)	15(1)	15(1)	0(1)	2(1)	4(1)
N(11)	14(1)	16(1)	26(1)	3(1)	8(1)	1(1)
N(12)	11(1)	13(1)	13(1)	0(1)	2(1)	4(1)
N(13)	11(1)	12(1)	19(1)	-2(1)	3(1)	3(1)
N(14)	13(1)	15(1)	13(1)	1(1)	3(1)	4(1)
C(1)	14(1)	27(2)	18(1)	3(1)	3(1)	7(1)
C(2)	13(1)	31(2)	21(1)	5(1)	5(1)	4(1)
C(3)	26(2)	19(2)	26(2)	6(1)	2(1)	-1(1)
C(4)	16(1)	17(1)	14(1)	2(1)	-1(1)	3(1)
C(5)	16(1)	17(1)	12(1)	1(1)	-1(1)	3(1)
C(6)	24(2)	18(1)	17(1)	2(1)	0(1)	8(1)
C(7)	26(2)	19(1)	18(1)	0(1)	0(1)	12(1)
C(8)	19(1)	26(2)	16(1)	0(1)	2(1)	12(1)
C(9)	14(1)	21(1)	10(1)	-1(1)	-1(1)	7(1)
C(10)	13(1)	24(1)	11(1)	0(1)	2(1)	7(1)
C(11)	16(1)	31(2)	23(1)	3(1)	8(1)	11(1)
C(12)	18(1)	23(2)	23(1)	7(1)	5(1)	4(1)
C(13)	17(1)	19(1)	23(1)	5(1)	3(1)	6(1)
C(14)	14(1)	18(1)	18(1)	3(1)	4(1)	5(1)
C(15)	14(1)	25(2)	17(1)	7(1)	1(1)	7(1)
C(16)	18(1)	27(2)	11(1)	2(1)	1(1)	4(1)
C(17)	18(1)	20(1)	13(1)	-1(1)	3(1)	6(1)
C(18)	11(1)	17(1)	14(1)	2(1)	3(1)	4(1)
C(19)	12(1)	16(1)	11(1)	0(1)	1(1)	3(1)
C(20)	16(1)	14(1)	14(1)	0(1)	4(1)	4(1)
C(21)	12(1)	13(1)	15(1)	2(1)	5(1)	3(1)
C(22)	11(1)	14(1)	15(1)	2(1)	2(1)	2(1)
C(23)	17(1)	16(1)	17(1)	0(1)	4(1)	5(1)
C(24)	17(1)	17(1)	24(1)	4(1)	6(1)	8(1)
C(25)	15(1)	17(1)	19(1)	6(1)	2(1)	4(1)
C(26)	15(1)	14(1)	15(1)	3(1)	1(1)	1(1)
C(27)	15(1)	16(1)	20(1)	-3(1)	-1(1)	3(1)
C(28)	16(1)	16(1)	28(2)	-3(1)	2(1)	2(1)
C(29)	26(2)	23(2)	32(2)	5(1)	16(1)	0(1)
C(30)	13(1)	14(1)	19(1)	3(1)	6(1)	2(1)
C(31)	15(1)	13(1)	19(1)	3(1)	5(1)	6(1)
C(32)	22(1)	20(1)	19(1)	4(1)	10(1)	7(1)
C(33)	25(2)	20(1)	12(1)	2(1)	6(1)	11(1)

C(34)	18(1)	16(1)	13(1)	-3(1)	-1(1)	8(1)
C(35)	12(1)	12(1)	17(1)	0(1)	2(1)	6(1)
C(36)	13(1)	14(1)	15(1)	-2(1)	2(1)	6(1)
C(37)	15(1)	22(1)	19(1)	-6(1)	-1(1)	1(1)
C(38)	15(1)	14(1)	23(1)	4(1)	9(1)	4(1)
C(39)	17(1)	16(1)	18(1)	4(1)	7(1)	6(1)
P(1)	18(1)	27(1)	18(1)	4(1)	4(1)	6(1)
F(1)	44(1)	56(1)	31(1)	12(1)	20(1)	25(1)
F(2)	44(1)	50(1)	31(1)	-5(1)	0(1)	-11(1)
F(3)	54(1)	44(1)	47(1)	20(1)	14(1)	28(1)
F(4)	27(1)	42(1)	36(1)	11(1)	-2(1)	-6(1)
F(5)	35(1)	56(1)	36(1)	18(1)	10(1)	28(1)
F(6)	30(1)	43(1)	23(1)	3(1)	11(1)	7(1)
P(2)	16(1)	21(1)	16(1)	3(1)	3(1)	6(1)
F(7)	22(1)	65(1)	29(1)	18(1)	12(1)	21(1)
F(8)	40(1)	23(1)	42(1)	-5(1)	10(1)	10(1)
F(9)	32(1)	44(1)	18(1)	11(1)	7(1)	20(1)
F(10)	36(1)	22(1)	42(1)	4(1)	-6(1)	-4(1)
F(11)	33(1)	46(1)	18(1)	7(1)	1(1)	18(1)
F(12)	18(1)	32(1)	24(1)	-7(1)	2(1)	9(1)
P(3)	24(1)	27(1)	18(1)	4(1)	-2(1)	-2(1)
F(13)	41(1)	55(1)	78(2)	21(1)	16(1)	28(1)
F(14)	38(1)	44(1)	42(1)	-11(1)	4(1)	-13(1)
F(15)	124(2)	39(1)	35(1)	20(1)	-22(1)	-11(1)
F(16)	45(1)	39(1)	43(1)	13(1)	-21(1)	-12(1)
F(17)	50(1)	42(1)	20(1)	3(1)	-3(1)	22(1)
F(18)	70(2)	52(1)	55(1)	-12(1)	38(1)	2(1)
O(3)	32(1)	23(1)	26(1)	0(1)	8(1)	3(1)
C(40)	46(2)	28(2)	29(2)	6(1)	7(2)	4(2)
C(41)	33(2)	19(2)	24(2)	-3(1)	5(1)	9(1)
C(42)	31(2)	36(2)	37(2)	5(1)	1(1)	7(2)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6**.

	x	y	z	U(eq)
H(1)	-238	344	3874	23
H(2)	-1207	-1510	4088	27
H(3A)	556	-3127	4048	38
H(3B)	-79	-3351	3168	38
H(3C)	-808	-3278	3873	38
H(6)	2085	-2892	3183	24
H(7)	3828	-2739	2674	25
H(8)	4948	-1114	2357	23
H(11A)	6464	563	2377	33
H(11B)	6763	1403	1773	33
H(11C)	5805	262	1501	33
H(12)	5734	2808	1881	26
H(13)	3998	2991	2443	23
H(14)	4265	638	4366	20
H(15)	5054	1435	5628	22
H(16)	4327	2705	6235	23
H(17)	2875	3214	5521	21
H(20)	1043	3507	4490	18
H(23)	-808	4112	3726	20
H(24)	-2079	4672	2886	22
H(25)	-2340	4093	1543	20
H(26)	-1342	2974	1072	18
H(27)	2636	4206	2763	22
H(28)	3978	5300	1965	25
H(29A)	3853	4039	111	42
H(29B)	4237	5236	542	42
H(29C)	3023	4756	-24	42
H(32)	1844	2990	-649	23
H(33)	272	1711	-1443	22
H(34)	-1230	584	-897	19
H(37A)	-3590	-1348	-113	31
H(37B)	-2472	-964	-550	31
H(37C)	-3224	-188	-375	31
H(38)	-3037	-1271	1346	21
H(39)	-1493	-89	2379	19
H(40A)	2094	5605	4243	54
H(40B)	3453	5768	4241	54
H(40C)	3040	6714	4622	54
H(42A)	4336	6659	5972	53
H(42B)	4679	5724	5508	53
H(42C)	4055	5519	6267	53
H(43D)	-851	4182	-1950	166
H(43E)	-1199	3255	-1417	166
H(43F)	144	3896	-1426	166
H(44C)	-1500	4589	-661	133
H(44D)	-474	5478	-946	133
H(45C)	932	4963	-159	133
H(45D)	-93	4075	126	133
H(46C)	304	6318	478	133
H(46D)	-722	5429	763	133

H(47D)	1598	5466	1232	166
H(47E)	498	5085	1686	166
H(47F)	1134	6327	1687	166
H(43A)	-553	4213	-1838	166
H(43B)	-1024	5067	-1381	166
H(43C)	-1654	3822	-1386	166
H(44A)	721	4563	-763	133
H(44B)	-305	3675	-478	133
H(45A)	93	5918	-126	133
H(45B)	-932	5030	159	133
H(46A)	474	4515	946	133
H(46B)	1499	5404	661	133
H(47A)	415	6617	1245	166
H(47B)	1416	6336	1768	166
H(47C)	74	5691	1779	166

Table S12. Torsion angles [°] for **6**.

N(7)-Co(1)-O(1)-O(2)	54.48(15)	N(5)-Co(1)-N(7)-N(8)	97.4(2)
N(3)-Co(1)-O(1)-O(2)	-130.53(14)	N(6)-Co(1)-N(7)-N(8)	-173.1(2)
N(1)-Co(1)-O(1)-O(2)	147.53(15)	O(1)-Co(1)-N(7)-C(19)	167.5(2)
N(5)-Co(1)-O(1)-O(2)	-48.96(15)	N(3)-Co(1)-N(7)-C(19)	61.8(11)
N(6)-Co(1)-O(1)-O(2)	62.3(6)	N(1)-Co(1)-N(7)-C(19)	79.7(2)
Co(1)-O(1)-O(2)-Co(2)	-90.08(14)	N(5)-Co(1)-N(7)-C(19)	-100.7(2)
N(8)-Co(2)-O(2)-O(1)	48.82(15)	N(6)-Co(1)-N(7)-C(19)	-11.16(19)
N(12)-Co(2)-O(2)-O(1)	-137.33(15)	C(19)-N(7)-N(8)-C(21)	2.3(3)
N(10)-Co(2)-O(2)-O(1)	141.24(15)	Co(1)-N(7)-N(8)-C(21)	165.78(18)
N(14)-Co(2)-O(2)-O(1)	-55.76(15)	C(19)-N(7)-N(8)-Co(2)	160.34(18)
N(9)-Co(2)-O(2)-O(1)	60.4(6)	Co(1)-N(7)-N(8)-Co(2)	-36.2(3)
N(7)-Co(1)-N(1)-C(4)	178.02(18)	O(2)-Co(2)-N(8)-N(7)	11.1(2)
O(1)-Co(1)-N(1)-C(4)	87.66(18)	N(12)-Co(2)-N(8)-N(7)	-64.9(9)
N(3)-Co(1)-N(1)-C(4)	-3.60(18)	N(10)-Co(2)-N(8)-N(7)	-76.9(2)
N(5)-Co(1)-N(1)-C(4)	-0.6(4)	N(14)-Co(2)-N(8)-N(7)	103.9(2)
N(6)-Co(1)-N(1)-C(4)	-101.75(18)	N(9)-Co(2)-N(8)-N(7)	-167.1(2)
N(7)-Co(1)-N(1)-C(1)	3.4(3)	O(2)-Co(2)-N(8)-C(21)	166.96(19)
O(1)-Co(1)-N(1)-C(1)	-87.0(3)	N(12)-Co(2)-N(8)-C(21)	91.0(8)
N(3)-Co(1)-N(1)-C(1)	-178.3(3)	N(10)-Co(2)-N(8)-C(21)	79.0(2)
N(5)-Co(1)-N(1)-C(1)	-175.2(3)	N(14)-Co(2)-N(8)-C(21)	-100.2(2)
N(6)-Co(1)-N(1)-C(1)	83.6(3)	N(9)-Co(2)-N(8)-C(21)	-11.19(19)
N(7)-Co(1)-N(3)-C(9)	-162.3(9)	N(8)-Co(2)-N(9)-C(26)	-174.5(2)
O(1)-Co(1)-N(3)-C(9)	91.92(19)	O(2)-Co(2)-N(9)-C(26)	173.7(4)
N(1)-Co(1)-N(3)-C(9)	179.54(19)	N(12)-Co(2)-N(9)-C(26)	11.8(2)
N(5)-Co(1)-N(3)-C(9)	0.41(18)	N(10)-Co(2)-N(9)-C(26)	93.1(2)
N(6)-Co(1)-N(3)-C(9)	-90.19(19)	N(14)-Co(2)-N(9)-C(26)	-70.0(2)
N(7)-Co(1)-N(3)-C(5)	20.9(11)	N(8)-Co(2)-N(9)-C(22)	6.44(17)
O(1)-Co(1)-N(3)-C(5)	-84.82(18)	O(2)-Co(2)-N(9)-C(22)	-5.4(6)
N(1)-Co(1)-N(3)-C(5)	2.79(18)	N(12)-Co(2)-N(9)-C(22)	-167.24(17)
N(5)-Co(1)-N(3)-C(5)	-176.34(19)	N(10)-Co(2)-N(9)-C(22)	-85.95(18)
N(6)-Co(1)-N(3)-C(5)	93.06(19)	N(14)-Co(2)-N(9)-C(22)	110.88(18)
N(7)-Co(1)-N(5)-C(10)	177.84(17)	N(8)-Co(2)-N(10)-C(30)	168.55(18)
O(1)-Co(1)-N(5)-C(10)	-91.27(18)	O(2)-Co(2)-N(10)-C(30)	77.15(18)
N(3)-Co(1)-N(5)-C(10)	-0.57(17)	N(12)-Co(2)-N(10)-C(30)	-10.12(18)
N(1)-Co(1)-N(5)-C(10)	-3.6(4)	N(14)-Co(2)-N(10)-C(30)	-14.2(4)
N(6)-Co(1)-N(5)-C(10)	97.52(18)	N(9)-Co(2)-N(10)-C(30)	-111.81(18)
N(7)-Co(1)-N(5)-C(13)	-6.3(3)	N(8)-Co(2)-N(10)-C(27)	-8.3(3)
O(1)-Co(1)-N(5)-C(13)	84.6(3)	O(2)-Co(2)-N(10)-C(27)	-99.7(3)
N(3)-Co(1)-N(5)-C(13)	175.3(3)	N(12)-Co(2)-N(10)-C(27)	173.0(3)
N(1)-Co(1)-N(5)-C(13)	172.2(3)	N(14)-Co(2)-N(10)-C(27)	169.0(3)
N(6)-Co(1)-N(5)-C(13)	-86.7(3)	N(9)-Co(2)-N(10)-C(27)	71.3(3)
N(7)-Co(1)-N(6)-C(14)	-172.3(2)	N(8)-Co(2)-N(12)-C(31)	-0.9(9)
O(1)-Co(1)-N(6)-C(14)	179.7(4)	O(2)-Co(2)-N(12)-C(31)	-77.11(19)
N(3)-Co(1)-N(6)-C(14)	12.7(2)	N(10)-Co(2)-N(12)-C(31)	11.26(18)
N(1)-Co(1)-N(6)-C(14)	94.8(2)	N(14)-Co(2)-N(12)-C(31)	-169.9(2)
N(5)-Co(1)-N(6)-C(14)	-69.0(2)	N(9)-Co(2)-N(12)-C(31)	100.07(19)
N(7)-Co(1)-N(6)-C(18)	7.58(18)	N(8)-Co(2)-N(12)-C(35)	170.4(7)
O(1)-Co(1)-N(6)-C(18)	-0.4(6)	O(2)-Co(2)-N(12)-C(35)	94.16(18)
N(3)-Co(1)-N(6)-C(18)	-167.39(18)	N(10)-Co(2)-N(12)-C(35)	-177.47(19)
N(1)-Co(1)-N(6)-C(18)	-85.29(18)	N(14)-Co(2)-N(12)-C(35)	1.34(18)
N(5)-Co(1)-N(6)-C(18)	110.89(18)	N(9)-Co(2)-N(12)-C(35)	-88.66(19)
O(1)-Co(1)-N(7)-N(8)	5.6(2)	N(8)-Co(2)-N(14)-C(36)	176.84(17)
N(3)-Co(1)-N(7)-N(8)	-100.2(10)	O(2)-Co(2)-N(14)-C(36)	-91.02(17)
N(1)-Co(1)-N(7)-N(8)	-82.2(2)	N(12)-Co(2)-N(14)-C(36)	-4.41(17)

N(10)-Co(2)-N(14)-C(36)	-0.4(4)	Co(1)-N(6)-C(14)-C(15)	-178.5(2)
N(9)-Co(2)-N(14)-C(36)	97.12(17)	N(6)-C(14)-C(15)-C(16)	0.4(4)
N(8)-Co(2)-N(14)-C(39)	-1.0(3)	C(14)-C(15)-C(16)-C(17)	-1.9(4)
O(2)-Co(2)-N(14)-C(39)	91.1(3)	C(15)-C(16)-C(17)-C(18)	1.5(4)
N(12)-Co(2)-N(14)-C(39)	177.7(3)	C(14)-N(6)-C(18)-C(17)	-2.0(4)
N(10)-Co(2)-N(14)-C(39)	-178.3(3)	Co(1)-N(6)-C(18)-C(17)	178.1(2)
N(9)-Co(2)-N(14)-C(39)	-80.8(3)	C(14)-N(6)-C(18)-C(19)	176.7(2)
C(4)-N(1)-C(1)-C(2)	-0.4(3)	Co(1)-N(6)-C(18)-C(19)	-3.3(3)
Co(1)-N(1)-C(1)-C(2)	174.5(2)	C(16)-C(17)-C(18)-N(6)	0.4(4)
N(1)-C(1)-C(2)-N(2)	-0.2(3)	C(16)-C(17)-C(18)-C(19)	-178.0(2)
C(4)-N(2)-C(2)-C(1)	0.8(3)	N(8)-N(7)-C(19)-C(20)	-1.6(3)
C(3)-N(2)-C(2)-C(1)	-178.4(2)	Co(1)-N(7)-C(19)-C(20)	-167.10(17)
C(1)-N(1)-C(4)-N(2)	0.9(3)	N(8)-N(7)-C(19)-C(18)	177.8(2)
Co(1)-N(1)-C(4)-N(2)	-175.40(16)	Co(1)-N(7)-C(19)-C(18)	12.4(3)
C(1)-N(1)-C(4)-C(5)	-179.7(2)	N(6)-C(18)-C(19)-N(7)	-5.1(3)
Co(1)-N(1)-C(4)-C(5)	3.9(3)	C(17)-C(18)-C(19)-N(7)	173.4(2)
C(2)-N(2)-C(4)-N(1)	-1.1(3)	N(6)-C(18)-C(19)-C(20)	174.1(3)
C(3)-N(2)-C(4)-N(1)	178.0(2)	C(17)-C(18)-C(19)-C(20)	-7.3(5)
C(2)-N(2)-C(4)-C(5)	179.7(3)	N(7)-C(19)-C(20)-C(21)	0.3(3)
C(3)-N(2)-C(4)-C(5)	-1.2(5)	C(18)-C(19)-C(20)-C(21)	-179.0(3)
C(9)-N(3)-C(5)-C(6)	1.2(4)	N(7)-N(8)-C(21)-C(20)	-2.2(3)
Co(1)-N(3)-C(5)-C(6)	177.83(18)	Co(2)-N(8)-C(21)-C(20)	-162.31(17)
C(9)-N(3)-C(5)-C(4)	-178.0(2)	N(7)-N(8)-C(21)-C(22)	173.7(2)
Co(1)-N(3)-C(5)-C(4)	-1.4(3)	Co(2)-N(8)-C(21)-C(22)	13.5(3)
N(1)-C(4)-C(5)-N(3)	-1.7(3)	C(19)-C(20)-C(21)-N(8)	1.1(3)
N(2)-C(4)-C(5)-N(3)	177.4(3)	C(19)-C(20)-C(21)-C(22)	-173.2(3)
N(1)-C(4)-C(5)-C(6)	179.2(3)	C(26)-N(9)-C(22)-C(23)	-0.4(4)
N(2)-C(4)-C(5)-C(6)	-1.6(5)	Co(2)-N(9)-C(22)-C(23)	178.8(2)
N(3)-C(5)-C(6)-C(7)	-0.4(4)	C(26)-N(9)-C(22)-C(21)	179.5(2)
C(4)-C(5)-C(6)-C(7)	178.6(3)	Co(2)-N(9)-C(22)-C(21)	-1.3(3)
C(5)-C(6)-C(7)-C(8)	-0.1(4)	N(8)-C(21)-C(22)-N(9)	-7.1(3)
C(6)-C(7)-C(8)-C(9)	-0.2(4)	C(20)-C(21)-C(22)-N(9)	167.1(3)
C(5)-N(3)-C(9)-C(8)	-1.5(4)	N(8)-C(21)-C(22)-C(23)	172.8(2)
Co(1)-N(3)-C(9)-C(8)	-178.09(18)	C(20)-C(21)-C(22)-C(23)	-13.0(5)
C(5)-N(3)-C(9)-C(10)	176.5(2)	N(9)-C(22)-C(23)-C(24)	-0.7(4)
Co(1)-N(3)-C(9)-C(10)	-0.2(3)	C(21)-C(22)-C(23)-C(24)	179.3(2)
C(7)-C(8)-C(9)-N(3)	1.0(4)	C(22)-C(23)-C(24)-C(25)	0.9(4)
C(7)-C(8)-C(9)-C(10)	-176.4(3)	C(23)-C(24)-C(25)-C(26)	0.0(4)
C(13)-N(5)-C(10)-N(4)	0.5(3)	C(22)-N(9)-C(26)-C(25)	1.4(4)
Co(1)-N(5)-C(10)-N(4)	177.72(16)	Co(2)-N(9)-C(26)-C(25)	-177.62(19)
C(13)-N(5)-C(10)-C(9)	-176.5(2)	C(24)-C(25)-C(26)-N(9)	-1.2(4)
Co(1)-N(5)-C(10)-C(9)	0.7(3)	C(30)-N(10)-C(27)-C(28)	-0.9(3)
C(12)-N(4)-C(10)-N(5)	-0.8(3)	Co(2)-N(10)-C(27)-C(28)	176.1(2)
C(11)-N(4)-C(10)-N(5)	177.6(2)	N(10)-C(27)-C(28)-N(11)	0.1(3)
C(12)-N(4)-C(10)-C(9)	175.7(3)	C(30)-N(11)-C(28)-C(27)	0.7(3)
C(11)-N(4)-C(10)-C(9)	-5.9(4)	C(29)-N(11)-C(28)-C(27)	-177.8(3)
N(3)-C(9)-C(10)-N(5)	-0.3(3)	C(27)-N(10)-C(30)-N(11)	1.4(3)
C(8)-C(9)-C(10)-N(5)	177.3(3)	Co(2)-N(10)-C(30)-N(11)	-176.50(17)
N(3)-C(9)-C(10)-N(4)	-176.6(3)	C(27)-N(10)-C(30)-C(31)	-174.1(2)
C(8)-C(9)-C(10)-N(4)	1.0(5)	Co(2)-N(10)-C(30)-C(31)	8.0(3)
C(10)-N(4)-C(12)-C(13)	0.7(3)	C(28)-N(11)-C(30)-N(10)	-1.3(3)
C(11)-N(4)-C(12)-C(13)	-177.8(2)	C(29)-N(11)-C(30)-N(10)	177.1(3)
C(10)-N(5)-C(13)-C(12)	-0.1(3)	C(28)-N(11)-C(30)-C(31)	173.2(3)
Co(1)-N(5)-C(13)-C(12)	-176.1(2)	C(29)-N(11)-C(30)-C(31)	-8.4(5)
N(4)-C(12)-C(13)-N(5)	-0.4(3)	C(35)-N(12)-C(31)-C(32)	0.9(4)
C(18)-N(6)-C(14)-C(15)	1.6(4)	Co(2)-N(12)-C(31)-C(32)	171.93(19)

C(35)-N(12)-C(31)-C(30)	179.5(2)
Co(2)-N(12)-C(31)-C(30)	-9.5(3)
N(10)-C(30)-C(31)-N(12)	0.7(3)
N(11)-C(30)-C(31)-N(12)	-173.6(3)
N(10)-C(30)-C(31)-C(32)	179.0(3)
N(11)-C(30)-C(31)-C(32)	4.8(5)
N(12)-C(31)-C(32)-C(33)	1.1(4)
C(30)-C(31)-C(32)-C(33)	-177.1(3)
C(31)-C(32)-C(33)-C(34)	-1.1(4)
C(32)-C(33)-C(34)-C(35)	-0.8(4)
C(31)-N(12)-C(35)-C(34)	-2.9(4)
Co(2)-N(12)-C(35)-C(34)	-173.84(18)
C(31)-N(12)-C(35)-C(36)	172.7(2)
Co(2)-N(12)-C(35)-C(36)	1.8(3)
C(33)-C(34)-C(35)-N(12)	2.8(4)
C(33)-C(34)-C(35)-C(36)	-171.7(3)
C(38)-N(13)-C(36)-N(14)	-1.1(3)
C(37)-N(13)-C(36)-N(14)	175.7(2)
C(38)-N(13)-C(36)-C(35)	173.8(3)
C(37)-N(13)-C(36)-C(35)	-9.4(4)
C(39)-N(14)-C(36)-N(13)	1.2(3)
Co(2)-N(14)-C(36)-N(13)	-177.39(16)
C(39)-N(14)-C(36)-C(35)	-174.6(2)
Co(2)-N(14)-C(36)-C(35)	6.9(3)
N(12)-C(35)-C(36)-N(13)	179.7(2)
C(34)-C(35)-C(36)-N(13)	-5.3(5)
N(12)-C(35)-C(36)-N(14)	-5.7(3)
C(34)-C(35)-C(36)-N(14)	169.3(2)
C(36)-N(13)-C(38)-C(39)	0.5(3)
C(37)-N(13)-C(38)-C(39)	-176.3(2)
C(36)-N(14)-C(39)-C(38)	-0.8(3)
Co(2)-N(14)-C(39)-C(38)	177.1(2)
N(13)-C(38)-C(39)-N(14)	0.2(3)
C(43)-C(44)-C(45)-C(46)	-180.0
C(44)-C(45)-C(46)-C(47)	180.0
C(43A)-C(44A)-C(45A)-C(46A)	-180.0
C(44A)-C(45A)-C(46A)-C(47A)	180.00(5)

Symmetry transformations used to generate equivalent atoms: