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Supporting Information

Metal Complexes of Dipyrromethenes Linked by Rigid Spacer Arms

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Contents

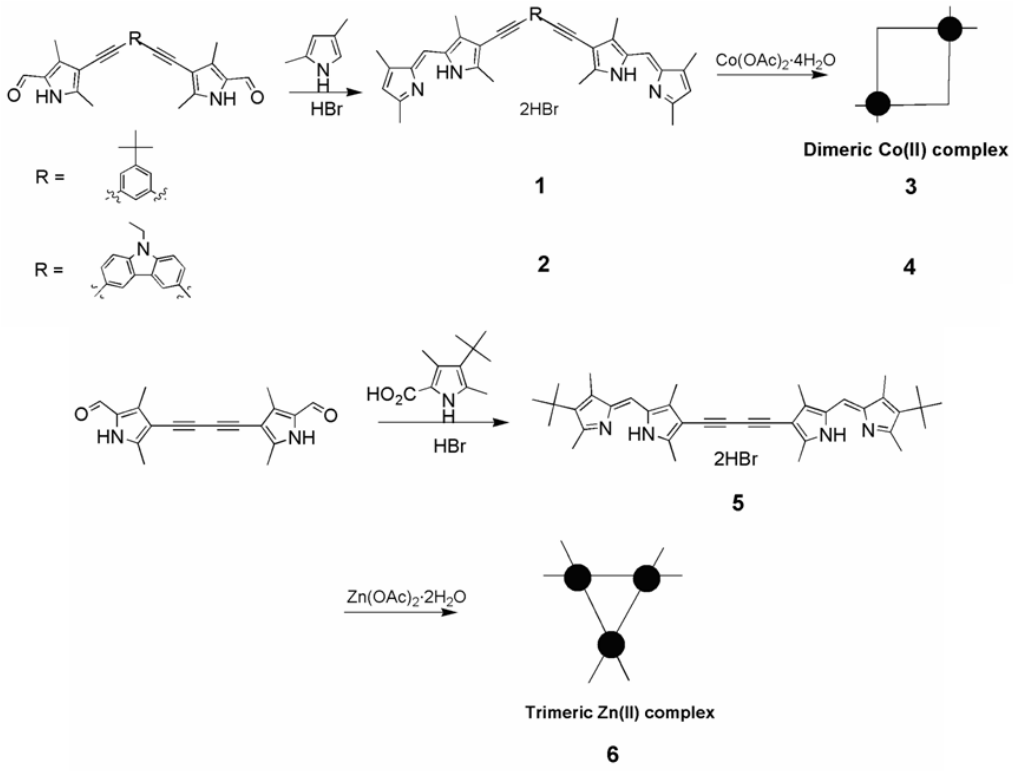
1. Experimental Procedure

General data

^{1}H and ^{13}C NMR spectra were recorded with a Bruker Advance 300 NMR spectrometer in CD_2Cl_2 or d_6-DMSO. Mass spectra were determined on a time-of-flight (TOF) mass spectrometer (Waters/Micromass LCT) equipped with electrospray (ESI). Bruke Biflex IV TOF spectrometer equipped with MALDI ion source was used for the molecular weight determination of trimeri zinc(II) complex. Carbon, nitrogen, and hydrogen ratios in the samples were determined on a Carlo Erba Elemental Analyzer EA 1108. Optical spectra were recorded with a Cary 50 UV-vis spectrophotometer using a 1 cm cell. The crystals were grown by slow vaporization of CH_2Cl_2 or $CHCl_3$ solutions. All chemicals were purchased from commercial suppliers and used without further purification.

Synthetic method and spectral data

Target compounds **3**, **4** and **6** were synthesized through the following routes.



General synthetic method for dipyrromethene ligands (1) and (2).

33% HBr in acetic acid (1.5 mL) was added to a solution of bispyrrole-2-aldehyde (0.38 mmol) and 2,4-dimethylpyrrole (0.88 mmol) in THF/CH_2Cl_2/MeOH (20/80/20 mL) and the reaction mixture was stirred for overnight. After the solvent was removed by rotary evaporation, the residue was dissolved in a small amount of $CHCl_3$/MeOH, and then diethyl ether was added to precipitate the target products. After storage in the fridge overnight and filtration, the orange solid **1** (89.5%) and red solid **2** (94.5%) were respectively obtained.
Spectral data for **1**. ^{1}H NMR at r.t. (d_6-DMSO, 300 MHz) δ = 12.49 (bs, 4H, NH), 7.61 (s, 3H, Ary-H), 7.58 (s, 2H, *meso*-H), 6.55 (s, 2H, β-H), 2.64 (s, 6H, Me), 2.57 (s, 6H, Me), 2.52 (s, 6H, Me), 2.44 (s, 6H, Me), 1.34 (s, 9H, *t*-Bu); HR ESIMS calcd. 579.3488, found 579.3491 [$(M+H)^+$]; UV-vis λ_{max} ($CHCl_3$, logε) /nm 396.0 (4.26), 506.0 (5.13).
Spectral data for **2**. ^{1}H NMR at r.t. (d_6-DMSO, 300 MHz) δ = 12.51 (bs, 2H, NH), 12.41 (bs, 2H, NH), 8.54 (s, 2H, Ary-H), 7.72 (dd, J = 8.3, ^{dd}J = 14.6, 4H, Ary-H), 7.58 (s, 2H, *meso*-H), 6.54 (s, 2H, β-H), 4.51 (m, 2H, Et), 2.68 (s, 6H, Me), 2.57 (s, 6H, Me), 2.56 (s, 6H, Me), 2.45 (s, 6H, Me), 1.35 (t, J = 7.3, 3H, Et); HR ESIMS calcd.640.3440, found 640.3450 [$(M+H)^+$]; UV-vis λ_{max} ($CHCl_3$, logε) /nm 490.0 (4.89).

General synthetic method for dimeric Co(II) complexes (3) and (4).

To a solution of dipyrromethene ligand (0.1 mmol) in $CHCl_3$/MeOH (20 mL/10 mL) was added a solution of $Co(OAc)_2 \cdot 4H_2O$ (0.15 mmol) in MeOH (1 mL). The reaction mixture was stirred for 1 h before a solution of NaOAc (1 mmol) in MeOH (1 mL) was added. After stirring overnight, the solvent was removed by rotary evaporation. A crude mixture of the metal complexes was obtained after filtration through a short column using silica gel and CH_2Cl_2. The target complexes

were separated by gel permeation chromatography using toluene as eluent to give green metallic solids **3** (11 mg, 17.3%) and **4** (15 mg, 21.5%).
Spectral data for **3**. MALDI-TOF calcd. 1270.5, found 1270.4 [$(M)^+$]; Elemental analysis (%) Calcd. 8.81 (N), 75.57 (C), 6.34 (H) found 8.69 (N), 75.58 (C), 6.62 (H); UV-vis λ_{max} ($CHCl_3$, logε) /nm 380.0 (4.51), 516.0 (5.35).
Spectral data for **4**. MALDI-TOF calcd. 1392.5, found 1392.3 [$(M)^+$]; UV-vis λ_{max} ($CHCl_3$, logε) /nm 380.1 (4.63), 515.0 (5.38).

1,4-bis(5-((Z)-(4-tert-butyl-3,5-dimethyl-2H-pyrrol-2-ylidene)methyl)-2,4-dimethyl-1H-pyrrol-3-yl)buta-1,3-diyne dihydrobromide (5).

4-tert-butyl-3,5-dimethyl-1H-pyrrole-2-carboxylic acid (332mg, 1.7 mmol) was added to a solution of 1,4-Bis(2,4-dimethyl-5-formyl-3-pyrryl)butadiyne (200 mg, 0.68 mmol) in THF/MeOH (70 mL/30 mL) at 75°C. After adding 33% HBr in acetic acid (2 mL), the reaction mixture was stirred for 4 h at 75°C. The solvent was removed by rotary evaporation, and the residue was dissolved in a small amount of CH_2Cl_2/MeOH. Ethyl ether was added to the resulting solution to precipitate the target product. After storage in the fridge overnight and filtration, the red solid **5** (370 mg, 76.0%) was isolated
Spectral data for ***5***.^{1}H NMR at r.t. (CD_2Cl_2, 300 MHz) δ = 13.49 (bs, 2H, NH), 13.18 (bs, 2H, NH), 7.18 (s, 2H, *meso*-H), 2.91 (s, 6H, Me), 2.73 (s, 6H, Me), 2.48 (s, 6H, Me), 2.44 (s, 6H, Me), 1.41 (s, 9H, *t*-Bu); ^{13}C NMR (CD_2Cl_2, 75.5 MHz) δ = 159.75, 156.33, 146.50, 144.27, 137.98, 128.60, 125.39, 119.99, 110.74, 80.30, 74.80, 33.84, 31.51, 18.04, 13.72, 13.63, 11.84; ESIMS 559.5 m/z ($[M+H]^+$); Elemental analysis (%) calcd. 7.77 (N), 63.34 (C), 6.71 (H) found 7.90 (N), 62.96 (C), 6.83 (H); UV-vis λ_{max} (CH_2Cl_2)/nm 528.0.

Trimeric Zn(II) complex (6).

To a solution of **5** (72 mg, 0.1 mmol) in $CHCl_3$/MeOH (20 mL/10 mL) was added a solution of $Zn(OAc)_2 \cdot 2H_2O$ (33 mg, 0.15 mmol) in MeOH (1 mL). The reaction mixture was stirred for 1 h before adding a solution of NaOAc (82 mg, 1 mmol) in MeOH (1 mL). After stirring overnight, the solvent was removed by rotary evaporation. A crude mixture of the metal complex was obtained after filtration through a short column using silica gel and CH_2Cl_2. The crude compound was then purified using gel permeation chromatography using toluene as eluent. The target metal complex **6** was obtained as a green metallic solid (12 mg, 20%).
Spectral data for ***6***. ^{1}H NMR at r.t. (CD_2Cl_2, 300 MHz) δ = 7.07 (s, 6H, *meso*-H), 2.39 (m, 18H, Me), 2.36 (m, 18H, Me), 2.35 (s, 18H, Me), 1.93 (m, 18H, Me), 1.34 (s, 27H, *t*-Bu), 1.33 (s, 27H, *t*-Bu); ^{13}C NMR (CD_2Cl_2, 75.5 MHz) δ = 162.12, 158.94, 142.17, 139.58, 138.58, 137.47, 134.89, 121.70, 109.64, 79.85, 78.40, 33.61 31.92, 20.30, 15.39, 13.33, 11.42; MALDI-TOF calcd. 1866.5, found 1866.9 [$(M)^+$]; Elemental analysis (%) calcd. 9.01 (N), 73.36 (C), 7.13 (H) found 8.76 (N), 73.35 (C), 7.36 (H); UV-vis λ_{max} (CH_2Cl_2)/nm 543.0.

NMR Spectra

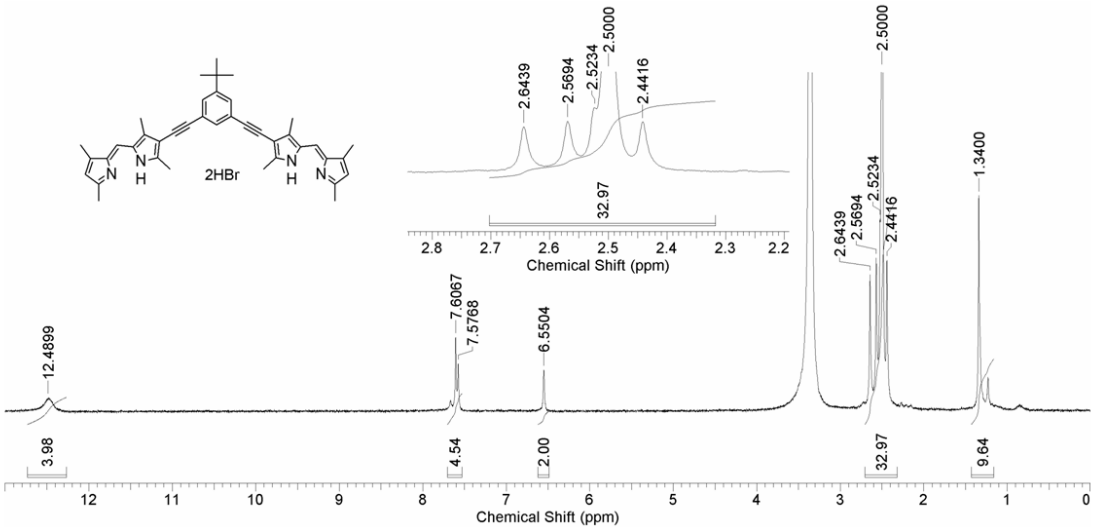


Fig. S1 ^{1}H NMR spectrum of ligand **1** in d_6-DMSO.

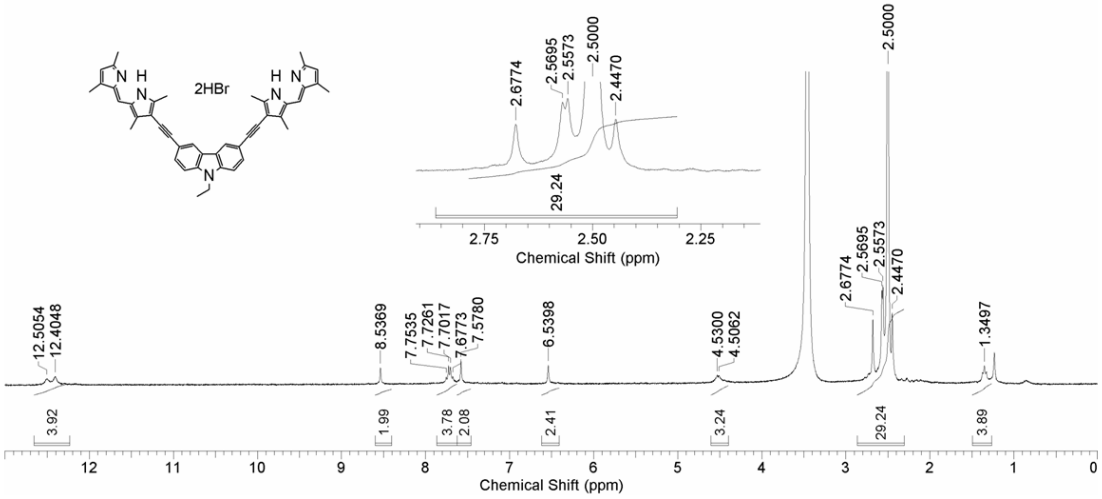


Fig. S2 ^{1}H NMR spectrum of ligand **2** in d_6-DMSO.

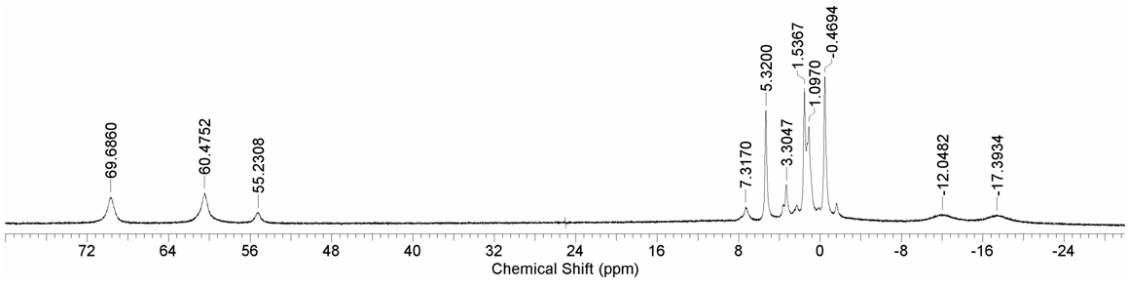


Fig. S3 ^{1}H NMR spectrum of Co(II) complex **3** in CD_2Cl_2.

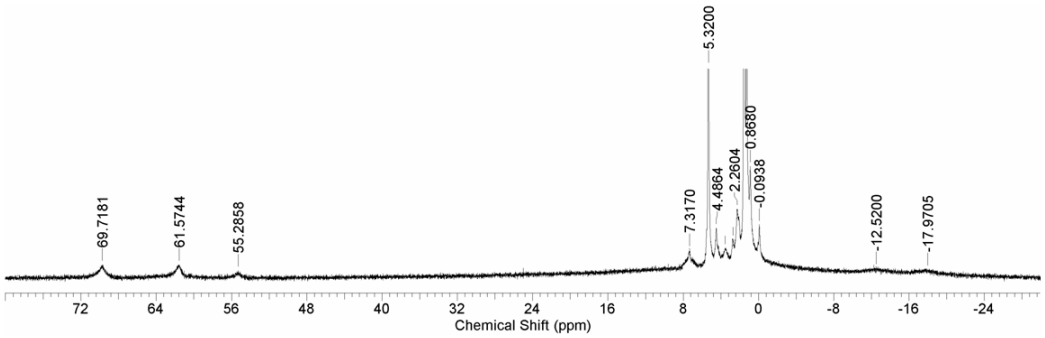


Fig. S4 ^{1}H NMR spectrum of Co(II) complex **4** in CD_2Cl_2.

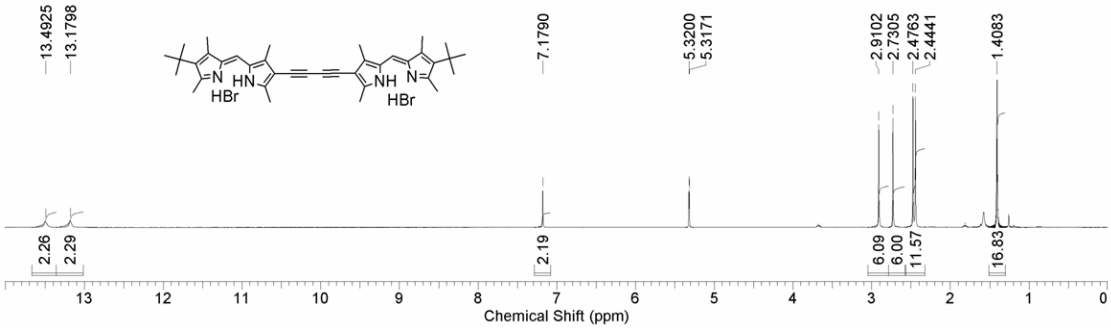


Fig. S5 ^{1}H NMR spectrum of ligand **5** in CD_2Cl_2.

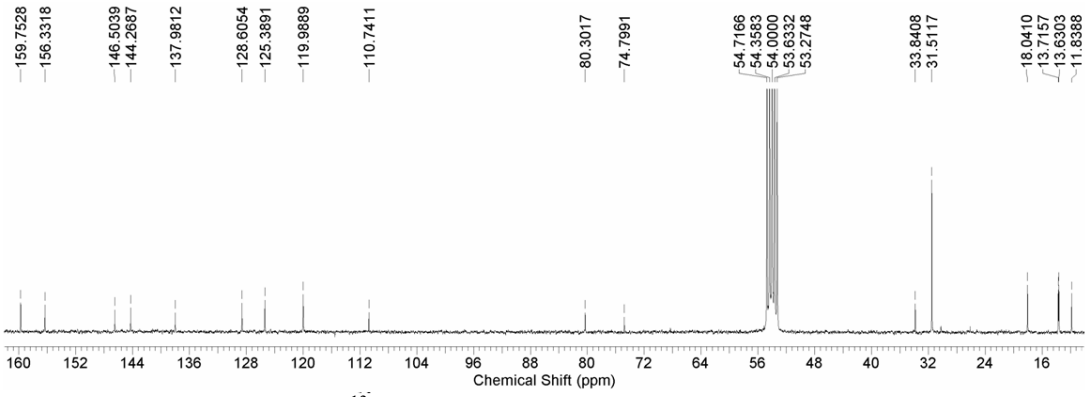


Fig. S6 ^{13}C NMR spectrum of ligand **5** in CD_2Cl_2.

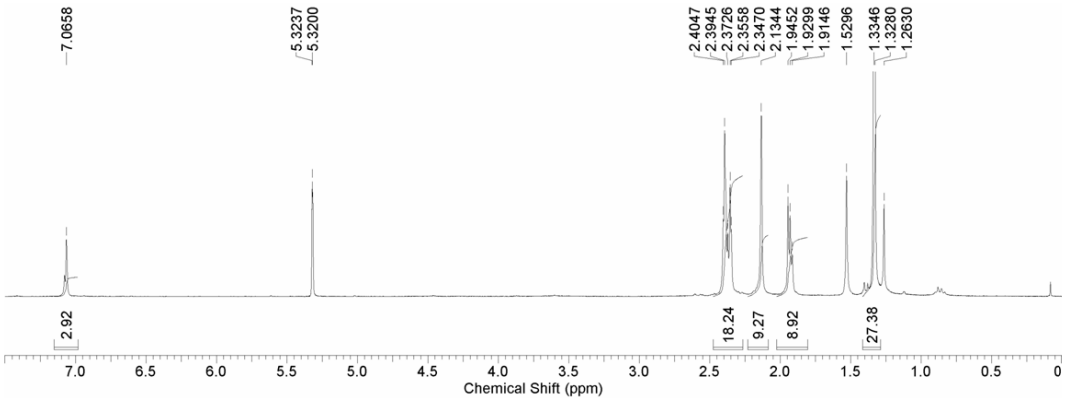


Fig. S7 ^{1}H NMR spectrum of Zn(II) complex **6** in CD_2Cl_2.

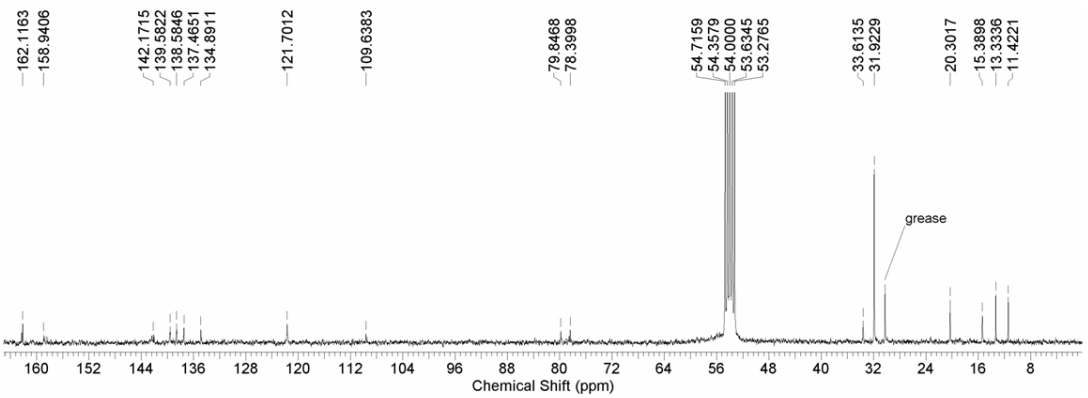


Fig. S8 ^{13}C NMR spectrum of Zn(II) complex **6** in CD_2Cl_2.

2. X-ray crystallographic data.

Complexes **3** and **4** were crystallized by slow vaporization of the solvent from $CHCl_3$ solutions. Similarly, complex **6** was obtained from a CH_2Cl_2 solution.

Crystallographic data for 3

A red plate crystal of $C_{80}H_{80}N_8Co_2 \cdot 5[CHCl_3]$ having approximate dimensions of 0.08 × 0.20 × 0.35 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX II diffractometer with graphite monochromated Mo-Kα radiation. The data were collected at a temperature of -100.0 ± 0.1ºC to a maximum 2θ value of 45.2º. Data were collected in a series of ϕ and ω scans in 0.50º oscillations with 50.0 second exposures. The crystal-to-detector distance was 36.00 mm.

Of the 38148 reflections that were collected, 11798 were unique (R_{int} = 0.063); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient μ, for Mo-Kα radiation is 8.58 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.638 and 0.934, respectively. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods[3]. The molecule crystallizes with $CHCl_3$ in the asymmetric unit. One solvent molecule was disordered and was modeled in two orientations. All non-hydrogen atoms were refined anisotropically, while all hydrogen atoms were placed in calculated positions and not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 11798 reflections and 1050 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors (R1 = 0.133 and wR2 = 0.256).

The standard deviation of an observation of unit weight[5] was 1.05. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.29 and -0.72 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All

refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

Crystallographic data for 4

A red plate crystal of $C_{88}H_{78}N_{10}Co_2 \cdot 2CHCl_3$ having approximate dimensions of 0.12 x 0.50 x 0.50 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX II diffractometer with graphite monochromated Mo-Kα radiation. The data were collected at a temperature of -100.0 ± 0.1ºC to a maximum 2θ value of 45.1º. Data were collected in a series of ϕ and ω scans in 0.50º oscillations with 15.0 second exposures. The crystal-to-detector distance was 36.00 mm.

Of the 51369 reflections that were collected, 15694 were unique (R_{int} = 0.073); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient μ, for Mo-Kα radiation is 4.45 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.803 and 0.948, respectively. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods[3]. The molecule crystallizes with $CHCl_3$ in the asymmetric unit. Two solvent molecules (one disordered) were modeled, however there remained a number of residual electron density peaks that could not be properly modeled. The PLATON/SQUEEZE[11] program was used to correct the raw data to remove these residual peaks, ultimately removing the equivalent of 223 electrons per unit cell (or 111.5 per asymmetric unit) or approximately four $CHCl_3$ molecules per unit cell. Please note, however, that the final formula, and subsequent calculations based on it, reflects only the two solvent molecules found and modeled. All non-hydrogen atoms except those found in the disordered solvent molecule fragments were refined anisotropically, while all hydrogen atoms were placed in calculated positions and not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 15694 reflections and 977 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors (R1 = 0.136 and wR2 = 0.221).

The standard deviation of an observation of unit weight[5] was 0.95. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.59 and -0.62 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

Crystallographic data for 6

A red prism crystal of $C_{114}H_{132}N_{12}Zn_3 \cdot 2CH_2Cl_2$ having approximate dimensions of 0.08 x 0.10 x 0.25 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX II diffractometer with graphite monochromated Mo-Kα radiation. The data were collected at a temperature of -100.0 ± 0.1ºC to a maximum 2θ value of 50.0º. Data were collected in a series of ϕ and ω scans in 0.50º oscillations with 30.0 second exposures. The crystal-to-detector distance was 36.00 mm.

Of the 25286 reflections that were collected, 3960 were unique (R_{int} = 0.045); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient μ, for Mo-Kα radiation is 6.53 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and

maximum transmission coefficients of 0.341 and 0.949, respectively. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods[3]. The molecule crystallizes about a three-fold axis located along the crystallographic c-axis. Additionally, the material crystallizes with several solvent molecules (either MeOH or CH_2C_2) in the lattice. The largest residual peaks, located on a three-fold axis at (1/3, 2/3, z) were modeled as a partially occupied by methylene chloride molecule. The residual R1 ($I > 2\sigma(I)$) improved from 8.05% to 6.6%. Any remaining residual electron density could not be satisfactorily modeled, thus the PLATON/SQUEEZE[11] program was used on the raw data set that removed the scattering contribution from any residual electron density found in the lattice. Ultimately a contribution of roughly 540 e^-/unit cell (or 45 e^- per asymmetric unit) was removed from the raw data. This amounts to roughly one CH_2Cl_2 molecule in each asymmetric unit. The residual R1 ($I > 2\sigma(I)$) improved from 6.70% to 4.5%. It is important to note that the formula and any values calculated from it do not reflect the solvent molecules in the lattice as they do not appear in the model. Finally, the one, unique, *t*-butyl group (C6 -> C9) was disordered about the C3-C6 bond. The disorder was modeled in two orientations. All non-hydrogen atoms were refined anisotropically, while all hydrogen atoms were placed in calculated positions and not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 3960 reflections and 235 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors (R1 = 0.066 and wR2 = 0.134).

The standard deviation of an observation of unit weight[5] was 1.06. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.61 and -0.59 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

Reference

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4. Least Squres function minimized: $\Sigma w(F_o^2 - F_c^2)^2$
5. Standard deviation of an observation of unit weight: $[\Sigma w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$
   Where: N_o = number of observations
   N_v = number of variables
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Table S1. Crystallographic Data of **3**, **4**, and **6**.

	3	**4**	**6**
Formula	$C_{80}H_{80}N_8Co_2 \cdot 5CHCl_3$	$C_{88}H_{78}N_{10}Co_2 \cdot 2CHCl_3$	$C_{114}H_{132}N_{12}Zn_3 \cdot 2CH_2Cl_2$
Mw	1868.22	1632.20	2036.28
cryst syst	triclinic	triclinic	trigonal
Space group	*P*-1(# 2)	*P*-1 (# 2)	*R*-3c(#167)
a/Å	16.7103(16)	13.5936(9)	19.650(10)
b/Å	17.1894(16)	18.5791(12)	19.650(10)
c/Å	18.881(3)	24.3507(17)	60.258(4)
α/deg	101.334(7)	90.743(3)	90.0
β/deg	101.137(7)	92.110(2)	90.0
γ/deg	116.285(5)	102.012(3)	120.0
V/Å^3	4519(1)	6009.9(7)	20150(2)
Z	2	2	6
D_c/g cm^{-3}	1.373	0.902	1.007
μ(MoK$\bar{\alpha}$) cm^{-1}	8.58	4.45	6.53
No. of obsd data (I>0.00σ(I))	11798	15694	3960
Reflection / Parameter Ratio	11.24	16.34	16.85
R1[a]; *wR2*[b]	0.133; 0.256	0.136; 0.221	0.066; 0.134
GOF	1.05	0.95	1.09
No. of obsd data (I>2σ(I))	7582	7524	2954
(*R1*; *wR2*) [c]	(0.083; 0.221)	(0.081; 0.205)	(0.045;0.127)

[a] $R1 = \Sigma\omega||Fo|-|Fc|| / \Sigma\omega|Fo|$, [b] $wR2 = \sqrt{\Sigma\{\omega(Fo^2-Fc^2)^2\} / \Sigma\omega(Fo^2)^2}$ [c] refined on F, I>2σ(I)

Table S2. Bond lengths [Å] and angles [°] for **3**.

C(1)-C(2)	1.493(13)	C(11)-C(14)	1.424(13)
C(1)-H(1A)	0.9800	C(11)-C(12)	1.429(12)
C(1)-H(1B)	0.9800	C(12)-N(2)	1.347(10)
C(1)-H(1C)	0.9800	C(12)-C(13)	1.478(11)
C(2)-N(1)	1.336(10)	C(13)-H(13A)	0.9800
C(2)-C(3)	1.385(12)	C(13)-H(13B)	0.9800
C(3)-C(4)	1.367(13)	C(13)-H(13C)	0.9800
C(3)-H(3)	0.9500	C(14)-C(15)	1.185(11)
C(4)-C(6)	1.448(12)	C(15)-C(16)	1.439(12)
C(4)-C(5)	1.456(13)	C(16)-C(17)	1.387(12)
C(5)-H(5A)	0.9800	C(16)-C(21)	1.398(11)
C(5)-H(5B)	0.9800	C(17)-C(18)	1.387(12)
C(5)-H(5C)	0.9800	C(17)-H(17)	0.9500
C(6)-C(7)	1.386(12)	C(18)-C(19)	1.385(11)
C(6)-N(1)	1.387(11)	C(18)-C(22)	1.534(12)
C(7)-C(8)	1.389(12)	C(19)-C(20)	1.382(12)
C(7)-H(7)	0.9500	C(19)-H(19)	0.9500
C(8)-N(2)	1.396(11)	C(20)-C(21)	1.393(12)
C(8)-C(9)	1.421(12)	C(20)-C(26)	1.407(12)
C(9)-C(11)	1.394(12)	C(21)-H(21)	0.9500
C(9)-C(10)	1.487(12)	C(22)-C(23)	1.518(13)
C(10)-H(10A)	0.9800	C(22)-C(24)	1.527(14)
C(10)-H(10B)	0.9800	C(22)-C(25)	1.530(13)
C(10)-H(10C)	0.9800	C(23)-H(23A)	0.9800

C(23)-H(23B)	0.9800	C(47)-H(47)	0.9500
C(23)-H(23C)	0.9800	C(48)-N(6)	1.389(10)
C(24)-H(24A)	0.9800	C(48)-C(49)	1.415(11)
C(24)-H(24B)	0.9800	C(49)-C(51)	1.381(11)
C(24)-H(24C)	0.9800	C(49)-C(50)	1.492(12)
C(25)-H(25A)	0.9800	C(50)-H(50A)	0.9800
C(25)-H(25B)	0.9800	C(50)-H(50B)	0.9800
C(25)-H(25C)	0.9800	C(50)-H(50C)	0.9800
C(26)-C(27)	1.222(12)	C(51)-C(52)	1.411(11)
C(27)-C(30)	1.416(12)	C(51)-C(54)	1.428(12)
C(28)-C(29)	1.470(12)	C(52)-N(6)	1.344(10)
C(28)-H(28A)	0.9800	C(52)-C(53)	1.475(12)
C(28)-H(28B)	0.9800	C(53)-H(53A)	0.9800
C(28)-H(28C)	0.9800	C(53)-H(53B)	0.9800
C(29)-N(3)	1.351(10)	C(53)-H(53C)	0.9800
C(29)-C(30)	1.413(12)	C(54)-C(55)	1.201(11)
C(30)-C(31)	1.380(12)	C(55)-C(56)	1.441(12)
C(31)-C(33)	1.399(11)	C(56)-C(61)	1.378(11)
C(31)-C(32)	1.491(13)	C(56)-C(57)	1.397(11)
C(32)-H(32A)	0.9800	C(57)-C(58)	1.393(11)
C(32)-H(32B)	0.9800	C(57)-H(57)	0.9500
C(32)-H(32C)	0.9800	C(58)-C(59)	1.397(11)
C(33)-C(34)	1.381(11)	C(58)-C(62)	1.534(11)
C(33)-N(3)	1.381(10)	C(59)-C(60)	1.378(11)
C(34)-C(35)	1.388(11)	C(59)-H(59)	0.9500
C(34)-H(34)	0.9500	C(60)-C(61)	1.386(11)
C(35)-N(4)	1.387(10)	C(60)-C(66)	1.424(12)
C(35)-C(36)	1.407(12)	C(61)-H(61)	0.9500
C(36)-C(38)	1.353(13)	C(62)-C(65)	1.518(12)
C(36)-C(37)	1.505(12)	C(62)-C(64)	1.524(12)
C(37)-H(37A)	0.9800	C(62)-C(63)	1.530(11)
C(37)-H(37B)	0.9800	C(63)-H(63A)	0.9800
C(37)-H(37C)	0.9800	C(63)-H(63B)	0.9800
C(38)-C(39)	1.411(13)	C(63)-H(63C)	0.9800
C(38)-H(38)	0.9500	C(64)-H(64A)	0.9800
C(39)-N(4)	1.321(10)	C(64)-H(64B)	0.9800
C(39)-C(40)	1.483(13)	C(64)-H(64C)	0.9800
C(40)-H(40A)	0.9800	C(65)-H(65A)	0.9800
C(40)-H(40B)	0.9800	C(65)-H(65B)	0.9800
C(40)-H(40C)	0.9800	C(65)-H(65C)	0.9800
C(41)-C(42)	1.483(12)	C(66)-C(67)	1.199(11)
C(41)-H(41A)	0.9800	C(67)-C(70)	1.428(12)
C(41)-H(41B)	0.9800	C(68)-C(69)	1.478(12)
C(41)-H(41C)	0.9800	C(68)-H(68A)	0.9800
C(42)-N(5)	1.330(10)	C(68)-H(68B)	0.9800
C(42)-C(43)	1.409(13)	C(68)-H(68C)	0.9800
C(43)-C(44)	1.362(12)	C(69)-N(7)	1.351(10)
C(43)-H(43)	0.9500	C(69)-C(70)	1.412(12)
C(44)-C(46)	1.424(11)	C(70)-C(71)	1.374(11)
C(44)-C(45)	1.498(13)	C(71)-C(73)	1.420(11)
C(45)-H(45A)	0.9800	C(71)-C(72)	1.492(12)
C(45)-H(45B)	0.9800	C(72)-H(72A)	0.9800
C(45)-H(45C)	0.9800	C(72)-H(72B)	0.9800
C(46)-C(47)	1.382(11)	C(72)-H(72C)	0.9800
C(46)-N(5)	1.391(10)	C(73)-N(7)	1.386(10)
C(47)-C(48)	1.384(11)	C(73)-C(74)	1.402(11)

C(74)-C(75)	1.383(11)	N(1)-C(2)-C(1)	121.9(8)
C(74)-H(74)	0.9500	C(3)-C(2)-C(1)	127.3(8)
C(75)-N(8)	1.386(10)	C(4)-C(3)-C(2)	109.6(8)
C(75)-C(76)	1.434(11)	C(4)-C(3)-H(3)	125.2
C(76)-C(78)	1.364(12)	C(2)-C(3)-H(3)	125.2
C(76)-C(77)	1.487(12)	C(3)-C(4)-C(6)	103.7(8)
C(77)-H(77A)	0.9800	C(3)-C(4)-C(5)	129.5(8)
C(77)-H(77B)	0.9800	C(6)-C(4)-C(5)	126.8(9)
C(77)-H(77C)	0.9800	C(4)-C(5)-H(5A)	109.5
C(78)-C(79)	1.406(11)	C(4)-C(5)-H(5B)	109.5
C(78)-H(78)	0.9500	H(5A)-C(5)-H(5B)	109.5
C(79)-N(8)	1.335(10)	C(4)-C(5)-H(5C)	109.5
C(79)-C(80)	1.468(12)	H(5A)-C(5)-H(5C)	109.5
C(80)-H(80A)	0.9800	H(5B)-C(5)-H(5C)	109.5
C(80)-H(80B)	0.9800	C(7)-C(6)-N(1)	124.8(7)
C(80)-H(80C)	0.9800	C(7)-C(6)-C(4)	125.4(8)
C(81)-Cl(2)	1.686(13)	N(1)-C(6)-C(4)	109.7(7)
C(81)-Cl(1)	1.696(13)	C(6)-C(7)-C(8)	129.0(8)
C(81)-Cl(3)	1.750(14)	C(6)-C(7)-H(7)	115.5
C(81)-H(81)	1.0000	C(8)-C(7)-H(7)	115.5
C(82)-Cl(4)	1.737(11)	C(7)-C(8)-N(2)	123.2(8)
C(82)-Cl(6)	1.741(11)	C(7)-C(8)-C(9)	127.2(8)
C(82)-Cl(5)	1.751(11)	N(2)-C(8)-C(9)	109.5(7)
C(82)-H(82)	1.0000	C(11)-C(9)-C(8)	105.4(7)
C(83)-Cl(9)	1.711(13)	C(11)-C(9)-C(10)	127.4(8)
C(83)-Cl(8)	1.712(14)	C(8)-C(9)-C(10)	127.1(8)
C(83)-Cl(7)	1.730(14)	C(9)-C(10)-H(10A)	109.5
C(83)-H(83)	1.0000	C(9)-C(10)-H(10B)	109.5
C(85)-Cl(15)	1.693(16)	H(10A)-C(10)-H(10B)	109.5
C(85)-Cl(14)	1.720(14)	C(9)-C(10)-H(10C)	109.5
C(85)-Cl(13)	1.757(17)	H(10A)-C(10)-H(10C)	109.5
C(85)-H(85)	1.0000	H(10B)-C(10)-H(10C)	109.5
N(1)-Co(1)	1.982(6)	C(9)-C(11)-C(14)	130.5(8)
N(2)-Co(1)	1.980(7)	C(9)-C(11)-C(12)	108.3(7)
N(3)-Co(2)	1.992(6)	C(14)-C(11)-C(12)	121.2(8)
N(4)-Co(2)	1.984(7)	N(2)-C(12)-C(11)	108.8(7)
N(5)-Co(1)	1.965(6)	N(2)-C(12)-C(13)	122.9(7)
N(6)-Co(1)	1.979(6)	C(11)-C(12)-C(13)	128.3(7)
N(7)-Co(2)	1.960(6)	C(12)-C(13)-H(13A)	109.5
N(8)-Co(2)	1.977(6)	C(12)-C(13)-H(13B)	109.5
C(84)-Cl(10)	1.654(9)	H(13A)-C(13)-H(13B)	109.5
C(84)-Cl(12)	1.655(9)	C(12)-C(13)-H(13C)	109.5
C(84)-Cl(11)	1.662(10)	H(13A)-C(13)-H(13C)	109.5
C(84)-H(84)	1.0000	H(13B)-C(13)-H(13C)	109.5
C(84B)-Cl(17)	1.657(11)	C(15)-C(14)-C(11)	172.0(9)
C(84B)-Cl(16)	1.657(11)	C(14)-C(15)-C(16)	172.2(10)
C(84B)-Cl(18)	1.659(11)	C(17)-C(16)-C(21)	119.5(8)
C(84B)-H(84B)	1.0000	C(17)-C(16)-C(15)	121.8(7)
		C(21)-C(16)-C(15)	118.5(8)
C(2)-C(1)-H(1A)	109.5	C(16)-C(17)-C(18)	121.8(7)
C(2)-C(1)-H(1B)	109.5	C(16)-C(17)-H(17)	119.1
H(1A)-C(1)-H(1B)	109.5	C(18)-C(17)-H(17)	119.1
C(2)-C(1)-H(1C)	109.5	C(19)-C(18)-C(17)	117.5(7)
H(1A)-C(1)-H(1C)	109.5	C(19)-C(18)-C(22)	120.3(8)
H(1B)-C(1)-H(1C)	109.5	C(17)-C(18)-C(22)	122.1(7)
N(1)-C(2)-C(3)	110.8(8)	C(20)-C(19)-C(18)	122.3(8)

C(20)-C(19)-H(19)	118.9	C(34)-C(33)-C(31)	126.6(8)
C(18)-C(19)-H(19)	118.9	N(3)-C(33)-C(31)	109.6(7)
C(19)-C(20)-C(21)	119.5(8)	C(33)-C(34)-C(35)	130.2(8)
C(19)-C(20)-C(26)	120.7(8)	C(33)-C(34)-H(34)	114.9
C(21)-C(20)-C(26)	119.8(8)	C(35)-C(34)-H(34)	114.9
C(20)-C(21)-C(16)	119.3(8)	N(4)-C(35)-C(34)	123.3(7)
C(20)-C(21)-H(21)	120.3	N(4)-C(35)-C(36)	109.4(7)
C(16)-C(21)-H(21)	120.3	C(34)-C(35)-C(36)	127.2(8)
C(23)-C(22)-C(24)	108.4(9)	C(38)-C(36)-C(35)	106.5(8)
C(23)-C(22)-C(25)	107.5(8)	C(38)-C(36)-C(37)	128.2(8)
C(24)-C(22)-C(25)	110.9(9)	C(35)-C(36)-C(37)	125.3(8)
C(23)-C(22)-C(18)	112.7(8)	C(36)-C(37)-H(37A)	109.5
C(24)-C(22)-C(18)	108.4(8)	C(36)-C(37)-H(37B)	109.5
C(25)-C(22)-C(18)	109.0(7)	H(37A)-C(37)-H(37B)	109.5
C(22)-C(23)-H(23A)	109.5	C(36)-C(37)-H(37C)	109.5
C(22)-C(23)-H(23B)	109.5	H(37A)-C(37)-H(37C)	109.5
H(23A)-C(23)-H(23B)	109.5	H(37B)-C(37)-H(37C)	109.5
C(22)-C(23)-H(23C)	109.5	C(36)-C(38)-C(39)	107.0(8)
H(23A)-C(23)-H(23C)	109.5	C(36)-C(38)-H(38)	126.5
H(23B)-C(23)-H(23C)	109.5	C(39)-C(38)-H(38)	126.5
C(22)-C(24)-H(24A)	109.5	N(4)-C(39)-C(38)	111.0(8)
C(22)-C(24)-H(24B)	109.5	N(4)-C(39)-C(40)	122.0(9)
H(24A)-C(24)-H(24B)	109.5	C(38)-C(39)-C(40)	127.0(8)
C(22)-C(24)-H(24C)	109.5	C(39)-C(40)-H(40A)	109.5
H(24A)-C(24)-H(24C)	109.5	C(39)-C(40)-H(40B)	109.5
H(24B)-C(24)-H(24C)	109.5	H(40A)-C(40)-H(40B)	109.5
C(22)-C(25)-H(25A)	109.5	C(39)-C(40)-H(40C)	109.5
C(22)-C(25)-H(25B)	109.5	H(40A)-C(40)-H(40C)	109.5
H(25A)-C(25)-H(25B)	109.5	H(40B)-C(40)-H(40C)	109.5
C(22)-C(25)-H(25C)	109.5	C(42)-C(41)-H(41A)	109.5
H(25A)-C(25)-H(25C)	109.5	C(42)-C(41)-H(41B)	109.5
H(25B)-C(25)-H(25C)	109.5	H(41A)-C(41)-H(41B)	109.5
C(27)-C(26)-C(20)	177.7(10)	C(42)-C(41)-H(41C)	109.5
C(26)-C(27)-C(30)	178.3(10)	H(41A)-C(41)-H(41C)	109.5
C(29)-C(28)-H(28A)	109.5	H(41B)-C(41)-H(41C)	109.5
C(29)-C(28)-H(28B)	109.5	N(5)-C(42)-C(43)	111.2(8)
H(28A)-C(28)-H(28B)	109.5	N(5)-C(42)-C(41)	122.0(8)
C(29)-C(28)-H(28C)	109.5	C(43)-C(42)-C(41)	126.8(8)
H(28A)-C(28)-H(28C)	109.5	C(44)-C(43)-C(42)	107.7(8)
H(28B)-C(28)-H(28C)	109.5	C(44)-C(43)-H(43)	126.2
N(3)-C(29)-C(30)	109.5(8)	C(42)-C(43)-H(43)	126.2
N(3)-C(29)-C(28)	122.9(7)	C(43)-C(44)-C(46)	105.5(8)
C(30)-C(29)-C(28)	127.6(8)	C(43)-C(44)-C(45)	127.6(8)
C(31)-C(30)-C(29)	107.2(7)	C(46)-C(44)-C(45)	126.9(8)
C(31)-C(30)-C(27)	128.2(8)	C(44)-C(45)-H(45A)	109.5
C(29)-C(30)-C(27)	124.6(8)	C(44)-C(45)-H(45B)	109.5
C(30)-C(31)-C(33)	106.6(7)	H(45A)-C(45)-H(45B)	109.5
C(30)-C(31)-C(32)	126.2(8)	C(44)-C(45)-H(45C)	109.5
C(33)-C(31)-C(32)	127.2(8)	H(45A)-C(45)-H(45C)	109.5
C(31)-C(32)-H(32A)	109.5	H(45B)-C(45)-H(45C)	109.5
C(31)-C(32)-H(32B)	109.5	C(47)-C(46)-N(5)	122.9(7)
H(32A)-C(32)-H(32B)	109.5	C(47)-C(46)-C(44)	127.3(8)
C(31)-C(32)-H(32C)	109.5	N(5)-C(46)-C(44)	109.8(7)
H(32A)-C(32)-H(32C)	109.5	C(46)-C(47)-C(48)	130.7(8)
H(32B)-C(32)-H(32C)	109.5	C(46)-C(47)-H(47)	114.7
C(34)-C(33)-N(3)	123.8(7)	C(48)-C(47)-H(47)	114.7

C(47)-C(48)-N(6)	122.5(7)	C(62)-C(64)-H(64A)	109.5
C(47)-C(48)-C(49)	127.9(8)	C(62)-C(64)-H(64B)	109.5
N(6)-C(48)-C(49)	109.4(7)	H(64A)-C(64)-H(64B)	109.5
C(51)-C(49)-C(48)	106.2(7)	C(62)-C(64)-H(64C)	109.5
C(51)-C(49)-C(50)	126.5(7)	H(64A)-C(64)-H(64C)	109.5
C(48)-C(49)-C(50)	127.2(8)	H(64B)-C(64)-H(64C)	109.5
C(49)-C(50)-H(50A)	109.5	C(62)-C(65)-H(65A)	109.5
C(49)-C(50)-H(50B)	109.5	C(62)-C(65)-H(65B)	109.5
H(50A)-C(50)-H(50B)	109.5	H(65A)-C(65)-H(65B)	109.5
C(49)-C(50)-H(50C)	109.5	C(62)-C(65)-H(65C)	109.5
H(50A)-C(50)-H(50C)	109.5	H(65A)-C(65)-H(65C)	109.5
H(50B)-C(50)-H(50C)	109.5	H(65B)-C(65)-H(65C)	109.5
C(49)-C(51)-C(52)	107.2(7)	C(67)-C(66)-C(60)	175.7(9)
C(49)-C(51)-C(54)	128.2(7)	C(66)-C(67)-C(70)	174.7(9)
C(52)-C(51)-C(54)	124.5(8)	C(69)-C(68)-H(68A)	109.5
N(6)-C(52)-C(51)	110.5(7)	C(69)-C(68)-H(68B)	109.5
N(6)-C(52)-C(53)	121.6(7)	H(68A)-C(68)-H(68B)	109.5
C(51)-C(52)-C(53)	127.9(7)	C(69)-C(68)-H(68C)	109.5
C(52)-C(53)-H(53A)	109.5	H(68A)-C(68)-H(68C)	109.5
C(52)-C(53)-H(53B)	109.5	H(68B)-C(68)-H(68C)	109.5
H(53A)-C(53)-H(53B)	109.5	N(7)-C(69)-C(70)	110.6(7)
C(52)-C(53)-H(53C)	109.5	N(7)-C(69)-C(68)	123.0(8)
H(53A)-C(53)-H(53C)	109.5	C(70)-C(69)-C(68)	126.4(8)
H(53B)-C(53)-H(53C)	109.5	C(71)-C(70)-C(69)	107.7(7)
C(55)-C(54)-C(51)	177.4(9)	C(71)-C(70)-C(67)	130.4(8)
C(54)-C(55)-C(56)	177.7(9)	C(69)-C(70)-C(67)	121.9(8)
C(61)-C(56)-C(57)	119.5(7)	C(70)-C(71)-C(73)	105.5(7)
C(61)-C(56)-C(55)	120.2(7)	C(70)-C(71)-C(72)	127.8(8)
C(57)-C(56)-C(55)	120.3(7)	C(73)-C(71)-C(72)	126.7(7)
C(58)-C(57)-C(56)	121.6(7)	C(71)-C(72)-H(72A)	109.5
C(58)-C(57)-H(57)	119.2	C(71)-C(72)-H(72B)	109.5
C(56)-C(57)-H(57)	119.2	H(72A)-C(72)-H(72B)	109.5
C(57)-C(58)-C(59)	117.0(7)	C(71)-C(72)-H(72C)	109.5
C(57)-C(58)-C(62)	123.0(7)	H(72A)-C(72)-H(72C)	109.5
C(59)-C(58)-C(62)	119.8(7)	H(72B)-C(72)-H(72C)	109.5
C(60)-C(59)-C(58)	122.0(7)	N(7)-C(73)-C(74)	122.0(7)
C(60)-C(59)-H(59)	119.0	N(7)-C(73)-C(71)	110.5(7)
C(58)-C(59)-H(59)	119.0	C(74)-C(73)-C(71)	127.6(8)
C(59)-C(60)-C(61)	119.6(7)	C(75)-C(74)-C(73)	129.4(8)
C(59)-C(60)-C(66)	120.9(7)	C(75)-C(74)-H(74)	115.3
C(61)-C(60)-C(66)	119.5(7)	C(73)-C(74)-H(74)	115.3
C(56)-C(61)-C(60)	120.2(8)	C(74)-C(75)-N(8)	124.6(7)
C(56)-C(61)-H(61)	119.9	C(74)-C(75)-C(76)	126.3(7)
C(60)-C(61)-H(61)	119.9	N(8)-C(75)-C(76)	109.1(7)
C(65)-C(62)-C(64)	109.8(7)	C(78)-C(76)-C(75)	105.4(7)
C(65)-C(62)-C(63)	108.6(7)	C(78)-C(76)-C(77)	128.1(8)
C(64)-C(62)-C(63)	107.6(7)	C(75)-C(76)-C(77)	126.5(8)
C(65)-C(62)-C(58)	108.5(7)	C(76)-C(77)-H(77A)	109.5
C(64)-C(62)-C(58)	110.5(7)	C(76)-C(77)-H(77B)	109.5
C(63)-C(62)-C(58)	111.8(6)	H(77A)-C(77)-H(77B)	109.5
C(62)-C(63)-H(63A)	109.5	C(76)-C(77)-H(77C)	109.5
C(62)-C(63)-H(63B)	109.5	H(77A)-C(77)-H(77C)	109.5
H(63A)-C(63)-H(63B)	109.5	H(77B)-C(77)-H(77C)	109.5
C(62)-C(63)-H(63C)	109.5	C(76)-C(78)-C(79)	108.3(7)
H(63A)-C(63)-H(63C)	109.5	C(76)-C(78)-H(78)	125.9
H(63B)-C(63)-H(63C)	109.5	C(79)-C(78)-H(78)	125.9

N(8)-C(79)-C(78)	110.3(7)	C(33)-N(3)-Co(2)	123.7(5)
N(8)-C(79)-C(80)	121.6(7)	C(39)-N(4)-C(35)	106.1(7)
C(78)-C(79)-C(80)	128.1(8)	C(39)-N(4)-Co(2)	129.7(6)
C(79)-C(80)-H(80A)	109.5	C(35)-N(4)-Co(2)	123.9(5)
C(79)-C(80)-H(80B)	109.5	C(42)-N(5)-C(46)	105.8(7)
H(80A)-C(80)-H(80B)	109.5	C(42)-N(5)-Co(1)	129.9(6)
C(79)-C(80)-H(80C)	109.5	C(46)-N(5)-Co(1)	124.2(5)
H(80A)-C(80)-H(80C)	109.5	C(52)-N(6)-C(48)	106.7(6)
H(80B)-C(80)-H(80C)	109.5	C(52)-N(6)-Co(1)	127.7(6)
Cl(2)-C(81)-Cl(1)	113.3(7)	C(48)-N(6)-Co(1)	123.9(5)
Cl(2)-C(81)-Cl(3)	111.7(8)	C(69)-N(7)-C(73)	105.8(7)
Cl(1)-C(81)-Cl(3)	110.0(8)	C(69)-N(7)-Co(2)	127.9(5)
Cl(2)-C(81)-H(81)	107.1	C(73)-N(7)-Co(2)	124.9(5)
Cl(1)-C(81)-H(81)	107.1	C(79)-N(8)-C(75)	106.9(6)
Cl(3)-C(81)-H(81)	107.1	C(79)-N(8)-Co(2)	130.0(6)
Cl(4)-C(82)-Cl(6)	110.8(6)	C(75)-N(8)-Co(2)	122.9(5)
Cl(4)-C(82)-Cl(5)	111.0(6)	Cl(10)-C(84)-Cl(12)	113.3(8)
Cl(6)-C(82)-Cl(5)	109.2(6)	Cl(10)-C(84)-Cl(11)	113.3(9)
Cl(4)-C(82)-H(82)	108.6	Cl(12)-C(84)-Cl(11)	112.5(8)
Cl(6)-C(82)-H(82)	108.6	Cl(10)-C(84)-H(84)	105.7
Cl(5)-C(82)-H(82)	108.6	Cl(12)-C(84)-H(84)	105.6
Cl(9)-C(83)-Cl(8)	113.3(8)	Cl(11)-C(84)-H(84)	105.5
Cl(9)-C(83)-Cl(7)	109.2(8)	N(5)-Co(1)-N(6)	94.8(3)
Cl(8)-C(83)-Cl(7)	109.7(8)	N(5)-Co(1)-N(2)	118.1(3)
Cl(9)-C(83)-H(83)	108.2	N(6)-Co(1)-N(2)	107.6(3)
Cl(8)-C(83)-H(83)	108.2	N(5)-Co(1)-N(1)	114.6(3)
Cl(7)-C(83)-H(83)	108.2	N(6)-Co(1)-N(1)	128.6(3)
Cl(15)-C(85)-Cl(14)	114.6(9)	N(2)-Co(1)-N(1)	94.7(3)
Cl(15)-C(85)-Cl(13)	110.5(8)	N(7)-Co(2)-N(8)	95.3(3)
Cl(14)-C(85)-Cl(13)	110.4(9)	N(7)-Co(2)-N(4)	124.0(3)
Cl(15)-C(85)-H(85)	107.0	N(8)-Co(2)-N(4)	111.9(3)
Cl(14)-C(85)-H(85)	107.0	N(7)-Co(2)-N(3)	108.2(3)
Cl(13)-C(85)-H(85)	107.0	N(8)-Co(2)-N(3)	125.1(3)
C(2)-N(1)-C(6)	106.2(7)	N(4)-Co(2)-N(3)	94.9(3)
C(2)-N(1)-Co(1)	130.0(6)	Cl(17)-C(84B)-Cl(16)	113.0(10)
C(6)-N(1)-Co(1)	123.4(5)	Cl(17)-C(84B)-Cl(18)	112.6(10)
C(12)-N(2)-C(8)	108.0(7)	Cl(16)-C(84B)-Cl(18)	112.9(10)
C(12)-N(2)-Co(1)	127.6(6)	Cl(17)-C(84B)-H(84B)	106.1
C(8)-N(2)-Co(1)	124.4(5)	Cl(16)-C(84B)-H(84B)	105.7
C(29)-N(3)-C(33)	107.1(7)	Cl(18)-C(84B)-H(84B)	105.8
C(29)-N(3)-Co(2)	129.0(6)		

Table S3. Bond lengths [Å] and angles [°] for **4**.

C(1)-C(2)	1.493(8)	C(5)-H(5A)	0.9800
C(1)-H(1A)	0.9800	C(5)-H(5B)	0.9800
C(1)-H(1B)	0.9800	C(5)-H(5C)	0.9800
C(1)-H(1C)	0.9800	C(6)-C(7)	1.386(8)
C(2)-N(1)	1.333(7)	C(6)-N(1)	1.408(7)
C(2)-C(3)	1.422(8)	C(7)-C(8)	1.373(7)
C(3)-C(4)	1.349(8)	C(7)-H(7)	0.9500
C(3)-H(3)	0.9500	C(8)-N(2)	1.399(7)
C(4)-C(6)	1.438(8)	C(8)-C(9)	1.408(7)
C(4)-C(5)	1.500(9)	C(9)-C(11)	1.376(8)

C(9)-C(10)	1.499(8)	C(38)-H(38)	0.9500
C(10)-H(10A)	0.9800	C(39)-C(41)	1.393(8)
C(10)-H(10B)	0.9800	C(39)-N(4)	1.407(7)
C(10)-H(10C)	0.9800	C(40)-C(41)	1.494(8)
C(11)-C(12)	1.421(8)	C(40)-H(40A)	0.9800
C(11)-C(14)	1.436(9)	C(40)-H(40B)	0.9800
C(12)-N(2)	1.350(7)	C(40)-H(40C)	0.9800
C(12)-C(13)	1.499(8)	C(41)-C(42)	1.379(8)
C(13)-H(13A)	0.9800	C(42)-C(43)	1.405(8)
C(13)-H(13B)	0.9800	C(42)-H(42)	0.9500
C(13)-H(13C)	0.9800	C(43)-N(4)	1.345(7)
C(14)-C(15)	1.193(8)	C(43)-C(44)	1.482(8)
C(15)-C(16)	1.431(8)	C(44)-H(44A)	0.9800
C(16)-C(17)	1.390(8)	C(44)-H(44B)	0.9800
C(16)-C(21)	1.391(7)	C(44)-H(44C)	0.9800
C(17)-C(18)	1.359(8)	C(45)-C(46)	1.494(8)
C(17)-H(17)	0.9500	C(45)-H(45A)	0.9800
C(18)-C(19)	1.405(7)	C(45)-H(45B)	0.9800
C(18)-H(18)	0.9500	C(45)-H(45C)	0.9800
C(19)-N(9)	1.397(7)	C(46)-N(5)	1.331(7)
C(19)-C(20)	1.406(8)	C(46)-C(47)	1.388(8)
C(20)-C(21)	1.389(7)	C(47)-C(48)	1.348(9)
C(20)-C(22)	1.406(8)	C(47)-H(47)	0.9500
C(23)-N(9)	1.377(7)	C(48)-C(50)	1.406(9)
C(23)-C(24)	1.380(8)	C(48)-C(49)	1.533(10)
C(24)-C(25)	1.383(8)	C(49)-H(49A)	0.9800
C(24)-H(24)	0.9500	C(49)-H(49B)	0.9800
C(25)-C(26)	1.393(9)	C(49)-H(49C)	0.9800
C(25)-H(25)	0.9500	C(50)-C(51)	1.372(9)
C(26)-C(27)	1.412(8)	C(50)-N(5)	1.396(7)
C(26)-C(30)	1.458(10)	C(51)-C(52)	1.377(9)
C(27)-H(27)	0.9500	C(51)-H(51)	0.9500
C(28)-N(9)	1.439(7)	C(52)-C(54)	1.414(8)
C(28)-C(29)	1.477(10)	C(52)-N(6)	1.432(7)
C(28)-H(28A)	0.9900	C(53)-C(54)	1.476(8)
C(28)-H(28B)	0.9900	C(53)-H(53A)	0.9800
C(29)-H(29A)	0.9800	C(53)-H(53B)	0.9800
C(29)-H(29B)	0.9800	C(53)-H(53C)	0.9800
C(29)-H(29C)	0.9800	C(54)-C(55)	1.426(9)
C(30)-C(31)	1.187(9)	C(55)-C(56)	1.419(8)
C(31)-C(34)	1.413(9)	C(55)-C(58)	1.421(9)
C(32)-C(33)	1.508(9)	C(56)-N(6)	1.342(7)
C(32)-H(32A)	0.9800	C(56)-C(57)	1.458(8)
C(32)-H(32B)	0.9800	C(57)-H(57A)	0.9800
C(32)-H(32C)	0.9800	C(57)-H(57B)	0.9800
C(33)-N(3)	1.311(7)	C(57)-H(57C)	0.9800
C(33)-C(34)	1.443(8)	C(58)-C(59)	1.197(9)
C(34)-C(35)	1.369(9)	C(59)-C(60)	1.423(9)
C(35)-C(37)	1.440(8)	C(60)-C(65)	1.404(7)
C(35)-C(36)	1.488(9)	C(60)-C(61)	1.418(9)
C(36)-H(36A)	0.9800	C(61)-C(62)	1.369(9)
C(36)-H(36B)	0.9800	C(61)-H(61)	0.9500
C(36)-H(36C)	0.9800	C(62)-C(63)	1.405(7)
C(37)-C(38)	1.364(8)	C(62)-H(62)	0.9500
C(37)-N(3)	1.391(7)	C(63)-N(10)	1.382(7)
C(38)-C(39)	1.404(8)	C(63)-C(64)	1.387(7)

C(64)-C(65)	1.376(7)	N(4)-Co(2)	1.983(5)
C(64)-C(66)	1.448(7)	N(5)-Co(1)	1.965(5)
C(65)-H(65)	0.9500	N(6)-Co(1)	1.980(5)
C(66)-C(67)	1.385(7)	N(7)-Co(2)	1.968(5)
C(66)-C(71)	1.414(7)	N(8)-Co(2)	1.974(4)
C(67)-C(68)	1.365(7)	C(89)-Cl(3)	1.708(6)
C(67)-N(10)	1.385(6)	C(89)-Cl(2)	1.719(6)
C(68)-C(69)	1.356(7)	C(89)-Cl(1)	1.720(6)
C(68)-H(68)	0.9500	C(89)-H(89)	1.0000
C(69)-C(70)	1.416(8)	C(90A)-Cl(4A)	1.701(7)
C(69)-H(69)	0.9500	C(90A)-Cl(5A)	1.703(7)
C(70)-C(71)	1.369(7)	C(90A)-Cl(6A)	1.708(7)
C(70)-C(74)	1.469(8)	C(90A)-H(90A)	1.0000
C(71)-H(71)	0.9500	C(90B)-Cl(6B)	1.695(7)
C(72)-N(10)	1.446(7)	C(90B)-Cl(4B)	1.704(7)
C(72)-C(73)	1.485(8)	C(90B)-Cl(5B)	1.705(7)
C(72)-H(72A)	0.9900	C(90B)-H(90B)	1.0000
C(72)-H(72B)	0.9900		
C(73)-H(73A)	0.9800	C(2)-C(1)-H(1A)	109.5
C(73)-H(73B)	0.9800	C(2)-C(1)-H(1B)	109.5
C(73)-H(73C)	0.9800	H(1A)-C(1)-H(1B)	109.5
C(74)-C(75)	1.189(7)	C(2)-C(1)-H(1C)	109.5
C(75)-C(78)	1.402(8)	H(1A)-C(1)-H(1C)	109.5
C(76)-C(77)	1.494(8)	H(1B)-C(1)-H(1C)	109.5
C(76)-H(76A)	0.9800	N(1)-C(2)-C(3)	111.1(5)
C(76)-H(76B)	0.9800	N(1)-C(2)-C(1)	121.3(6)
C(76)-H(76C)	0.9800	C(3)-C(2)-C(1)	127.6(6)
C(77)-N(7)	1.334(6)	C(4)-C(3)-C(2)	107.6(5)
C(77)-C(78)	1.410(8)	C(4)-C(3)-H(3)	126.2
C(78)-C(79)	1.400(8)	C(2)-C(3)-H(3)	126.2
C(79)-C(81)	1.409(7)	C(3)-C(4)-C(6)	106.6(6)
C(79)-C(80)	1.503(8)	C(3)-C(4)-C(5)	128.1(6)
C(80)-H(80A)	0.9800	C(6)-C(4)-C(5)	125.3(6)
C(80)-H(80B)	0.9800	C(4)-C(5)-H(5A)	109.5
C(80)-H(80C)	0.9800	C(4)-C(5)-H(5B)	109.5
C(81)-N(7)	1.386(7)	H(5A)-C(5)-H(5B)	109.5
C(81)-C(82)	1.395(7)	C(4)-C(5)-H(5C)	109.5
C(82)-C(83)	1.394(8)	H(5A)-C(5)-H(5C)	109.5
C(82)-H(82)	0.9500	H(5B)-C(5)-H(5C)	109.5
C(83)-N(8)	1.409(7)	C(7)-C(6)-N(1)	124.0(5)
C(83)-C(85)	1.419(7)	C(7)-C(6)-C(4)	127.4(6)
C(84)-C(85)	1.502(8)	N(1)-C(6)-C(4)	108.6(5)
C(84)-H(84A)	0.9800	C(8)-C(7)-C(6)	129.9(6)
C(84)-H(84B)	0.9800	C(8)-C(7)-H(7)	115.1
C(84)-H(84C)	0.9800	C(6)-C(7)-H(7)	115.1
C(85)-C(86)	1.382(8)	C(7)-C(8)-N(2)	123.2(5)
C(86)-C(87)	1.400(7)	C(7)-C(8)-C(9)	127.1(6)
C(86)-H(86)	0.9500	N(2)-C(8)-C(9)	109.6(5)
C(87)-N(8)	1.345(6)	C(11)-C(9)-C(8)	107.1(5)
C(87)-C(88)	1.461(8)	C(11)-C(9)-C(10)	125.6(5)
C(88)-H(88A)	0.9800	C(8)-C(9)-C(10)	127.3(5)
C(88)-H(88B)	0.9800	C(9)-C(10)-H(10A)	109.5
C(88)-H(88C)	0.9800	C(9)-C(10)-H(10B)	109.5
N(1)-Co(1)	1.973(4)	H(10A)-C(10)-H(10B)	109.5
N(2)-Co(1)	1.961(4)	C(9)-C(10)-H(10C)	109.5
N(3)-Co(2)	1.983(5)	H(10A)-C(10)-H(10C)	109.5

H(10B)-C(10)-H(10C)	109.5	H(28A)-C(28)-H(28B)	107.7
C(9)-C(11)-C(12)	106.6(5)	C(28)-C(29)-H(29A)	109.5
C(9)-C(11)-C(14)	126.5(6)	C(28)-C(29)-H(29B)	109.5
C(12)-C(11)-C(14)	126.9(6)	H(29A)-C(29)-H(29B)	109.5
N(2)-C(12)-C(11)	110.8(5)	C(28)-C(29)-H(29C)	109.5
N(2)-C(12)-C(13)	120.9(6)	H(29A)-C(29)-H(29C)	109.5
C(11)-C(12)-C(13)	128.3(6)	H(29B)-C(29)-H(29C)	109.5
C(12)-C(13)-H(13A)	109.5	C(31)-C(30)-C(26)	179.3(8)
C(12)-C(13)-H(13B)	109.5	C(30)-C(31)-C(34)	179.3(8)
H(13A)-C(13)-H(13B)	109.5	C(33)-C(32)-H(32A)	109.5
C(12)-C(13)-H(13C)	109.5	C(33)-C(32)-H(32B)	109.5
H(13A)-C(13)-H(13C)	109.5	H(32A)-C(32)-H(32B)	109.5
H(13B)-C(13)-H(13C)	109.5	C(33)-C(32)-H(32C)	109.5
C(15)-C(14)-C(11)	176.6(8)	H(32A)-C(32)-H(32C)	109.5
C(14)-C(15)-C(16)	177.9(8)	H(32B)-C(32)-H(32C)	109.5
C(17)-C(16)-C(21)	120.2(5)	N(3)-C(33)-C(34)	110.7(6)
C(17)-C(16)-C(15)	119.8(5)	N(3)-C(33)-C(32)	122.9(6)
C(21)-C(16)-C(15)	119.9(6)	C(34)-C(33)-C(32)	126.4(6)
C(18)-C(17)-C(16)	122.5(5)	C(35)-C(34)-C(31)	128.4(6)
C(18)-C(17)-H(17)	118.8	C(35)-C(34)-C(33)	106.6(6)
C(16)-C(17)-H(17)	118.8	C(31)-C(34)-C(33)	125.0(7)
C(17)-C(18)-C(19)	117.6(6)	C(34)-C(35)-C(37)	106.2(6)
C(17)-C(18)-H(18)	121.2	C(34)-C(35)-C(36)	125.3(6)
C(19)-C(18)-H(18)	121.2	C(37)-C(35)-C(36)	128.5(7)
N(9)-C(19)-C(18)	129.2(5)	C(35)-C(36)-H(36A)	109.5
N(9)-C(19)-C(20)	109.7(5)	C(35)-C(36)-H(36B)	109.5
C(18)-C(19)-C(20)	121.1(5)	H(36A)-C(36)-H(36B)	109.5
C(21)-C(20)-C(19)	119.8(5)	C(35)-C(36)-H(36C)	109.5
C(21)-C(20)-C(22)	134.1(6)	H(36A)-C(36)-H(36C)	109.5
C(19)-C(20)-C(22)	106.1(5)	H(36B)-C(36)-H(36C)	109.5
C(20)-C(21)-C(16)	118.8(6)	C(38)-C(37)-N(3)	125.0(5)
C(20)-C(21)-H(21)	120.6	C(38)-C(37)-C(35)	126.4(6)
C(16)-C(21)-H(21)	120.6	N(3)-C(37)-C(35)	108.6(6)
C(27)-C(22)-C(23)	120.2(5)	C(37)-C(38)-C(39)	129.7(6)
C(27)-C(22)-C(20)	133.1(6)	C(37)-C(38)-H(38)	115.1
C(23)-C(22)-C(20)	106.5(5)	C(39)-C(38)-H(38)	115.1
N(9)-C(23)-C(24)	128.7(6)	C(41)-C(39)-C(38)	128.0(6)
N(9)-C(23)-C(22)	110.0(5)	C(41)-C(39)-N(4)	109.4(5)
C(24)-C(23)-C(22)	121.3(6)	C(38)-C(39)-N(4)	122.6(6)
C(23)-C(24)-C(25)	118.3(6)	C(41)-C(40)-H(40A)	109.5
C(23)-C(24)-H(24)	120.9	C(41)-C(40)-H(40B)	109.5
C(25)-C(24)-H(24)	120.9	H(40A)-C(40)-H(40B)	109.5
C(24)-C(25)-C(26)	121.8(6)	C(41)-C(40)-H(40C)	109.5
C(24)-C(25)-H(25)	119.1	H(40A)-C(40)-H(40C)	109.5
C(26)-C(25)-H(25)	119.1	H(40B)-C(40)-H(40C)	109.5
C(25)-C(26)-C(27)	119.6(6)	C(42)-C(41)-C(39)	106.7(6)
C(25)-C(26)-C(30)	120.8(6)	C(42)-C(41)-C(40)	127.0(6)
C(27)-C(26)-C(30)	119.5(6)	C(39)-C(41)-C(40)	126.3(6)
C(22)-C(27)-C(26)	118.8(6)	C(41)-C(42)-C(43)	107.5(5)
C(22)-C(27)-H(27)	120.6	C(41)-C(42)-H(42)	126.3
C(26)-C(27)-H(27)	120.6	C(43)-C(42)-H(42)	126.3
N(9)-C(28)-C(29)	113.7(7)	N(4)-C(43)-C(42)	110.2(5)
N(9)-C(28)-H(28A)	108.8	N(4)-C(43)-C(44)	120.8(5)
C(29)-C(28)-H(28A)	108.8	C(42)-C(43)-C(44)	128.9(6)
N(9)-C(28)-H(28B)	108.8	C(43)-C(44)-H(44A)	109.5
C(29)-C(28)-H(28B)	108.8	C(43)-C(44)-H(44B)	109.5

H(44A)-C(44)-H(44B)	109.5	C(58)-C(59)-C(60)	176.0(7)
C(43)-C(44)-H(44C)	109.5	C(65)-C(60)-C(61)	117.7(6)
H(44A)-C(44)-H(44C)	109.5	C(65)-C(60)-C(59)	123.4(6)
H(44B)-C(44)-H(44C)	109.5	C(61)-C(60)-C(59)	118.9(5)
C(46)-C(45)-H(45A)	109.5	C(62)-C(61)-C(60)	122.5(6)
C(46)-C(45)-H(45B)	109.5	C(62)-C(61)-H(61)	118.7
H(45A)-C(45)-H(45B)	109.5	C(60)-C(61)-H(61)	118.7
C(46)-C(45)-H(45C)	109.5	C(61)-C(62)-C(63)	117.7(6)
H(45A)-C(45)-H(45C)	109.5	C(61)-C(62)-H(62)	121.2
H(45B)-C(45)-H(45C)	109.5	C(63)-C(62)-H(62)	121.2
N(5)-C(46)-C(47)	111.5(5)	N(10)-C(63)-C(64)	110.5(5)
N(5)-C(46)-C(45)	121.9(6)	N(10)-C(63)-C(62)	128.0(6)
C(47)-C(46)-C(45)	126.5(7)	C(64)-C(63)-C(62)	121.4(6)
C(48)-C(47)-C(46)	107.7(7)	C(65)-C(64)-C(63)	120.1(5)
C(48)-C(47)-H(47)	126.2	C(65)-C(64)-C(66)	134.8(5)
C(46)-C(47)-H(47)	126.1	C(63)-C(64)-C(66)	105.1(5)
C(47)-C(48)-C(50)	106.3(6)	C(64)-C(65)-C(60)	120.6(6)
C(47)-C(48)-C(49)	127.5(7)	C(64)-C(65)-H(65)	119.7
C(50)-C(48)-C(49)	126.2(7)	C(60)-C(65)-H(65)	119.7
C(48)-C(49)-H(49A)	109.5	C(67)-C(66)-C(71)	119.8(5)
C(48)-C(49)-H(49B)	109.5	C(67)-C(66)-C(64)	107.8(5)
H(49A)-C(49)-H(49B)	109.5	C(71)-C(66)-C(64)	132.4(6)
C(48)-C(49)-H(49C)	109.5	C(68)-C(67)-C(66)	121.1(5)
H(49A)-C(49)-H(49C)	109.5	C(68)-C(67)-N(10)	130.1(6)
H(49B)-C(49)-H(49C)	109.5	C(66)-C(67)-N(10)	108.7(5)
C(51)-C(50)-N(5)	122.6(6)	C(69)-C(68)-C(67)	120.0(6)
C(51)-C(50)-C(48)	128.1(6)	C(69)-C(68)-H(68)	120.0
N(5)-C(50)-C(48)	109.4(6)	C(67)-C(68)-H(68)	120.0
C(50)-C(51)-C(52)	131.7(6)	C(68)-C(69)-C(70)	120.1(6)
C(50)-C(51)-H(51)	114.1	C(68)-C(69)-H(69)	119.9
C(52)-C(51)-H(51)	114.1	C(70)-C(69)-H(69)	119.9
C(51)-C(52)-C(54)	128.0(7)	C(71)-C(70)-C(69)	120.7(5)
C(51)-C(52)-N(6)	122.4(6)	C(71)-C(70)-C(74)	120.2(6)
C(54)-C(52)-N(6)	109.6(6)	C(69)-C(70)-C(74)	119.2(5)
C(54)-C(53)-H(53A)	109.5	C(70)-C(71)-C(66)	118.2(6)
C(54)-C(53)-H(53B)	109.5	C(70)-C(71)-H(71)	120.9
H(53A)-C(53)-H(53B)	109.5	C(66)-C(71)-H(71)	120.9
C(54)-C(53)-H(53C)	109.5	N(10)-C(72)-C(73)	113.0(5)
H(53A)-C(53)-H(53C)	109.5	N(10)-C(72)-H(72A)	109.0
H(53B)-C(53)-H(53C)	109.5	C(73)-C(72)-H(72A)	109.0
C(52)-C(54)-C(55)	104.9(5)	N(10)-C(72)-H(72B)	109.0
C(52)-C(54)-C(53)	130.9(7)	C(73)-C(72)-H(72B)	109.0
C(55)-C(54)-C(53)	124.1(6)	H(72A)-C(72)-H(72B)	107.8
C(56)-C(55)-C(58)	123.0(7)	C(72)-C(73)-H(73A)	109.5
C(56)-C(55)-C(54)	108.3(6)	C(72)-C(73)-H(73B)	109.5
C(58)-C(55)-C(54)	128.6(6)	H(73A)-C(73)-H(73B)	109.5
N(6)-C(56)-C(55)	109.9(6)	C(72)-C(73)-H(73C)	109.5
N(6)-C(56)-C(57)	120.8(5)	H(73A)-C(73)-H(73C)	109.5
C(55)-C(56)-C(57)	129.2(7)	H(73B)-C(73)-H(73C)	109.5
C(56)-C(57)-H(57A)	109.5	C(75)-C(74)-C(70)	177.6(7)
C(56)-C(57)-H(57B)	109.5	C(74)-C(75)-C(78)	178.1(7)
H(57A)-C(57)-H(57B)	109.5	C(77)-C(76)-H(76A)	109.5
C(56)-C(57)-H(57C)	109.5	C(77)-C(76)-H(76B)	109.5
H(57A)-C(57)-H(57C)	109.5	H(76A)-C(76)-H(76B)	109.5
H(57B)-C(57)-H(57C)	109.5	C(77)-C(76)-H(76C)	109.5
C(59)-C(58)-C(55)	179.0(8)	H(76A)-C(76)-H(76C)	109.5

H(76B)-C(76)-H(76C)	109.5	C(23)-N(9)-C(28)	126.5(5)
N(7)-C(77)-C(78)	111.6(5)	C(19)-N(9)-C(28)	125.8(5)
N(7)-C(77)-C(76)	122.2(6)	C(33)-N(3)-C(37)	107.8(5)
C(78)-C(77)-C(76)	126.2(5)	C(33)-N(3)-Co(2)	128.4(5)
C(79)-C(78)-C(75)	127.6(6)	C(37)-N(3)-Co(2)	123.1(4)
C(79)-C(78)-C(77)	106.0(5)	C(43)-N(4)-C(39)	106.2(5)
C(75)-C(78)-C(77)	126.4(6)	C(43)-N(4)-Co(2)	129.6(4)
C(78)-C(79)-C(81)	106.1(5)	C(39)-N(4)-Co(2)	123.8(4)
C(78)-C(79)-C(80)	126.6(6)	C(46)-N(5)-C(50)	105.1(5)
C(81)-C(79)-C(80)	127.3(5)	C(46)-N(5)-Co(1)	130.2(4)
C(79)-C(80)-H(80A)	109.5	C(50)-N(5)-Co(1)	124.7(4)
C(79)-C(80)-H(80B)	109.5	C(56)-N(6)-C(52)	107.3(5)
H(80A)-C(80)-H(80B)	109.5	C(56)-N(6)-Co(1)	129.5(4)
C(79)-C(80)-H(80C)	109.5	C(52)-N(6)-Co(1)	122.9(4)
H(80A)-C(80)-H(80C)	109.5	C(63)-N(10)-C(67)	107.7(5)
H(80B)-C(80)-H(80C)	109.5	C(63)-N(10)-C(72)	125.9(5)
N(7)-C(81)-C(82)	123.4(5)	C(67)-N(10)-C(72)	126.0(5)
N(7)-C(81)-C(79)	109.9(5)	C(77)-N(7)-C(81)	106.4(5)
C(82)-C(81)-C(79)	126.7(6)	C(77)-N(7)-Co(2)	128.7(4)
C(83)-C(82)-C(81)	129.1(6)	C(81)-N(7)-Co(2)	124.8(3)
C(83)-C(82)-H(82)	115.4	C(87)-N(8)-C(83)	105.7(4)
C(81)-C(82)-H(82)	115.4	C(87)-N(8)-Co(2)	130.9(4)
C(82)-C(83)-N(8)	123.9(5)	C(83)-N(8)-Co(2)	123.3(4)
C(82)-C(83)-C(85)	126.7(6)	N(2)-Co(1)-N(5)	120.5(2)
N(8)-C(83)-C(85)	109.5(5)	N(2)-Co(1)-N(1)	95.73(19)
C(85)-C(84)-H(84A)	109.5	N(5)-Co(1)-N(1)	115.82(19)
C(85)-C(84)-H(84B)	109.5	N(2)-Co(1)-N(6)	110.11(19)
H(84A)-C(84)-H(84B)	109.5	N(5)-Co(1)-N(6)	95.6(2)
C(85)-C(84)-H(84C)	109.5	N(1)-Co(1)-N(6)	120.83(19)
H(84A)-C(84)-H(84C)	109.5	N(7)-Co(2)-N(8)	95.48(18)
H(84B)-C(84)-H(84C)	109.5	N(7)-Co(2)-N(3)	108.37(18)
C(86)-C(85)-C(83)	105.8(5)	N(8)-Co(2)-N(3)	122.50(19)
C(86)-C(85)-C(84)	128.1(5)	N(7)-Co(2)-N(4)	119.60(18)
C(83)-C(85)-C(84)	126.1(6)	N(8)-Co(2)-N(4)	117.35(18)
C(85)-C(86)-C(87)	107.8(5)	N(3)-Co(2)-N(4)	95.1(2)
C(85)-C(86)-H(86)	126.1	Cl(3)-C(89)-Cl(2)	113.6(4)
C(87)-C(86)-H(86)	126.1	Cl(3)-C(89)-Cl(1)	112.4(4)
N(8)-C(87)-C(86)	111.2(5)	Cl(2)-C(89)-Cl(1)	113.1(4)
N(8)-C(87)-C(88)	120.5(5)	Cl(3)-C(89)-H(89)	105.6
C(86)-C(87)-C(88)	128.3(5)	Cl(2)-C(89)-H(89)	105.6
C(87)-C(88)-H(88A)	109.5	Cl(1)-C(89)-H(89)	105.6
C(87)-C(88)-H(88B)	109.5	Cl(4A)-C(90A)-Cl(5A)	112.2(6)
H(88A)-C(88)-H(88B)	109.5	Cl(4A)-C(90A)-Cl(6A)	114.6(6)
C(87)-C(88)-H(88C)	109.5	Cl(5A)-C(90A)-Cl(6A)	112.8(6)
H(88A)-C(88)-H(88C)	109.5	Cl(4A)-C(90A)-H(90A)	105.4
H(88B)-C(88)-H(88C)	109.5	Cl(5A)-C(90A)-H(90A)	105.4
C(2)-N(1)-C(6)	106.1(5)	Cl(6A)-C(90A)-H(90A)	105.4
C(2)-N(1)-Co(1)	131.2(4)	Cl(6B)-C(90B)-Cl(4B)	116.1(7)
C(6)-N(1)-Co(1)	122.7(4)	Cl(6B)-C(90B)-Cl(5B)	114.1(7)
C(12)-N(2)-C(8)	105.9(5)	Cl(4B)-C(90B)-Cl(5B)	112.8(7)
C(12)-N(2)-Co(1)	129.5(4)	Cl(6B)-C(90B)-H(90B)	104.0
C(8)-N(2)-Co(1)	124.3(4)	Cl(4B)-C(90B)-H(90B)	104.0
C(23)-N(9)-C(19)	107.7(5)	Cl(5B)-C(90B)-H(90B)	104.0

Table S4. Bond lengths [Å] and angles [°] for **6**.

C(1)-C(2)	1.486(5)	N(2)-Zn(1)	1.977(2)
C(1)-H(1A)	0.9800	Zn(1)-N(2)#2	1.977(2)
C(1)-H(1B)	0.9800	Zn(1)-N(1)#2	1.991(2)
C(1)-H(1C)	0.9800	C(7B)-H(7B1)	0.9800
C(2)-N(1)	1.333(3)	C(7B)-H(7B2)	0.9800
C(2)-C(3)	1.438(4)	C(7B)-H(7B3)	0.9800
C(3)-C(4)	1.375(4)	C(8B)-H(8B1)	0.9800
C(3)-C(6)	1.535(4)	C(8B)-H(8B2)	0.9800
C(4)-C(10)	1.437(4)	C(8B)-H(8B3)	0.9800
C(4)-C(5)	1.507(4)	C(9B)-H(9B1)	0.9800
C(5)-H(5A)	0.9800	C(9B)-H(9B2)	0.9800
C(5)-H(5B)	0.9800	C(9B)-H(9B3)	0.9800
C(5)-H(5C)	0.9800	Cl(1)-C(20)	1.806(15)
C(5)-H(5D)	0.9800	Cl(1)-C(20)#3	1.806(15)
C(5)-H(5E)	0.9800	Cl(1)-C(20)#4	1.806(15)
C(5)-H(5F)	0.9800	Cl(2)-C(20)	1.469(16)
C(6)-C(7B)	1.499(7)	Cl(2)-C(20)#3	1.469(16)
C(6)-C(8)	1.510(6)	Cl(2)-C(20)#4	1.469(16)
C(6)-C(8B)	1.527(8)	C(20)-H(20A)	0.9900
C(6)-C(9)	1.531(6)	C(20)-H(20B)	0.9900
C(6)-C(9B)	1.544(7)		
C(6)-C(7)	1.554(6)	C(2)-C(1)-H(1A)	109.5
C(7)-H(7A)	0.9800	C(2)-C(1)-H(1B)	109.5
C(7)-H(7B)	0.9800	H(1A)-C(1)-H(1B)	109.5
C(7)-H(7C)	0.9800	C(2)-C(1)-H(1C)	109.5
C(8)-H(8A)	0.9800	H(1A)-C(1)-H(1C)	109.5
C(8)-H(8B)	0.9800	H(1B)-C(1)-H(1C)	109.5
C(8)-H(8C)	0.9800	N(1)-C(2)-C(3)	111.4(3)
C(9)-H(9A)	0.9800	N(1)-C(2)-C(1)	117.7(3)
C(9)-H(9B)	0.9800	C(3)-C(2)-C(1)	130.9(3)
C(9)-H(9C)	0.9800	C(4)-C(3)-C(2)	105.7(3)
C(10)-C(11)	1.378(4)	C(4)-C(3)-C(6)	127.4(3)
C(10)-N(1)	1.394(4)	C(2)-C(3)-C(6)	126.9(3)
C(11)-C(12)	1.394(4)	C(3)-C(4)-C(10)	107.3(3)
C(11)-H(11)	0.9500	C(3)-C(4)-C(5)	131.3(3)
C(12)-N(2)	1.391(4)	C(10)-C(4)-C(5)	121.3(3)
C(12)-C(14)	1.420(4)	C(4)-C(5)-H(5A)	109.5
C(13)-C(14)	1.510(4)	C(4)-C(5)-H(5B)	109.5
C(13)-H(13A)	0.9800	H(5A)-C(5)-H(5B)	109.5
C(13)-H(13B)	0.9800	C(4)-C(5)-H(5C)	109.5
C(13)-H(13C)	0.9800	H(5A)-C(5)-H(5C)	109.5
C(14)-C(15)	1.383(4)	H(5B)-C(5)-H(5C)	109.5
C(15)-C(16)	1.415(4)	C(4)-C(5)-H(5D)	109.5
C(15)-C(18)	1.425(4)	H(5A)-C(5)-H(5D)	141.1
C(16)-N(2)	1.337(3)	H(5B)-C(5)-H(5D)	56.3
C(16)-C(17)	1.487(4)	H(5C)-C(5)-H(5D)	56.3
C(17)-H(17A)	0.9800	C(4)-C(5)-H(5E)	109.5
C(17)-H(17B)	0.9800	H(5A)-C(5)-H(5E)	56.3
C(17)-H(17C)	0.9800	H(5B)-C(5)-H(5E)	141.1
C(17)-H(17D)	0.9800	H(5C)-C(5)-H(5E)	56.3
C(17)-H(17E)	0.9800	H(5D)-C(5)-H(5E)	109.5
C(17)-H(17F)	0.9800	C(4)-C(5)-H(5F)	109.5
C(18)-C(19)	1.198(4)	H(5A)-C(5)-H(5F)	56.3
C(19)-C(19)#1	1.374(6)	H(5B)-C(5)-H(5F)	56.3
N(1)-Zn(1)	1.991(2)	H(5C)-C(5)-H(5F)	141.1

H(5D)-C(5)-H(5F)	109.5	C(15)-C(14)-C(12)	106.7(3)
H(5E)-C(5)-H(5F)	109.5	C(15)-C(14)-C(13)	126.7(3)
C(7B)-C(6)-C(8)	135.2(7)	C(12)-C(14)-C(13)	126.6(3)
C(7B)-C(6)-C(8B)	112.7(9)	C(14)-C(15)-C(16)	106.8(2)
C(8)-C(6)-C(8B)	42.6(8)	C(14)-C(15)-C(18)	128.1(3)
C(7B)-C(6)-C(9)	64.5(7)	C(16)-C(15)-C(18)	125.1(3)
C(8)-C(6)-C(9)	112.9(7)	N(2)-C(16)-C(15)	110.4(3)
C(8B)-C(6)-C(9)	145.7(7)	N(2)-C(16)-C(17)	122.5(3)
C(7B)-C(6)-C(3)	108.4(5)	C(15)-C(16)-C(17)	127.1(3)
C(8)-C(6)-C(3)	113.3(5)	C(16)-C(17)-H(17A)	109.5
C(8B)-C(6)-C(3)	102.8(6)	C(16)-C(17)-H(17B)	109.5
C(9)-C(6)-C(3)	110.5(4)	H(17A)-C(17)-H(17B)	109.5
C(7B)-C(6)-C(9B)	109.5(7)	C(16)-C(17)-H(17C)	109.5
C(8)-C(6)-C(9B)	69.5(7)	H(17A)-C(17)-H(17C)	109.5
C(8B)-C(6)-C(9B)	111.6(9)	H(17B)-C(17)-H(17C)	109.5
C(9)-C(6)-C(9B)	48.2(7)	C(16)-C(17)-H(17D)	109.5
C(3)-C(6)-C(9B)	111.6(5)	H(17A)-C(17)-H(17D)	141.1
C(7B)-C(6)-C(7)	42.8(5)	H(17B)-C(17)-H(17D)	56.3
C(8)-C(6)-C(7)	102.8(6)	H(17C)-C(17)-H(17D)	56.3
C(8B)-C(6)-C(7)	70.2(8)	C(16)-C(17)-H(17E)	109.5
C(9)-C(6)-C(7)	102.1(7)	H(17A)-C(17)-H(17E)	56.3
C(3)-C(6)-C(7)	114.4(4)	H(17B)-C(17)-H(17E)	141.1
C(9B)-C(6)-C(7)	132.1(6)	H(17C)-C(17)-H(17E)	56.3
C(6)-C(7)-H(7A)	109.5	H(17D)-C(17)-H(17E)	109.5
C(6)-C(7)-H(7B)	109.5	C(16)-C(17)-H(17F)	109.5
H(7A)-C(7)-H(7B)	109.5	H(17A)-C(17)-H(17F)	56.3
C(6)-C(7)-H(7C)	109.5	H(17B)-C(17)-H(17F)	56.3
H(7A)-C(7)-H(7C)	109.5	H(17C)-C(17)-H(17F)	141.1
H(7B)-C(7)-H(7C)	109.5	H(17D)-C(17)-H(17F)	109.5
C(6)-C(8)-H(8A)	109.5	H(17E)-C(17)-H(17F)	109.5
C(6)-C(8)-H(8B)	109.5	C(19)-C(18)-C(15)	179.0(4)
H(8A)-C(8)-H(8B)	109.5	C(18)-C(19)-C(19)#1	179.1(4)
C(6)-C(8)-H(8C)	109.5	C(2)-N(1)-C(10)	107.0(2)
H(8A)-C(8)-H(8C)	109.5	C(2)-N(1)-Zn(1)	130.0(2)
H(8B)-C(8)-H(8C)	109.5	C(10)-N(1)-Zn(1)	122.83(18)
C(6)-C(9)-H(9A)	109.5	C(16)-N(2)-C(12)	107.5(2)
C(6)-C(9)-H(9B)	109.5	C(16)-N(2)-Zn(1)	130.10(19)
H(9A)-C(9)-H(9B)	109.5	C(12)-N(2)-Zn(1)	122.26(17)
C(6)-C(9)-H(9C)	109.5	N(2)#2-Zn(1)-N(2)	111.43(12)
H(9A)-C(9)-H(9C)	109.5	N(2)#2-Zn(1)-N(1)#2	96.32(9)
H(9B)-C(9)-H(9C)	109.5	N(2)-Zn(1)-N(1)#2	120.86(9)
C(11)-C(10)-N(1)	123.4(3)	N(2)#2-Zn(1)-N(1)	120.86(9)
C(11)-C(10)-C(4)	128.0(3)	N(2)-Zn(1)-N(1)	96.31(9)
N(1)-C(10)-C(4)	108.5(3)	N(1)#2-Zn(1)-N(1)	112.87(13)
C(10)-C(11)-C(12)	130.3(3)	C(6)-C(7B)-H(7B1)	109.5
C(10)-C(11)-H(11)	114.8	C(6)-C(7B)-H(7B2)	109.5
C(12)-C(11)-H(11)	114.8	H(7B1)-C(7B)-H(7B2)	109.5
N(2)-C(12)-C(11)	124.5(2)	C(6)-C(7B)-H(7B3)	109.5
N(2)-C(12)-C(14)	108.6(2)	H(7B1)-C(7B)-H(7B3)	109.5
C(11)-C(12)-C(14)	126.8(3)	H(7B2)-C(7B)-H(7B3)	109.5
C(14)-C(13)-H(13A)	109.5	C(6)-C(8B)-H(8B1)	109.5
C(14)-C(13)-H(13B)	109.5	C(6)-C(8B)-H(8B2)	109.5
H(13A)-C(13)-H(13B)	109.5	H(8B1)-C(8B)-H(8B2)	109.5
C(14)-C(13)-H(13C)	109.5	C(6)-C(8B)-H(8B3)	109.5
H(13A)-C(13)-H(13C)	109.5	H(8B1)-C(8B)-H(8B3)	109.5
H(13B)-C(13)-H(13C)	109.5	H(8B2)-C(8B)-H(8B3)	109.5

C(6)-C(9B)-H(9B1)	109.5	C(20)-Cl(2)-C(20)#3	65.3(12)
C(6)-C(9B)-H(9B2)	109.5	C(20)-Cl(2)-C(20)#4	65.3(12)
H(9B1)-C(9B)-H(9B2)	109.5	C(20)#3-Cl(2)-C(20)#4	65.3(12)
C(6)-C(9B)-H(9B3)	109.5	Cl(2)-C(20)-Cl(1)	111.0(13)
H(9B1)-C(9B)-H(9B3)	109.5	Cl(2)-C(20)-H(20A)	109.4
H(9B2)-C(9B)-H(9B3)	109.5	Cl(1)-C(20)-H(20A)	109.4
C(20)-Cl(1)-C(20)#3	52.1(11)	Cl(2)-C(20)-H(20B)	109.4
C(20)-Cl(1)-C(20)#4	52.1(11)	Cl(1)-C(20)-H(20B)	109.4
C(20)#3-Cl(1)-C(20)#4	52.1(11)	H(20A)-C(20)-H(20B)	108.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+4/3,-x+y+2/3,-z+1/6 #2 y-2/3,x+2/3,-z+1/6
#3 -x+y,-x+1,z #4 -y+1,x-y+1,z

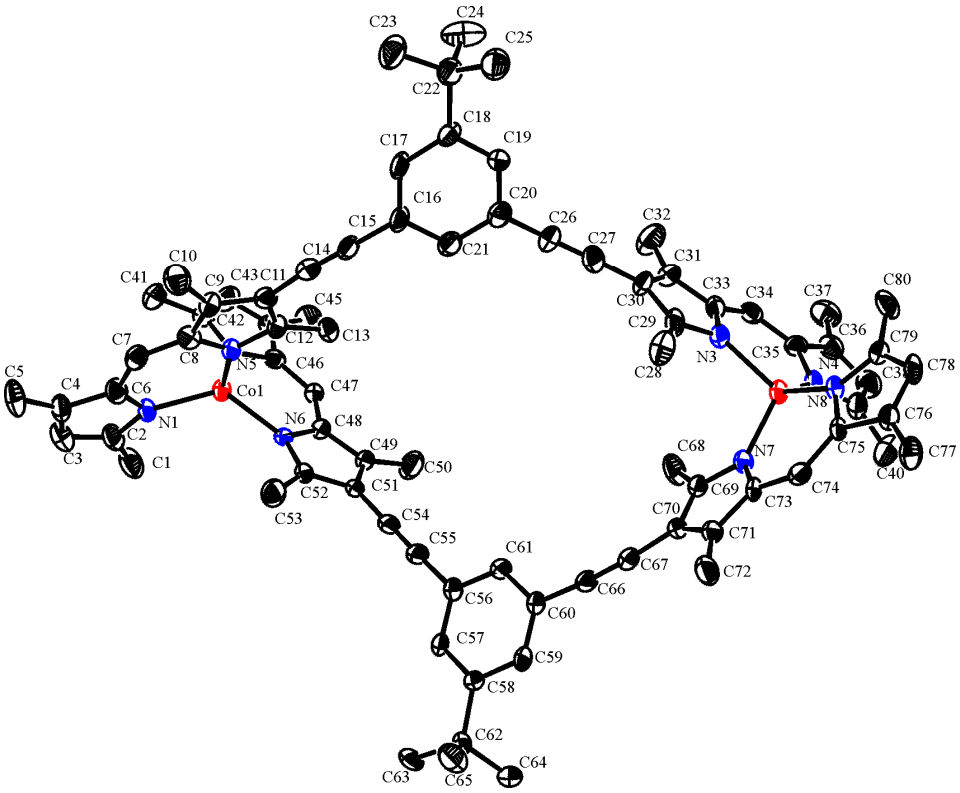

Fig. S9 ORTEP structure of **3** with numbering.

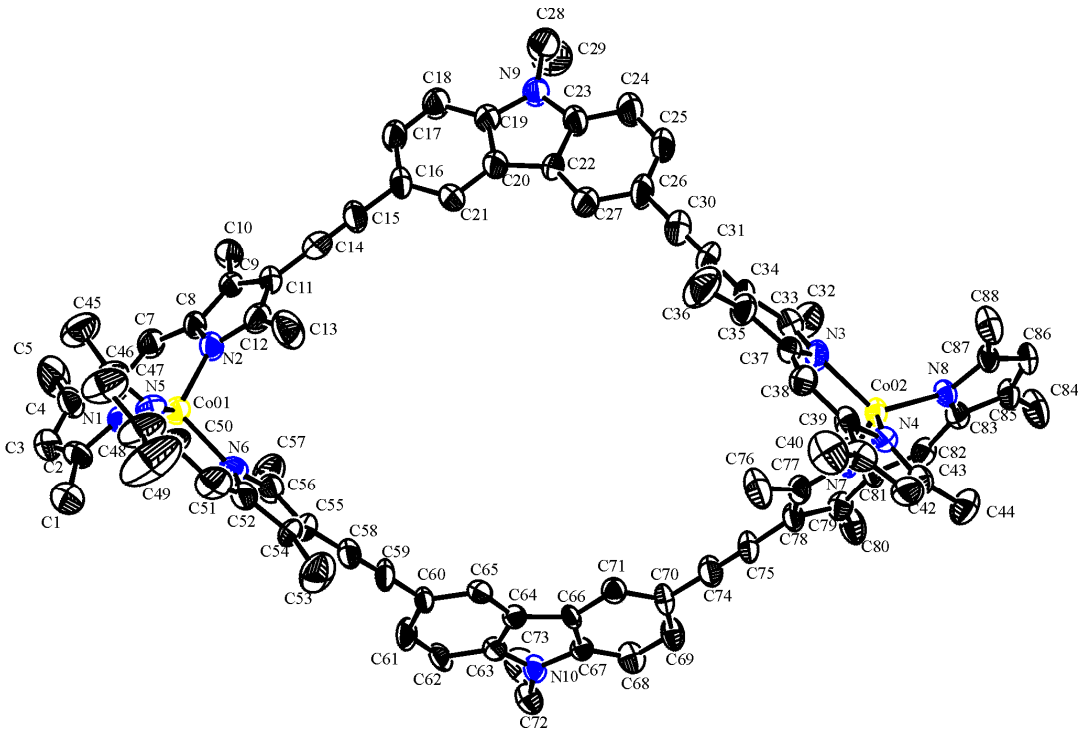

Fig. S10 ORTEP structure of **4** with numbering.

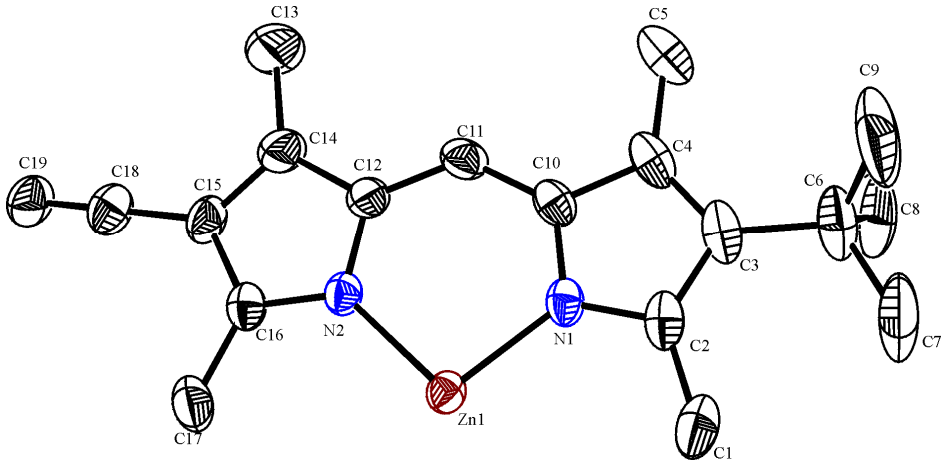

Fig. S11 ORTEP structure for a fragment of **6** with numbering.

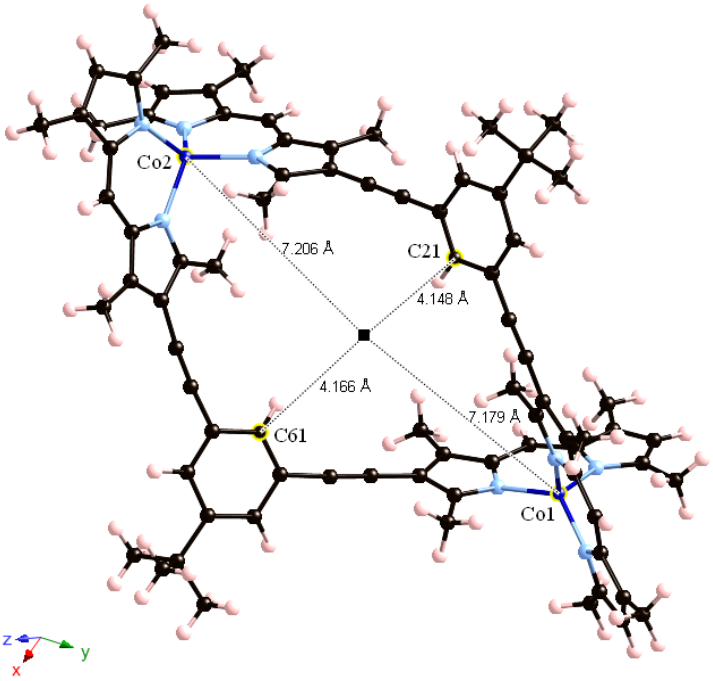

Fig. S12 Distances between the center and atoms of **3**.

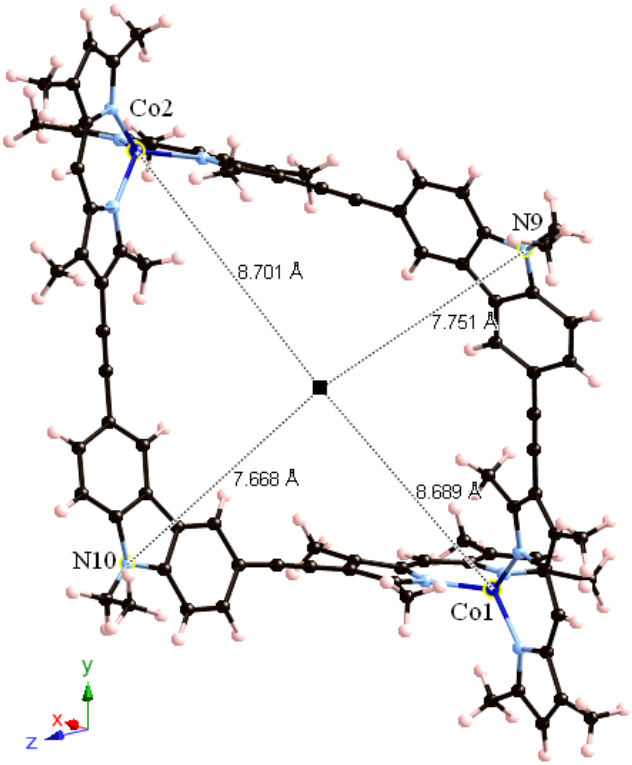

Fig. S13 Distances between the center and atoms of **4**.

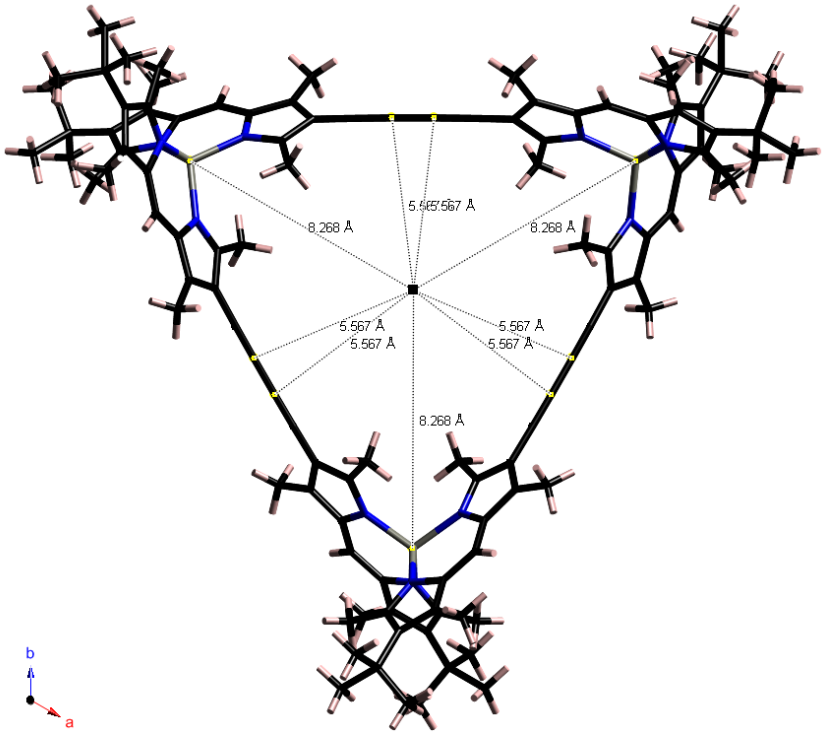

Fig. S14 Distances between the center and atoms of **6**.

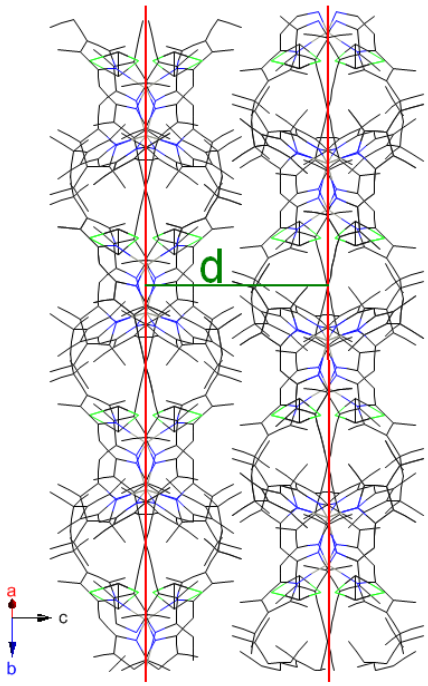

Fig. S15 Side view of the packing diagram of **6**; distance between the mean planes of each layer: d = 10.05 Å.

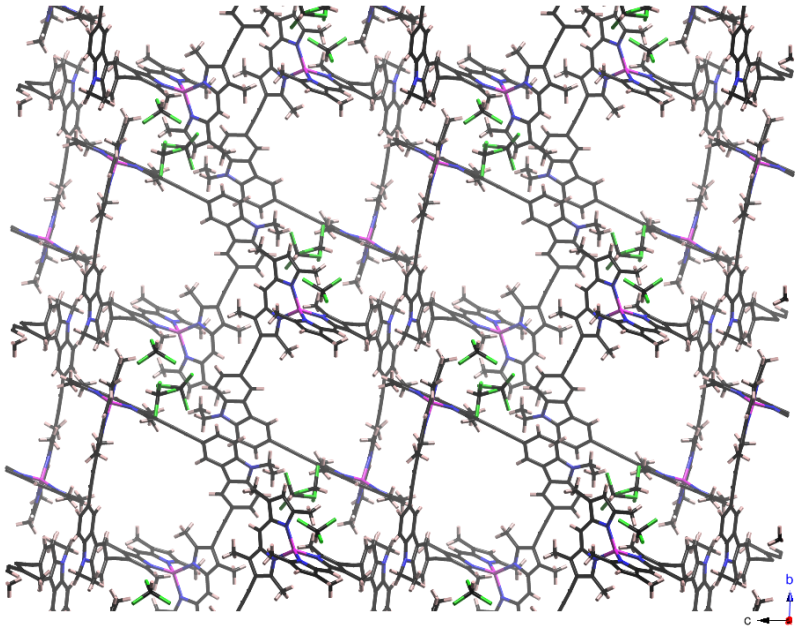

Fig. S16 Packing diagram of compound **4** including solvent molecules.

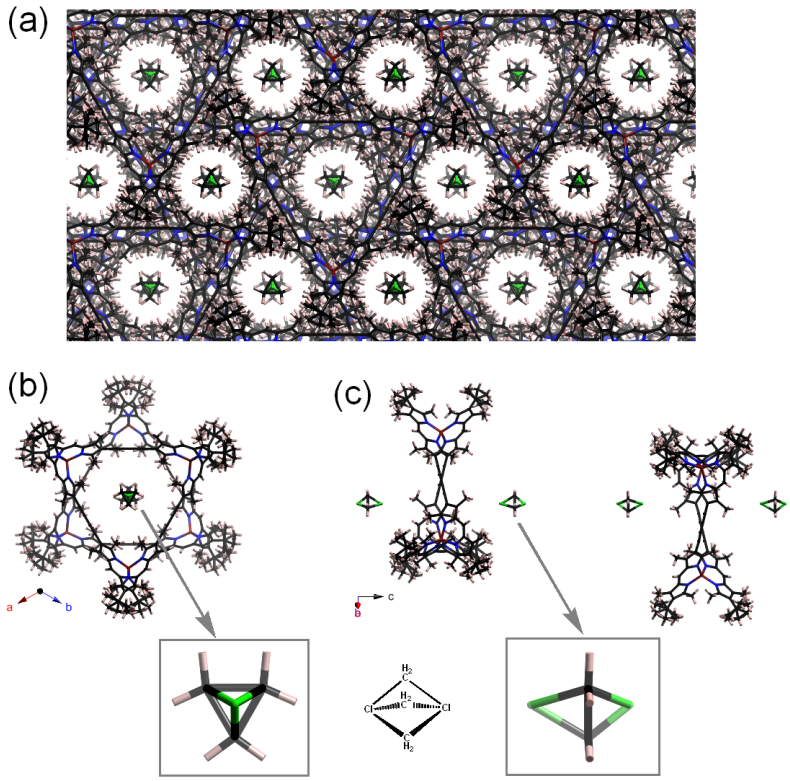

Fig. S17 (a) Packing diagram of compound **6** including solvent molecules; (b) top view and (c) side view for a portion of the packing diagram.