Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Facile Routes to Abnormal-NHC Cobalt(II) Complexes

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Experimental

Materials and Methods: All syntheses and manipulations were performed under an inert gas (N_2 or Ar) atmosphere using Schlenk techniques or a glove box. Solvents THF, C_6H_6, Et_2O, *n*-hexane (Na-K/ benzophenone), CH_2Cl_2 (CaH_2) were dried by refluxing over an appropriate drying agent, distilled under a N_2 atmosphere, and stored over 3Å molecular sieves. ^1H, ^{11}B, and ^{13}C NMR spectra were recorded using a Bruker Avance III 300, a Bruker Avance III 500 or a Bruker Avance DRX 500 spectrometer. Melting points were measured with a Büchi B-545 melting point apparatus. Toluene solution of $Na[HBEt_3]$ (Sigma Aldrich) was used as received. (IPr^{Ph})I (**1**)[1] and $Co\{N(SiMe_3)_2\}_2$[2] were prepared by employing literature methods.

Synthesis of (aIPr^{Ph})$_2$CoI$_2$ (2): To a Schleck flask containing (IPr^{Ph})I (**1**) (3.90 g, 6.58 mmol) and $Co\{N(SiMe_3)_2\}_2$ (1.25 g, 3.29 mmol) was added 150 mL of toluene and the resulting slurry was stirred at 110 °C for 5 h. The dark green solution was filtered while hot and the filtrate was stored at 4 °C for one day. Turquoise crystals were extracted by filtration and dried under vacuum. The mother liquor was concentrated to 40 mL and kept at –30 °C for one week to give a second crop of compound **2**. Combined yield found: 3.26 g, 79%. Mp. 244 – 246 °C. Elemental analysis (%) calcd for $C_{66}H_{80}N_4CoI_2$ (1242): C 63.82, H 6.49, N 4.51; found: C 63.52, H 6.32, N 4.13. ^1H NMR (500 MHz, C_6D_6, 25 °C): δ 26.51 (s, 1H); 9.70 (s, 4H); 9.35 (s, 2H); 9.28 (s, 2H); 4.96 (s, 1H); 4.84 (s, 2H); 3.03 (s, 6H); 2.30 (s, 6H); 2.24 (s, 6H); 1.41 (s, 4H); 0.91 (m, 2H); –3.35 (s, 6H) ppm.

Synthesis of (aIPr^{Ph})BEt$_3$ (3): To a 100 mL toluene suspension of (IPr^{Ph})I (**1**) (3.0 g, 5.06 mmol) was added a 1.0 M toluene solution of $Na\{HBEt_3\}$ (5.1 mL. 5.1 mmol) at room temperature. The resulting dark slurry was stirred under reflux for 4h and then brought to room temperature. Filtration through a plug of Celite yielded a yellow solution, which was dried under vacuum to afford a light yellow sticky solid. The residue was dissolved in a minimum amount (ca. 10 mL) of Et_2O and combined with 10 mL of *n*-hexane and stored at –30 °C for one week. Colorless crystals of compound **3** were isolated and dried under vacuum. The mother liquor was combined with 10 mL of *n*-hexane and kept at –30 °C for the second crop. Combined yield: 2.13 g, 75%. Mp. 253 – 256 °C (dec.). Elemental analysis (%) calcd for $C_{39}H_{55}N_2B$ (562): C, 83.25; H, 9.85; N, 4.98; found: C, 82.71; H, 9.42; N, 4.61. ^1H NMR (500 MHz, C_6D_6, 25 °C): δ 7.23 (t, J = 7.8 Hz, 1H, *p*-C_6H_3); 7.16 (s, 1H, *H*CCN, overlaps with the residual C_6H_6 peak); 7.06 (m, 3H, *p*-C_6H_3, *m*-C_6H_3); 6.90 (d, J = 7.3 Hz, 2H, *m*-C_6H_3); 6.81 (d, 2H, C_6H_5); 6.52 (m, 3H, C_6H_5); 3.08 (sept, J = 6.8 Hz, 2H, *H*CMe_2); 2.71 (sept, J = 6.8 Hz, 2H, *H*CMe_2); 1.48 (d, J = 6.7 Hz, 6H, HC*Me*$_2$); 1.37 (t, J = 7.6 Hz, 9H, H_2C*Me*); 1.10 (d, J = 6.5 Hz, 6H, *H*$_2$CMe_2); 0.85 (q, J = 7.6 Hz, 6H, H_2C*Me*$_2$); 0.82 (d, J = 7.6 Hz, 6H, HC*Me*$_2$); 0.72 (d, J = 6.9 Hz, 6H, HC*Me*$_2$) ppm. ^1H NMR (300 MHz, CD_2Cl_2, 25 °C): δ 7.49 (tt, J = 8.5, 4.3 Hz, 2H, *p*-C_6H_3); 7.29 (d, J = 7.8 Hz, 2H, *p*-C_6H_3); 7.23 (d, J = 7.8 Hz, 2H, *p*-C_6H_3); 7.22 – 7.12 (m, 1H, C_6H_5); 7.03 (d, J = 8.3 Hz, 2H C_6H_5); 6.98 (s, 1H, *H*CCN); 6.76 (d, J = 7.5 Hz, 2H, C_6H_5); 2.79 (sept, 2H, *H*CMe_2); 2.62 (sept, 2H, *H*CMe_2); 1.33 (d, J = 6.7 Hz, 6H, HC*Me*$_2$); 1.24 (d, J = 6.8 Hz, 6H, HC*Me*$_2$);

0.97 (d, J = 6.9 Hz, 6H, HCMe_2); 0.70 (d, J = 6.8 Hz, 6H, HCMe_2); 0.64 (t, J = 7.7 Hz, 9H, H_2CMe); 0.06 (q, J = 7.6 Hz, 6H, H_2CMe) ppm. ^{13}C NMR (75 MHz, CD_2Cl_2, 25 °C): δ 146.00, 145.48, 135.41, 133.30, 131.28, 130.53, 129.79, 128.69, 127.74, 125.34, 124.82, 124.17, 29.37, 28.60, 25.63, 24.65, 23.89, 22.77, 16.30, 11.29 ppm. ^{11}B NMR (96 MHz, CD_2Cl_2, 25 °C): δ –14.36 ppm.

Synthesis of (aIPr^{Ph})Co{N(SiMe$_3$)$_2$}$_2$ (4): To a Schlenk flask containing **3** (0.78 g, 1.38 mmol) and Co{N(SiMe$_3$)$_2$}$_2$ (0.53 g, 1.39 mmol) was added 20 mL of toluene and the resulting solution was stirred at 110 °C for 4 h. The volatiles were removed under vacuum to afford a dark residue, which was extracted 10 mL of toluene and stored at –30 °C for one week to obtain green crystals of compound **4**. Yield: 0.44 g (37%). Mp. 178 – 181 °C (dec.). ^{1}H NMR (500 MHz, C_6D_6, 25 °C): δ 44.83 (s, 2H), 35.60 (br, 1H), 32.08 (s, 1H), 24.18 (s, 2H), 18.27 (s, 2H), 18.11 (s, 1H), 17.16 (s, 7H); 14.17 (s, 2H); 11.53 (s, 1H), 10.30 (s, 6H), 0.09 (s, 2H), –5.23 (s, 6H), –19.08 (s, 36H); –26.10 (s, 6H).

NMR Spectra

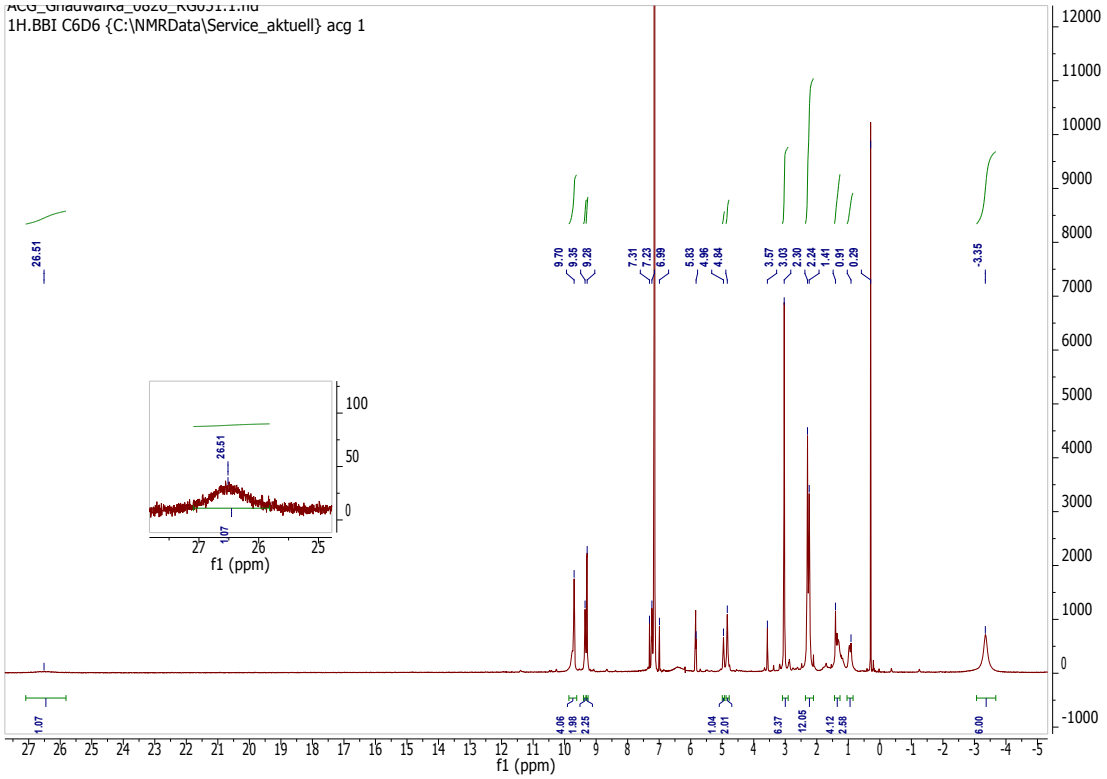


Figure S1. ^{1}H NMR spectrum of **2** in C_6D_6.

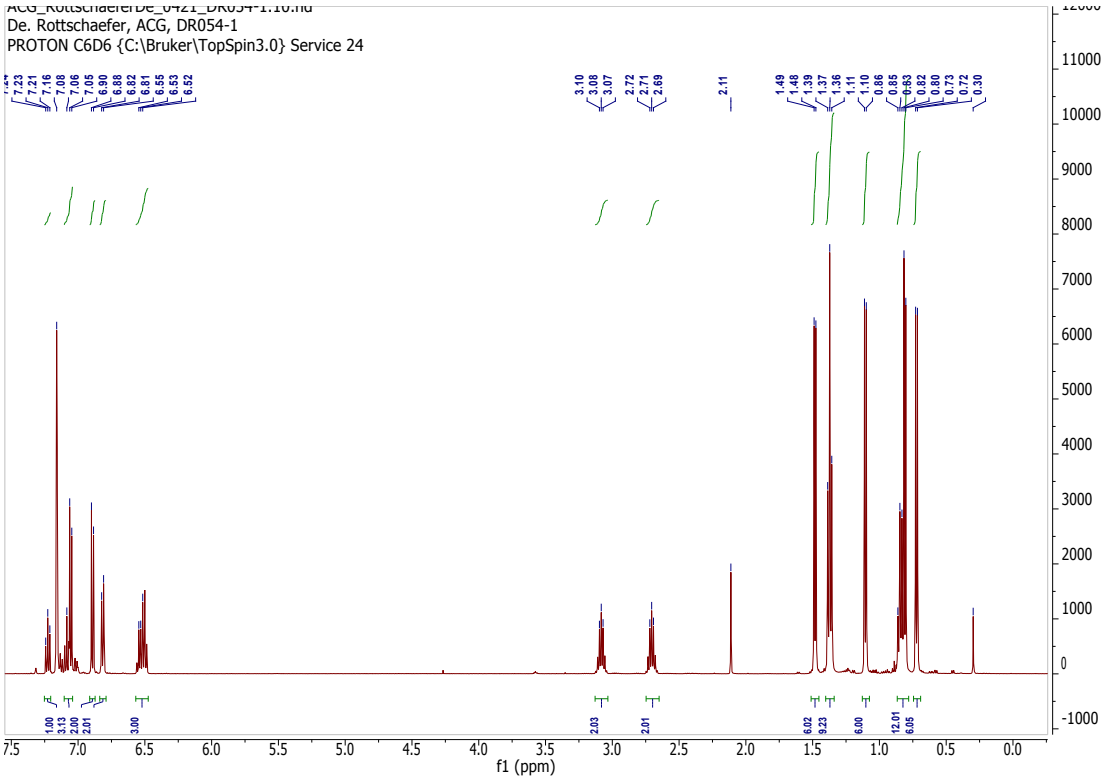


Figure S2. ^{1}H NMR spectrum of **3** in C_6D_6.

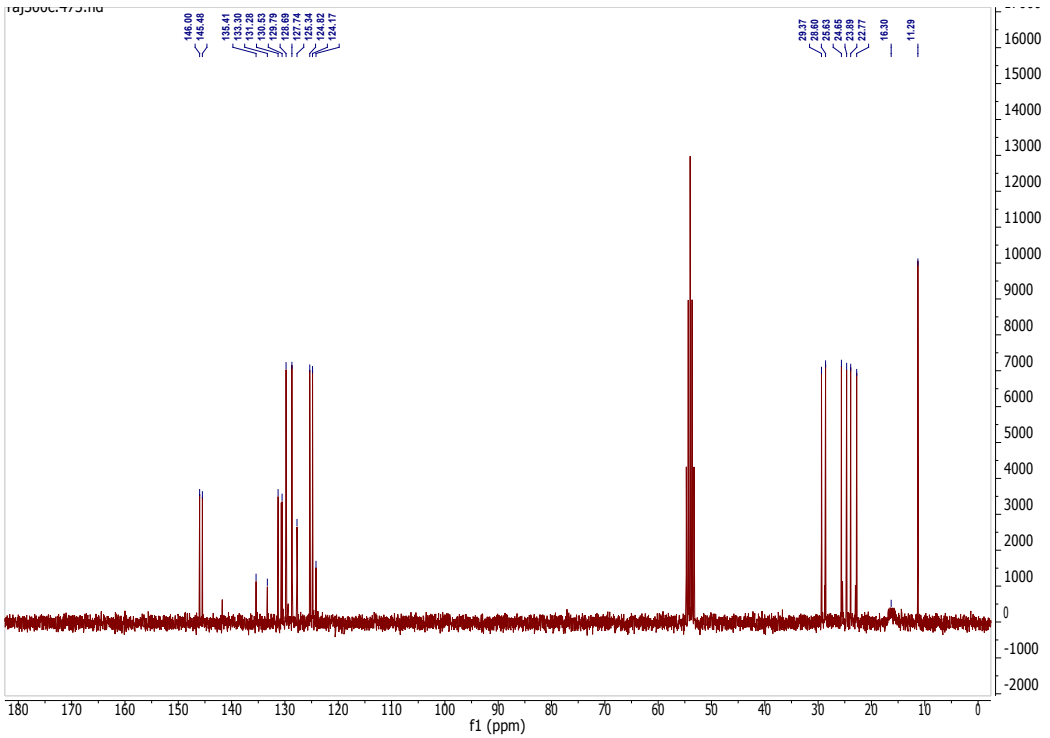


Figure S3. ^{13}C NMR spectrum of **3** in CD_2Cl_2.

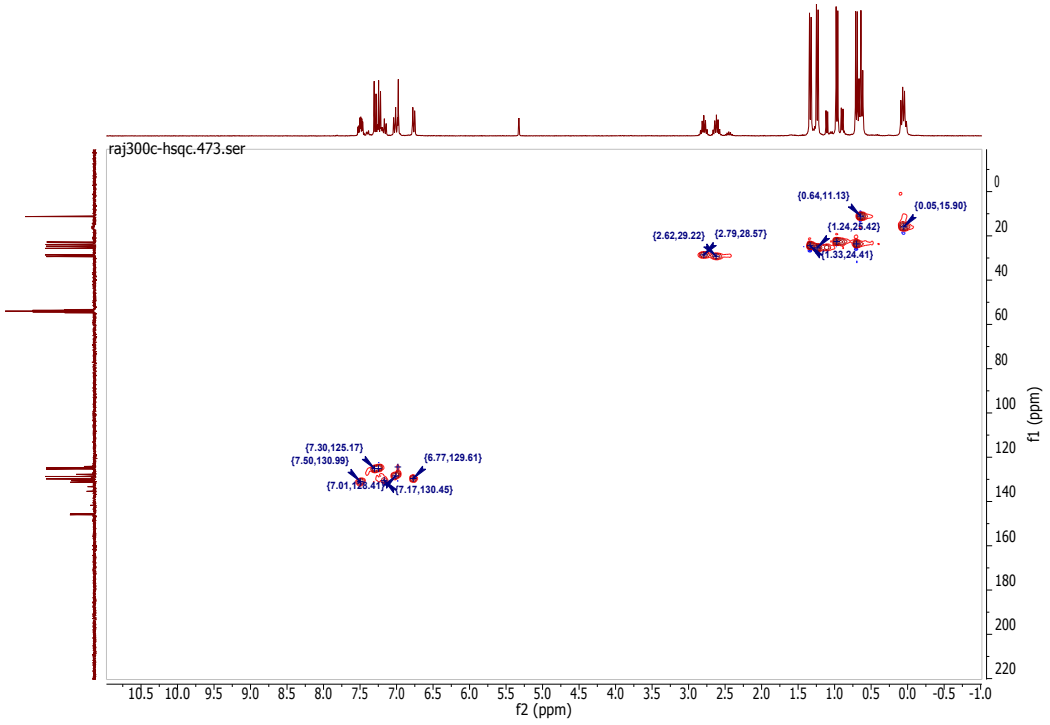


Figure S4. ^{1}H -^{13}C-HSQC NMR spectrum of **3** in CD_2Cl_2.

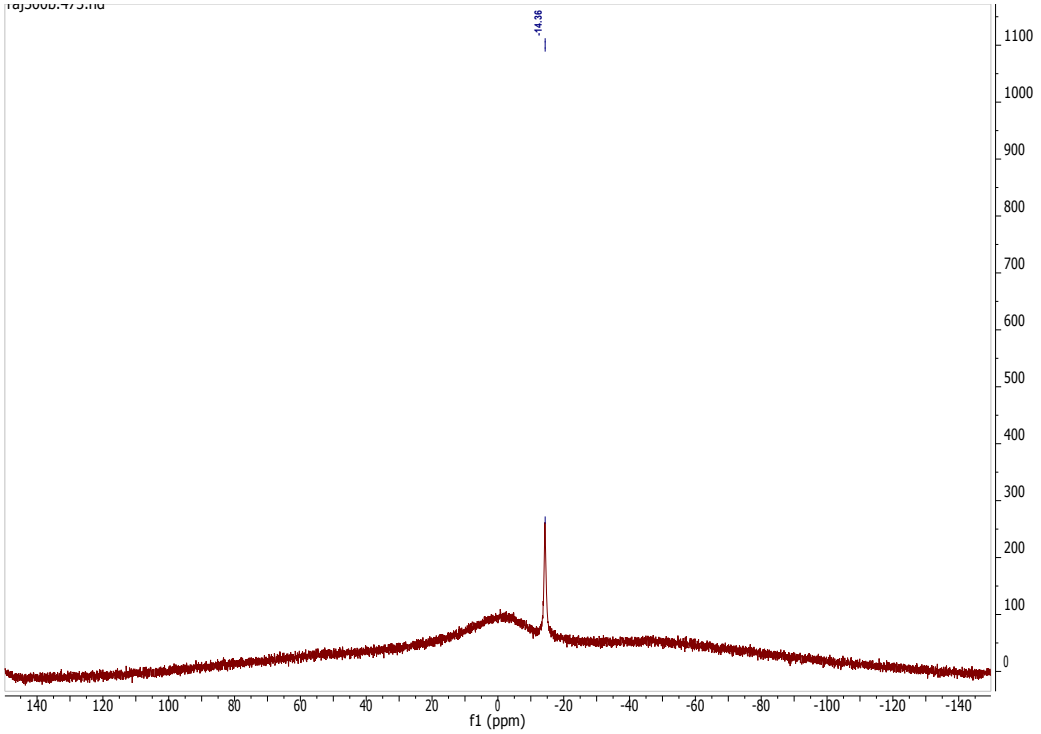


Figure S5. ^{11}B NMR spectrum of **3** in CD_2Cl_2.

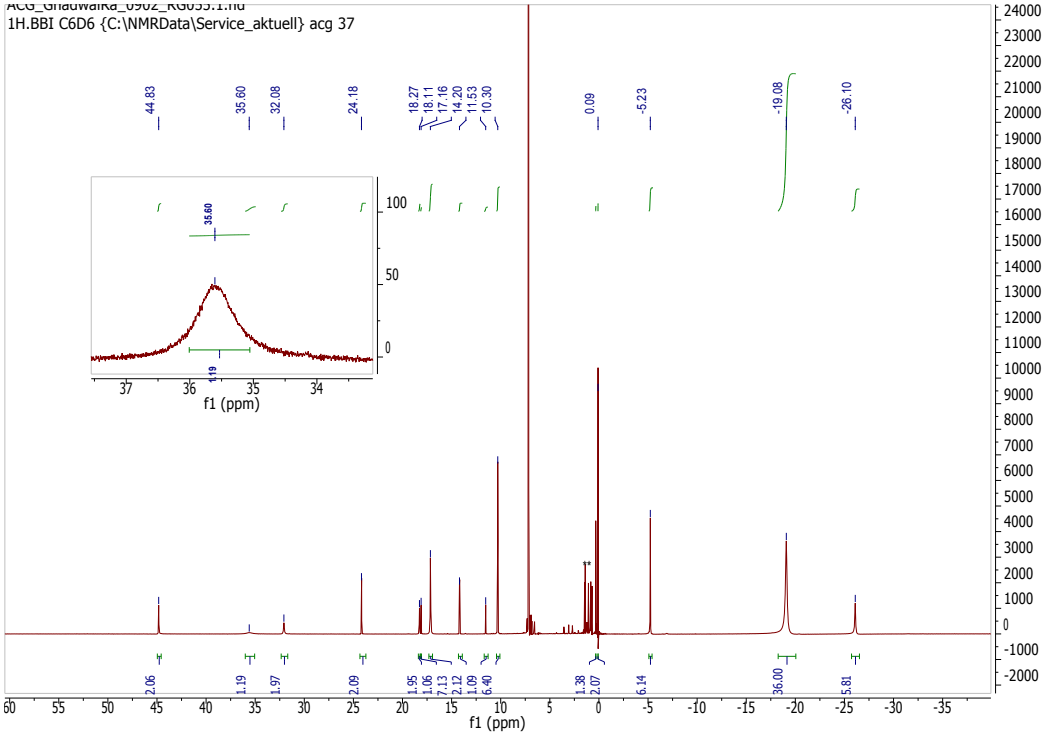


Figure S6. ^{1}H NMR spectrum of **4** in C_6D_6 [**trace of (aIPr^{Ph})BEt$_3$].

UV/vis spectroscopy

The UV/vis spectrum (Figure S7) of each of the complexes **2** and **4** exhibits three low intensity absorptions in the λ = 600 – 750 nm region, which corresponds to the expected three d–d transitions.

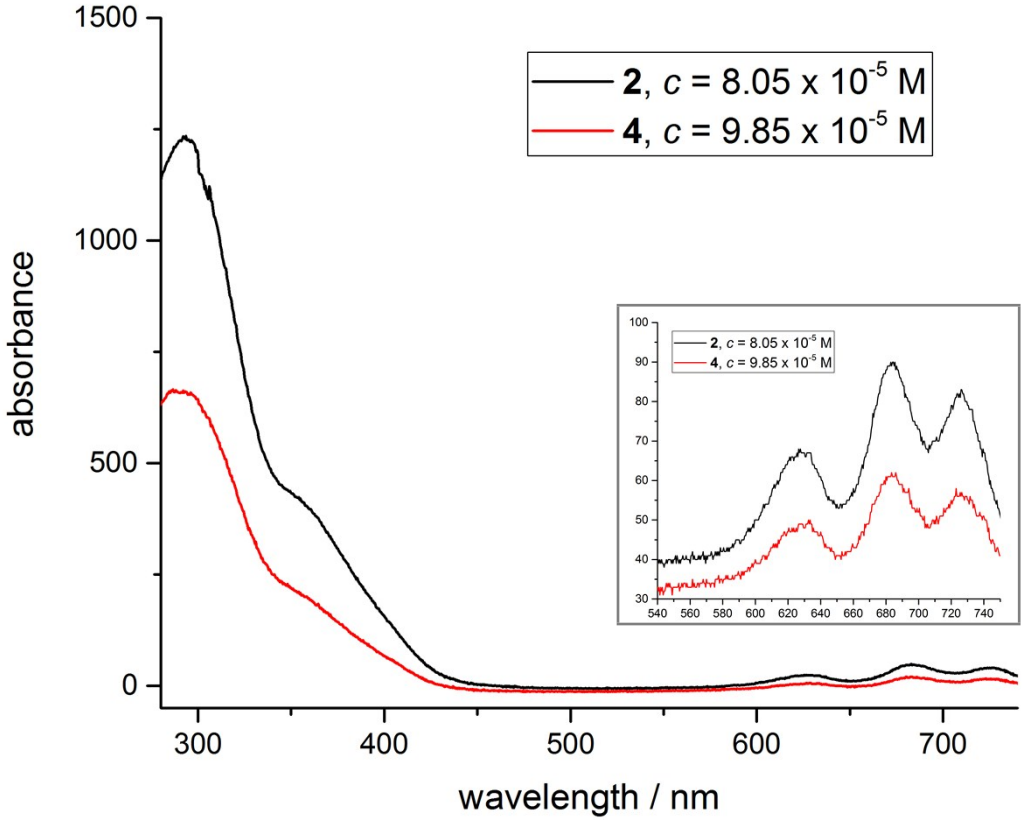


Figure S7. UV/vis spectra of **2** and **4** in THF.

SQUID Magnetic Measurements for 2

Temperature-dependent magnetic susceptibility measurements of **2** were carried out with a *Quantum-Design* MPMS-XL-5 SQUID magnetometer equipped with a 5 Tesla magnet in the range from 200 to 2 K in a magnetic field of 0.5 T. The polycrystalline sample was contained in a gel bucket, covered with a few drops of low viscosity perfluoropolyether based inert oil Fomblin YL VAC 25/6 to fix the crystals, and fixed in a non-magnetic sample holder. The maximum measuring temperature of 200 K was chosen because of the pour point of the oil, in order to keep the oil in the frozen state and to avoid therefore the orientation of the crystals parallel to the magnetic field. Each raw data file for the measured magnetic moment was corrected for the diamagnetic contribution of the gel bucket and of the inert oil according to $M^{dia} = \chi_g \cdot m \cdot H$, with experimentally obtained gram susceptibility of gel bucket [$\chi_g = -5.70 \cdot 10^{-7}$ emu/(g·Oe)] and of the oil [$\chi_g = -3.51 \cdot 10^{-7}$ emu/(g·Oe)]. The molar susceptibility data were corrected for the diamagnetic contribution according to χ^{dia}(sample) = $-0.5 \cdot M \cdot 10^{-6}$ cm^3 mol^{-1}.[3] Full-matrix diagonalization of the spin Hamiltonian for zero-field splitting and Zeeman splitting was performed with the *julX* program (E. Bill, Max-Planck Institute for Chemical Energy Conversion, Mülheim/Ruhr, Germany, **2008**). Matrix diagonalization is done with the routine *ZHEEV* from the *LAPACK* numerical package. Parameter optimization is performed with the simplex routine *AMOEBA* from *NUMERICAL RECIPES*. Temperature-independent paramagnetism (*TIP*) was included according to $\chi_{calc} = \chi + TIP$. Before simulation, the experimental data were corrected for *TIP* = $1420 \cdot 10^{-6}$ cm^{3}mol^{-1}.

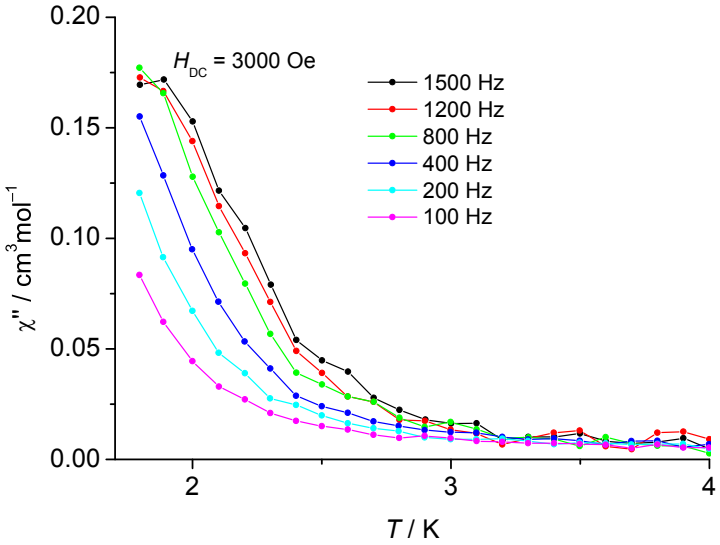


Figure S8. Temperature dependence of χ '' at various frequencies with an applied DC field of *H*DC = 3000 Oe.

The $\chi_M T$ value remains constant up to 20 K and then drops to 1.23 cm^3 mol^{-1} K at 2 K, indicating the presence of zero-field splitting, which was calculated to |D| = 7.3 cm^{-1}. In agreement with the small D value the frequency dependent alternating current (AC) susceptibility could be obtained only under applied DC field of 3000 Oe (Figure S9).

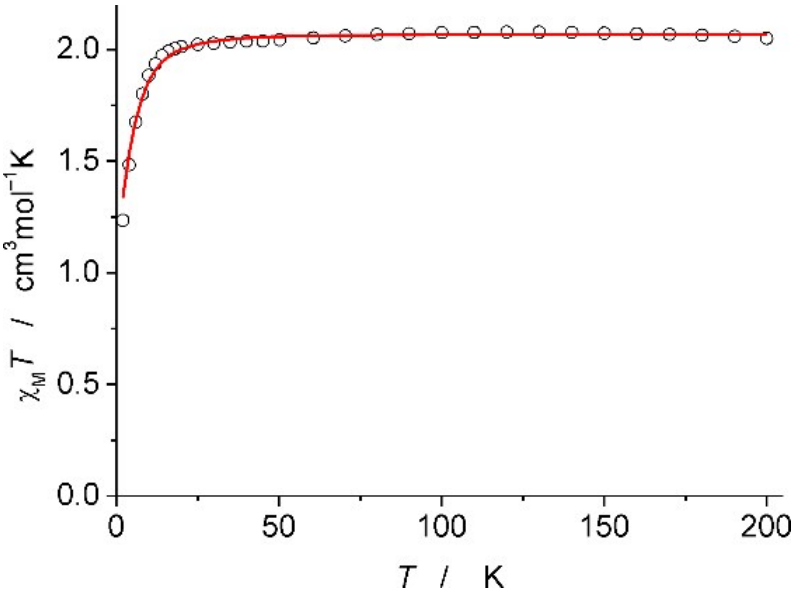
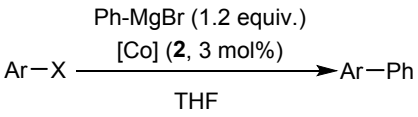


Figure S9. $\chi_M T$ *vs.* T plot for **2**. Red solid line represents the best simulation with $|D| = 7.3$ cm^{-1} and $g = 2.10$.

Catalysis

Compound **2** was tested in Kumada cross-coupling reactions using various aryl halides (Ar–X) and phenylmagnesium bromide (Scheme S1).

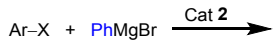


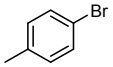
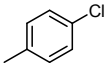
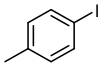
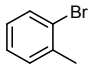
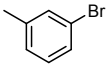
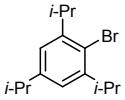
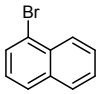
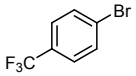
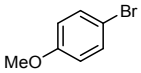
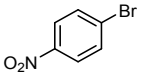
Scheme S1.

All catalytic reactions were carried out under an inert atmosphere (N_2 or Ar). Dried and degassed THF was used. GC/MS analyses were performed using a Shimadzu GCMS-QP2010 SE apparatus (Column: Rtx®-200 Crossbond trifluoropropylmethyl polysiloxane, 30 m 0.25 mm, 0.25 µm). 4-Bromotoluene (TCI Chemicals), 4-chlorotoluene (Merck), 4-iodotoluene (Fluka), 2-bromotoluene, 3-bromotoluene (both Acros Organics), 1-bromo-naphthalene (Sigma-Aldrich), 4-bromobenzotrifluoride (Lancester), 4-bromoanisole (Acros Organics) and 1-bromo-4-nitrobenzene (Merck) were used without further purification. 2-Bromo-1,3,5-triisopropylbenzene (abcr) was distilled prior to use. Liquid aryl halides were added using a 100 µL syringe (HAMILTON, Bonaduz, Switzerland). Phenylmagnesium bromide (3 M in Et_2O) was purchased from Sigma-Aldrich.

Method: In a reaction vessel, the compound **2** (19 mg, 3 mol%) and the aryl halide Ar–X (0.5 mmol) were dissolved in dry THF (6 mL). Phenylmagnesium bromide (3 M in Et_2O; 0.2 mL, 0.6 mmol, 1.2 eq.) was added in one portion to the turquoise solution. The resulting mixture was stirred at ambient temperature (20 °C). After 20 h, an aliquot (0.7 mL) of the reaction mixture was removed *via* a syringe and quenched with 1 mL of water. Organic contents were extracted with dichloromethane (2 mL) and GC-MS analyzed. Results are listed in Table S1.

Table S1. Catalytic activity of **2** in Kumada coupling reactions.



Entry	Ar–X	Conversion, %[a] Ar–H / Ar–X / Ar–Ph
1		60.2 / – / 39.8
2		17.8 / 75.6 / 6.6
3		73.0 / 27.0 / –
4		20.7 / – / 79.3
5		35.9 / – / 64.1
6		100.0 / – / –
7		79.6 / – / 20.4
8		28.2 / 58.8 / 13.0
9		78.9 / – / 21.1
10		unidentified products

[a]after 20 h, determined by GC-MS.

Low-temperature monitoring: In a reaction vessel, compound **2** (19 mg, 3 mol%) and 4-bromotoluene (89 mg, 0.52 mmol) were dissolved in dry THF (6 mL) and cooled to –78 °C. Phenylmagnesium bromide (3 M in Et_2O; 0.17 mL, 0.51 mmol, 1.2 eq.) was added in one portion to the turquoise solution. The resulting mixture was stirred for 1.5 h and meanwhile warmed to –50 °C. An aliquot (0.7 mL) of the reaction mixture, still turquoise, was removed *via* a syringe and quenched with 1 mL of water. Organic contents were extracted with dichloromethane (2 mL) and GC-MS analyzed. Further stirring for 1 h at –20 °C) resulted in a bright green solution (total reaction time: 2.5 h. An aliquot (0.7 mL) of the reaction mixture was removed *via* a syringe and quenched with 1 mL of water. Organic contents were extracted with dichloromethane (2 mL) and GC-MS analyzed. After a total reaction time of 20 h, an aliquot (0.7 mL) of the dark green-brownish reaction mixture was

removed *via* a syringe and quenched with 1 mL of water. Organic contents were extracted with dichloromethane (2 mL) and GC-MS analyzed. Results are listed in Table S2.

Table S2.

Entry	Reaction time, h	Reaction temp., °C	Conversion, %[a] Tol–H / Tol–Br / Tol–Ph
1	1.5	–50 °C	3.2 / 96.5 / 0.3
2	2.5	–20 °C	16.6 / 70.1 / 13.3
3	20	r.t.	32.3 / 33.7 / 34.4

[a]after 20 h, determined by GC-MS.

Single Crystal X-Ray Crystallography:

Suitable single crystals were selected from the mother liquor under Schlenk conditions and covered with perfluorinated polyether oil on a microscope slide, which was cooled with a nitrogen gas flow using the X-Temp2 device.[4] The diffraction data of compound **2** and **4** were collected at 100 K on a Bruker D8 three circle diffractometer, equipped with a SMART APEX II CCD detector and an INCOATEC microfocus source (Ag K_α radiation) with INCOATEC Quazar mirror optics. The diffraction data of compound **3** were collected at 100 K on a Bruker D8 three circle diffractom-eter, equipped with a Bruker Smart APEX II CCD detector and a Bruker Rotating Anode (Mo Kα radiation) with MONTEL Graded multilayer optics. The data were integrated with SAINT[5] and a multi-scan absorption correction with SADABS[6] was applied. For compound **3** also a 3λ-correction[6] was applied. The structure solution was performed with SHELXT[7] and structure refinement was performed with SHELXL,[8] using the graphical user interface SHELXLE.[9] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were assigned to ideal positions and refined using a riding model with U_{iso} constrained to 1.2 (1.5) times the U_{eq} value of the parent carbon atom. Crystallographic data has been deposited with the Cambridge Crystallographic Centre. Copies of the data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S3. Crystal Data and Struicture Refinement Details for **2**, **3**, and **4**.

Compound	**2**	**3**	**4**
CCDC Number	1503206	1503204	1503205
Empirical formula	$C_{70.50}H_{87.50}CoI_2N_4O_{0.75}$	$C_{39.50}H_{55.92}BClN_2$	$C_{45}H_{76}CoN_4Si_4$
Formula weight [g/mol]	1315.67	605.04	844.38
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.56086	0.71073	0.56086
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$
Unit cell dimensions [Å]	a = 10.437(2)	a = 21.075(2)	a = 13.047(2)
	b = 21.065(3)	b = 17.000(2)	b = 19.641(2)
	c = 30.004(3)	c = 21.788(3)	c = 20.141(3)
α [°]	90.142(2)	90	85.11(2)
β [°]	91.419(2)	107.71(2)	79.66(2)
γ [°]	90.082(2)	90	89.90(2)
Volume [Å^3]	6594.5(17)	7436.2(17)	89.90(2)°
Z	4	8	4
Absorption coefficient [mm^{-1}]	0.661	0.130	0.247
F(000)	2710	2631	1828
Crystal size [mm^3]	0.259 x 0.088 x 0.088	0.177 x 0.156 x 0.070	0.364 x 0.325 x 0.162
Theta range for data collection [°]	1.540 to 21.490	1.014 to 25.729	1.205 to 19.751
Reflections collected / unique	292417/ 30586	132794/ 14184	156211 / 18549
R_{int}	0.0768	0.0390	0.0398
Completeness	100.0	100.0	100.0
Max. and min. transmission	0.7446 and 0.7071	0.7453 and 0.6857	0.7445 and 0.7255
Data / restraints / parameters	30586 / 1079 / 1644	14184 / 673 / 979	18549 / 1098 / 1140
Goodness-of-fit on F^2	1.033	1.015	1.031
Final R indices [I>2sigma(I)]	$R1$ = 0.0343, $wR2$ = 0.0677	$R1$ = 0.0421, $wR2$ = 0.0964	$R1$ = 0.0299, $wR2$ = 0.0707
R indices (all data)	$R1$ = 0.0535, $wR2$ = 0.0743	$R1$ = 0.0598, $wR2$ = 0.1068	$R1$ = 0.0406, $wR2$ = 0.0769
Largest diff. peak and hole (e.A^{-3})	0.672 and -0.682	0.352 and -0.222	0.316 and -0.300

Compound **2**

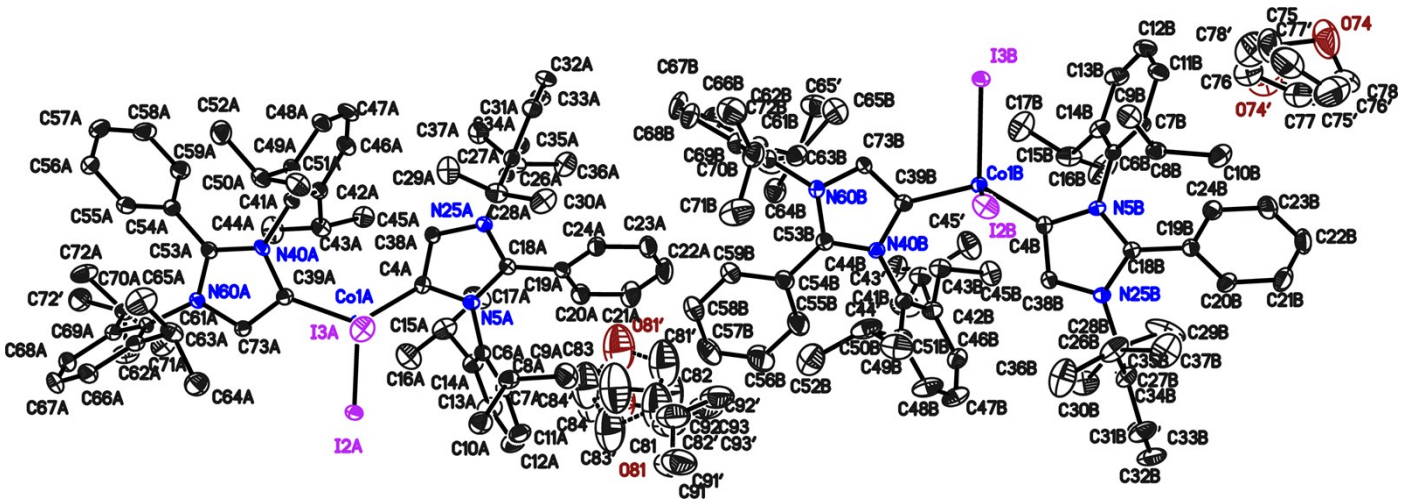


Figure S10. Molecular structure of **2**. Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity.

Bond lengths [Å] and angles [°] for Compound 2

Symmetry transformations used to		C(83')-C(84')	1.496(15)	C(8A)-C(9A)	1.531(4)
generate equivalent atoms:		C(91)-C(92)#1	1.369(5)	C(11A)-C(12A)	1.382(4)
#1 -x+2,-y,-z+1		C(91)-C(93)	1.376(6)	C(12A)-C(13A)	1.377(4)
O(74)-C(75)	1.408(7)	C(92)-C(91)#1	1.369(5)	C(13A)-C(14A)	1.390(4)
O(74)-C(78)	1.441(7)	C(92)-C(93)	1.381(6)	C(14A)-C(15A)	1.530(4)
C(75)-C(76)	1.479(8)	C(91')-C(92')#1	1.369(5)	C(15A)-C(17A)	1.514(4)
C(76)-C(77)	1.575(9)	C(91')-C(93')	1.375(6)	C(15A)-C(16A)	1.525(4)
C(77)-C(78)	1.537(7)	C(92')-C(91')#1	1.369(5)	C(18A)-N(25A)	1.346(3)
O(74')-C(78')	1.404(14)	C(92')-C(93')	1.379(6)	C(18A)-C(19A)	1.472(3)
O(74')-C(75')	1.440(14)	Co(1A)-C(4A)	2.021(2)	C(19A)-C(24A)	1.391(4)
C(75')-C(76')	1.499(14)	Co(1A)-C(39A)	2.037(2)	C(19A)-C(20A)	1.392(4)
C(76')-C(77')	1.549(17)	Co(1A)-I(2A)	2.6067(5)	C(20A)-C(21A)	1.381(4)
C(77')-C(78')	1.485(14)	Co(1A)-I(3A)	2.6259(6)	C(21A)-C(22A)	1.382(4)
O(81)-C(84)	1.403(12)	C(4A)-C(38A)	1.369(3)	C(22A)-C(23A)	1.379(4)
O(81)-C(81)	1.414(11)	C(4A)-N(5A)	1.416(3)	C(23A)-C(24A)	1.387(4)
C(81)-C(82)	1.480(14)	N(5A)-C(18A)	1.353(3)	N(25A)-C(38A)	1.384(3)
C(82)-C(83)	1.558(15)	N(5A)-C(6A)	1.455(3)	N(25A)-C(26A)	1.447(3)
C(83)-C(84)	1.467(13)	C(6A)-C(7A)	1.397(4)	C(26A)-C(27A)	1.398(4)
O(81')-C(84')	1.400(15)	C(6A)-C(14A)	1.398(4)	C(26A)-C(34A)	1.399(3)
O(81')-C(81')	1.401(14)	C(7A)-C(11A)	1.393(4)	C(27A)-C(31A)	1.398(4)
C(81')-C(82')	1.479(15)	C(7A)-C(8A)	1.515(4)	C(27A)-C(28A)	1.517(4)
C(82')-C(83')	1.557(18)	C(8A)-C(10A)	1.531(4)	C(28A)-C(29A)	1.524(4)

C(28A)-C(30A)	1.535(4)	C(63A)-C(64A)	1.533(4)	N(25B)-C(38B)	1.385(3)
C(31A)-C(32A)	1.380(4)	C(66A)-C(67A)	1.379(4)	N(25B)-C(26B)	1.447(3)
C(32A)-C(33A)	1.380(4)	C(67A)-C(68A)	1.379(4)	C(26B)-C(27B)	1.391(4)
C(33A)-C(34A)	1.394(4)	C(68A)-C(69A)	1.405(4)	C(26B)-C(34B)	1.397(4)
C(34A)-C(35A)	1.515(4)	C(69A)-C(70')	1.511(4)	C(27B)-C(31B)	1.399(4)
C(35A)-C(37A)	1.526(4)	C(69A)-C(70A)	1.511(4)	C(27B)-C(28B)	1.522(4)
C(35A)-C(36A)	1.531(4)	C(70A)-C(72A)	1.527(5)	C(28B)-C(29B)	1.525(5)
C(39A)-C(73A)	1.363(3)	C(70A)-C(71A)	1.528(5)	C(28B)-C(30B)	1.526(4)
C(39A)-N(40A)	1.412(3)	C(70')-C(72')	1.520(9)	C(31B)-C(32B)	1.375(4)
N(40A)-C(53A)	1.359(3)	C(70')-C(71')	1.556(9)	C(32B)-C(33B)	1.372(4)
N(40A)-C(41A)	1.448(3)	Co(1B)-C(39B)	2.036(2)	C(33B)-C(34B)	1.390(4)
C(41A)-C(49A)	1.405(4)	Co(1B)-C(4B)	2.037(2)	C(34B)-C(35B)	1.519(4)
C(41A)-C(42A)	1.408(4)	Co(1B)-I(3B)	2.6315(5)	C(35B)-C(37B)	1.524(4)
C(42A)-C(46A)	1.391(4)	Co(1B)-I(2B)	2.6388(6)	C(35B)-C(36B)	1.531(5)
C(42A)-C(43A)	1.530(4)	C(4B)-C(38B)	1.365(3)	C(39B)-C(73B)	1.367(3)
C(43A)-C(44A)	1.526(4)	C(4B)-N(5B)	1.406(3)	C(39B)-N(40B)	1.412(3)
C(43A)-C(45A)	1.531(4)	N(5B)-C(18B)	1.357(3)	N(40B)-C(53B)	1.358(3)
C(46A)-C(47A)	1.383(4)	N(5B)-C(6B)	1.453(3)	N(40B)-C(41B)	1.449(3)
C(47A)-C(48A)	1.378(4)	C(6B)-C(7B)	1.395(4)	C(41B)-C(49B)	1.395(4)
C(48A)-C(49A)	1.394(3)	C(6B)-C(14B)	1.401(4)	C(41B)-C(42B)	1.399(4)
C(49A)-C(50A)	1.519(4)	C(7B)-C(11B)	1.393(4)	C(42B)-C(46B)	1.386(4)
C(50A)-C(51A)	1.524(4)	C(7B)-C(8B)	1.521(4)	C(42B)-C(43B)	1.538(4)
C(50A)-C(52A)	1.531(4)	C(8B)-C(9B)	1.532(4)	C(42B)-C(43')	1.559(13)
C(53A)-N(60A)	1.344(3)	C(8B)-C(10B)	1.534(4)	C(43B)-C(45B)	1.520(5)
C(53A)-C(54A)	1.473(3)	C(11B)-C(12B)	1.377(4)	C(43B)-C(44B)	1.526(5)
C(54A)-C(59A)	1.394(4)	C(12B)-C(13B)	1.378(4)	C(43')-C(45')	1.517(13)
C(54A)-C(55A)	1.399(4)	C(13B)-C(14B)	1.392(4)	C(43')-C(44')	1.528(13)
C(55A)-C(56A)	1.393(4)	C(14B)-C(15B)	1.515(4)	C(46B)-C(47B)	1.378(4)
C(56A)-C(57A)	1.381(4)	C(15B)-C(17B)	1.520(4)	C(47B)-C(48B)	1.377(4)
C(57A)-C(58A)	1.389(4)	C(15B)-C(16B)	1.528(4)	C(48B)-C(49B)	1.401(4)
C(58A)-C(59A)	1.383(4)	C(18B)-N(25B)	1.351(3)	C(49B)-C(50B)	1.522(4)
N(60A)-C(73A)	1.385(3)	C(18B)-C(19B)	1.470(3)	C(50B)-C(51B)	1.524(4)
N(60A)-C(61A)	1.455(3)	C(19B)-C(20B)	1.398(4)	C(50B)-C(52B)	1.544(5)
C(61A)-C(69A)	1.390(4)	C(19B)-C(24B)	1.399(4)	C(53B)-N(60B)	1.346(3)
C(61A)-C(62A)	1.400(4)	C(20B)-C(21B)	1.383(4)	C(53B)-C(54B)	1.480(4)
C(62A)-C(66A)	1.403(4)	C(21B)-C(22B)	1.377(4)	C(54B)-C(55B)	1.384(4)
C(62A)-C(63A)	1.519(4)	C(22B)-C(23B)	1.378(4)	C(54B)-C(59B)	1.407(4)
C(63A)-C(65A)	1.525(4)	C(23B)-C(24B)	1.383(4)	C(55B)-C(56B)	1.389(4)

C(56B)-C(57B)	1.365(5)	C(81')-C(82')-C(83')	103.0(13)	C(16A)-C(15A)-C(14A)	111.6(3)
C(57B)-C(58B)	1.370(5)	C(84')-C(83')-C(82')	102.1(12)	N(25A)-C(18A)-N(5A)	106.5(2)
C(58B)-C(59B)	1.379(4)	O(81')-C(84')-C(83')	109.4(14)	N(25A)-C(18A)-C(19A)	124.2(2)
N(60B)-C(73B)	1.383(3)	C(92)#1-C(91)-C(93)	119.8(8)	N(5A)-C(18A)-C(19A)	129.3(2)
N(60B)-C(61B)	1.450(3)	C(91)#1-C(92)-C(93)	119.6(8)	C(24A)-C(19A)-C(20A)	118.6(2)
C(61B)-C(62B)	1.386(4)	C(91)-C(93)-C(92)	120.6(8)	C(24A)-C(19A)-C(18A)	119.1(2)
C(61B)-C(69B)	1.417(4)	C(92')#1-C(91')-C(93')	118.9(7)	C(20A)-C(19A)-C(18A)	122.3(2)
C(62B)-C(66B)	1.393(4)	C(91')#1-C(92')-C(93')	121.0(7)	C(21A)-C(20A)-C(19A)	120.4(3)
C(62B)-C(63B)	1.526(4)	C(91')-C(93')-C(92')	120.1(7)	C(20A)-C(21A)-C(22A)	120.4(3)
C(62B)-C(63')	1.526(4)	C(4A)-Co(1A)-C(39A)	125.01(10)	C(23A)-C(22A)-C(21A)	120.0(3)
C(63B)-C(65B)	1.516(5)	C(4A)-Co(1A)-I(2A)	111.95(7)	C(22A)-C(23A)-C(24A)	119.7(3)
C(63B)-C(64B)	1.527(4)	C(39A)-Co(1A)-I(2A)	102.65(7)	C(23A)-C(24A)-C(19A)	121.0(3)
C(63')-C(65')	1.533(13)	C(4A)-Co(1A)-I(3A)	103.70(7)	C(18A)-N(25A)-C(38A)	108.5(2)
C(63')-C(64')	1.546(13)	C(39A)-Co(1A)-I(3A)	101.28(7)	C(18A)-N(25A)-C(26A)	128.0(2)
C(66B)-C(67B)	1.385(5)	I(2A)-Co(1A)-I(3A)	111.722(14)	C(38A)-N(25A)-C(26A)	123.5(2)
C(67B)-C(68B)	1.384(5)	C(38A)-C(4A)-N(5A)	102.3(2)	C(27A)-C(26A)-C(34A)	123.7(2)
C(68B)-C(69B)	1.396(4)	C(38A)-C(4A)-Co(1A)	123.72(18)	C(27A)-C(26A)-N(25A)	117.5(2)
C(69B)-C(70B)	1.524(4)	N(5A)-C(4A)-Co(1A)	131.16(18)	C(34A)-C(26A)-N(25A)	118.7(2)
C(70B)-C(71B)	1.521(5)	C(18A)-N(5A)-C(4A)	112.0(2)	C(26A)-C(27A)-C(31A)	116.7(2)
C(70B)-C(72B)	1.524(4)	C(18A)-N(5A)-C(6A)	122.2(2)	C(26A)-C(27A)-C(28A)	122.4(2)
		C(4A)-N(5A)-C(6A)	125.8(2)	C(31A)-C(27A)-C(28A)	120.9(2)
C(75)-O(74)-C(78)	109.5(4)	C(7A)-C(6A)-C(14A)	123.4(2)	C(27A)-C(28A)-C(29A)	110.5(2)
O(74)-C(75)-C(76)	109.0(5)	C(7A)-C(6A)-N(5A)	118.3(2)	C(27A)-C(28A)-C(30A)	112.0(2)
C(75)-C(76)-C(77)	103.3(5)	C(14A)-C(6A)-N(5A)	118.3(2)	C(29A)-C(28A)-C(30A)	110.4(2)
C(78)-C(77)-C(76)	105.5(5)	C(11A)-C(7A)-C(6A)	116.8(3)	C(32A)-C(31A)-C(27A)	121.1(3)
O(74)-C(78)-C(77)	103.7(5)	C(11A)-C(7A)-C(8A)	119.7(2)	C(33A)-C(32A)-C(31A)	120.4(3)
C(78')-O(74')-C(75')	108.4(13)	C(6A)-C(7A)-C(8A)	123.4(2)	C(32A)-C(33A)-C(34A)	121.3(3)
O(74')-C(75')-C(76')	104.6(12)	C(7A)-C(8A)-C(10A)	111.0(2)	C(33A)-C(34A)-C(26A)	116.7(2)
C(75')-C(76')-C(77')	109.9(11)	C(7A)-C(8A)-C(9A)	111.6(2)	C(33A)-C(34A)-C(35A)	120.7(2)
C(78')-C(77')-C(76')	99.6(11)	C(10A)-C(8A)-C(9A)	110.3(2)	C(26A)-C(34A)-C(35A)	122.7(2)
O(74')-C(78')-C(77')	112.5(13)	C(12A)-C(11A)-C(7A)	121.3(3)	C(34A)-C(35A)-C(37A)	110.2(2)
C(84)-O(81)-C(81)	107.1(10)	C(13A)-C(12A)-C(11A)	120.0(3)	C(34A)-C(35A)-C(36A)	110.8(2)
O(81)-C(81)-C(82)	107.8(11)	C(12A)-C(13A)-C(14A)	121.6(3)	C(37A)-C(35A)-C(36A)	111.4(2)
C(81)-C(82)-C(83)	106.1(10)	C(13A)-C(14A)-C(6A)	116.7(3)	C(4A)-C(38A)-N(25A)	110.7(2)
C(84)-C(83)-C(82)	101.3(10)	C(13A)-C(14A)-C(15A)	120.3(3)	C(73A)-C(39A)-N(40A)	102.6(2)
O(81)-C(84)-C(83)	113.0(11)	C(6A)-C(14A)-C(15A)	122.9(2)	C(73A)-C(39A)-Co(1A)	120.80(18)
C(84')-O(81')-C(81')	109.9(15)	C(17A)-C(15A)-C(16A)	109.6(3)	N(40A)-C(39A)-Co(1A)	135.10(18)
O(81')-C(81')-C(82')	107.8(13)	C(17A)-C(15A)-C(14A)	113.3(3)	C(53A)-N(40A)-C(39A)	112.1(2)

C(53A)-N(40A)-C(41A)	124.4(2)	C(61A)-C(62A)-C(63A)	123.7(2)	C(7B)-C(8B)-C(9B)	110.2(2)
C(39A)-N(40A)-C(41A)	123.21(19)	C(66A)-C(62A)-C(63A)	119.7(3)	C(7B)-C(8B)-C(10B)	111.6(2)
C(49A)-C(41A)-C(42A)	123.6(2)	C(62A)-C(63A)-C(65A)	111.2(2)	C(9B)-C(8B)-C(10B)	110.8(2)
C(49A)-C(41A)-N(40A)	118.4(2)	C(62A)-C(63A)-C(64A)	112.0(2)	C(12B)-C(11B)-C(7B)	121.4(3)
C(42A)-C(41A)-N(40A)	118.0(2)	C(65A)-C(63A)-C(64A)	110.6(3)	C(11B)-C(12B)-C(13B)	120.1(3)
C(46A)-C(42A)-C(41A)	116.3(2)	C(67A)-C(66A)-C(62A)	120.4(3)	C(12B)-C(13B)-C(14B)	121.5(3)
C(46A)-C(42A)-C(43A)	120.9(2)	C(68A)-C(67A)-C(66A)	121.4(3)	C(13B)-C(14B)-C(6B)	116.6(3)
C(41A)-C(42A)-C(43A)	122.8(2)	C(67A)-C(68A)-C(69A)	120.7(3)	C(13B)-C(14B)-C(15B)	119.9(2)
C(44A)-C(43A)-C(42A)	113.3(2)	C(61A)-C(69A)-C(68A)	116.4(3)	C(6B)-C(14B)-C(15B)	123.5(2)
C(44A)-C(43A)-C(45A)	109.1(2)	C(61A)-C(69A)-C(70')	123.8(2)	C(14B)-C(15B)-C(17B)	112.3(2)
C(42A)-C(43A)-C(45A)	113.3(2)	C(68A)-C(69A)-C(70')	119.8(2)	C(14B)-C(15B)-C(16B)	112.1(3)
C(47A)-C(46A)-C(42A)	121.7(3)	C(61A)-C(69A)-C(70A)	123.8(2)	C(17B)-C(15B)-C(16B)	109.9(2)
C(48A)-C(47A)-C(46A)	120.2(2)	C(68A)-C(69A)-C(70A)	119.8(2)	N(25B)-C(18B)-N(5B)	106.1(2)
C(47A)-C(48A)-C(49A)	121.5(3)	C(69A)-C(70A)-C(72A)	110.0(3)	N(25B)-C(18B)-C(19B)	126.4(2)
C(48A)-C(49A)-C(41A)	116.5(2)	C(69A)-C(70A)-C(71A)	110.4(2)	N(5B)-C(18B)-C(19B)	127.3(2)
C(48A)-C(49A)-C(50A)	119.1(2)	C(72A)-C(70A)-C(71A)	109.7(3)	C(20B)-C(19B)-C(24B)	118.2(2)
C(41A)-C(49A)-C(50A)	124.4(2)	C(69A)-C(70')-C(72')	118.1(6)	C(20B)-C(19B)-C(18B)	120.3(2)
C(49A)-C(50A)-C(51A)	112.1(2)	C(69A)-C(70')-C(71')	112.4(5)	C(24B)-C(19B)-C(18B)	121.5(2)
C(49A)-C(50A)-C(52A)	110.3(2)	C(72')-C(70')-C(71')	109.7(7)	C(21B)-C(20B)-C(19B)	120.6(3)
C(51A)-C(50A)-C(52A)	109.8(2)	C(39A)-C(73A)-N(60A)	110.5(2)	C(22B)-C(21B)-C(20B)	120.4(3)
N(60A)-C(53A)-N(40A)	106.0(2)	C(39B)-Co(1B)-C(4B)	120.02(10)	C(21B)-C(22B)-C(23B)	119.8(3)
N(60A)-C(53A)-C(54A)	126.1(2)	C(39B)-Co(1B)-I(3B)	101.15(7)	C(22B)-C(23B)-C(24B)	120.5(3)
N(40A)-C(53A)-C(54A)	127.9(2)	C(4B)-Co(1B)-I(3B)	115.77(7)	C(23B)-C(24B)-C(19B)	120.5(3)
C(59A)-C(54A)-C(55A)	119.3(2)	C(39B)-Co(1B)-I(2B)	109.76(7)	C(18B)-N(25B)-C(38B)	108.3(2)
C(59A)-C(54A)-C(53A)	120.2(2)	C(4B)-Co(1B)-I(2B)	102.31(7)	C(18B)-N(25B)-C(26B)	128.4(2)
C(55A)-C(54A)-C(53A)	120.5(2)	I(3B)-Co(1B)-I(2B)	107.441(13)	C(38B)-N(25B)-C(26B)	123.2(2)
C(56A)-C(55A)-C(54A)	119.8(3)	C(38B)-C(4B)-N(5B)	102.7(2)	C(27B)-C(26B)-C(34B)	123.6(2)
C(57A)-C(56A)-C(55A)	120.5(3)	C(38B)-C(4B)-Co(1B)	122.79(18)	C(27B)-C(26B)-N(25B)	119.3(2)
C(56A)-C(57A)-C(58A)	119.8(3)	N(5B)-C(4B)-Co(1B)	132.20(17)	C(34B)-C(26B)-N(25B)	117.0(2)
C(59A)-C(58A)-C(57A)	120.2(3)	C(18B)-N(5B)-C(4B)	112.14(19)	C(26B)-C(27B)-C(31B)	116.7(3)
C(58A)-C(59A)-C(54A)	120.4(3)	C(18B)-N(5B)-C(6B)	123.92(19)	C(26B)-C(27B)-C(28B)	122.4(2)
C(53A)-N(60A)-C(73A)	108.9(2)	C(4B)-N(5B)-C(6B)	123.93(19)	C(31B)-C(27B)-C(28B)	120.8(3)
C(53A)-N(60A)-C(61A)	129.4(2)	C(7B)-C(6B)-C(14B)	123.4(2)	C(27B)-C(28B)-C(29B)	112.3(3)
C(73A)-N(60A)-C(61A)	121.6(2)	C(7B)-C(6B)-N(5B)	118.6(2)	C(27B)-C(28B)-C(30B)	111.0(3)
C(69A)-C(61A)-C(62A)	124.4(2)	C(14B)-C(6B)-N(5B)	118.0(2)	C(29B)-C(28B)-C(30B)	109.9(3)
C(69A)-C(61A)-N(60A)	119.0(2)	C(11B)-C(7B)-C(6B)	116.9(2)	C(32B)-C(31B)-C(27B)	121.2(3)
C(62A)-C(61A)-N(60A)	116.5(2)	C(11B)-C(7B)-C(8B)	119.4(2)	C(33B)-C(32B)-C(31B)	120.3(3)
C(61A)-C(62A)-C(66A)	116.6(3)	C(6B)-C(7B)-C(8B)	123.7(2)	C(32B)-C(33B)-C(34B)	121.6(3)

C(33B)-C(34B)-C(26B)	116.6(3)	N(40B)-C(53B)-C(54B)	128.5(2)
C(33B)-C(34B)-C(35B)	119.9(3)	C(55B)-C(54B)-C(59B)	117.6(3)
C(26B)-C(34B)-C(35B)	123.4(2)	C(55B)-C(54B)-C(53B)	122.0(2)
C(34B)-C(35B)-C(37B)	112.1(2)	C(59B)-C(54B)-C(53B)	120.3(3)
C(34B)-C(35B)-C(36B)	109.7(3)	C(54B)-C(55B)-C(56B)	120.8(3)
C(37B)-C(35B)-C(36B)	110.8(3)	C(57B)-C(56B)-C(55B)	120.6(3)
C(4B)-C(38B)-N(25B)	110.7(2)	C(56B)-C(57B)-C(58B)	119.6(3)
C(73B)-C(39B)-N(40B)	102.6(2)	C(57B)-C(58B)-C(59B)	120.7(3)
C(73B)-C(39B)-Co(1B)	122.08(19)	C(58B)-C(59B)-C(54B)	120.6(3)
N(40B)-C(39B)-Co(1B)	135.03(18)	C(53B)-N(60B)-C(73B)	109.3(2)
C(53B)-N(40B)-C(39B)	112.3(2)	C(53B)-N(60B)-C(61B)	128.2(2)
C(53B)-N(40B)-C(41B)	125.7(2)	C(73B)-N(60B)-C(61B)	122.4(2)
C(39B)-N(40B)-C(41B)	122.0(2)	C(62B)-C(61B)-C(69B)	124.8(2)
C(49B)-C(41B)-C(42B)	123.4(2)	C(62B)-C(61B)-N(60B)	118.2(2)
C(49B)-C(41B)-N(40B)	119.0(2)	C(69B)-C(61B)-N(60B)	116.9(2)
C(42B)-C(41B)-N(40B)	117.7(2)	C(61B)-C(62B)-C(66B)	116.2(3)
C(46B)-C(42B)-C(41B)	117.1(2)	C(61B)-C(62B)-C(63B)	122.9(2)
C(46B)-C(42B)-C(43B)	120.2(3)	C(66B)-C(62B)-C(63B)	120.7(3)
C(41B)-C(42B)-C(43B)	122.4(3)	C(61B)-C(62B)-C(63')	122.9(2)
C(46B)-C(42B)-C(43')	121.1(6)	C(66B)-C(62B)-C(63')	120.7(3)
C(41B)-C(42B)-C(43')	118.8(6)	C(65B)-C(63B)-C(62B)	111.2(3)
C(45B)-C(43B)-C(44B)	108.6(3)	C(65B)-C(63B)-C(64B)	110.6(3)
C(45B)-C(43B)-C(42B)	113.9(3)	C(62B)-C(63B)-C(64B)	112.7(3)
C(44B)-C(43B)-C(42B)	110.9(3)	C(62B)-C(63')-C(65')	110.4(10)
C(45')-C(43')-C(44')	111.1(12)	C(62B)-C(63')-C(64')	111.3(10)
C(45')-C(43')-C(42B)	103.9(10)	C(65')-C(63')-C(64')	107.4(13)
C(44')-C(43')-C(42B)	116.7(10)	C(67B)-C(66B)-C(62B)	121.1(3)
C(47B)-C(46B)-C(42B)	121.5(3)	C(68B)-C(67B)-C(66B)	121.0(3)
C(48B)-C(47B)-C(46B)	119.9(3)	C(67B)-C(68B)-C(69B)	120.9(3)
C(47B)-C(48B)-C(49B)	121.6(3)	C(68B)-C(69B)-C(61B)	115.6(3)
C(41B)-C(49B)-C(48B)	116.4(3)	C(68B)-C(69B)-C(70B)	122.1(3)
C(41B)-C(49B)-C(50B)	123.2(2)	C(61B)-C(69B)-C(70B)	122.3(2)
C(48B)-C(49B)-C(50B)	120.3(3)	C(71B)-C(70B)-C(69B)	113.4(3)
C(49B)-C(50B)-C(51B)	112.7(3)	C(71B)-C(70B)-C(72B)	109.8(3)
C(49B)-C(50B)-C(52B)	110.7(3)	C(69B)-C(70B)-C(72B)	113.0(3)
C(51B)-C(50B)-C(52B)	109.0(3)	C(39B)-C(73B)-N(60B)	110.2(2)
N(60B)-C(53B)-N(40B)	105.6(2)		
N(60B)-C(53B)-C(54B)	125.9(2)		

Compound **3**

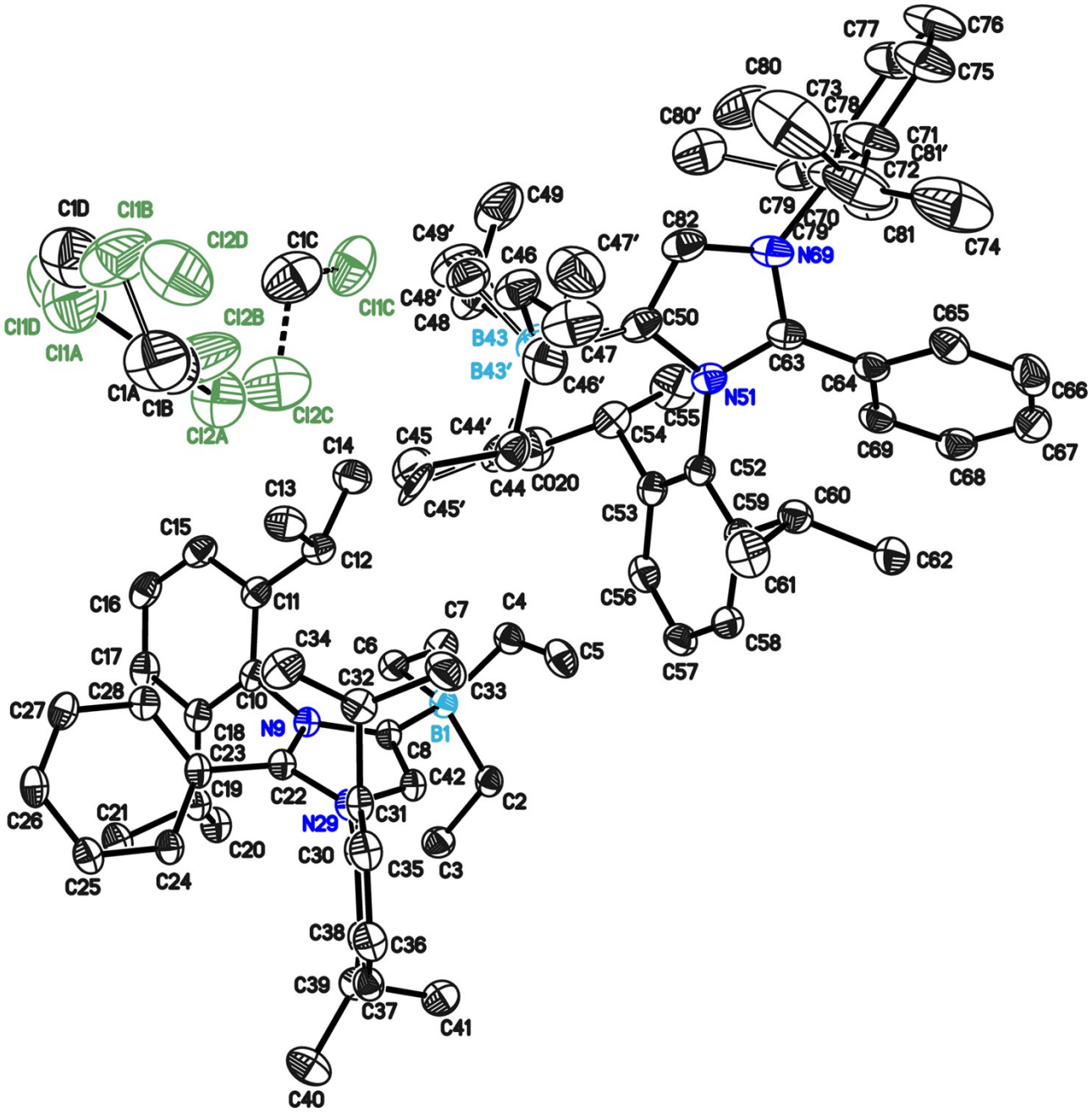


Figure S11. Molecular structure of aNHC-borane (aIPr^{Ph})BEt$_3$ (**3**). Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity.

Bond lengths [Å] and angles [°] for Compound 3

C(1A)-Cl(2A)	1.730(3)	C(1C)-Cl(1C)	1.720(15)	B(1)-C(4)	1.657(2)
C(1A)-Cl(1A)	1.754(6)	C(1D)-Cl(1D)	1.704(16)	B(1)-C(8)	1.661(2)
C(1B)-Cl(2B)	1.704(16)	C(1D)-Cl(2D)	1.727(16)	C(2)-C(3)	1.530(2)
C(1B)-Cl(1B)	1.717(16)	B(1)-C(6)	1.641(2)	C(4)-C(5)	1.525(2)
C(1C)-Cl(2C)	1.717(15)	B(1)-C(2)	1.648(2)	C(6)-C(7)	1.5359(19)

C(8)-C(42)	1.3592(19)	C(39)-C(41)	1.533(2)	N(69)-C(82)	1.375(2)
C(8)-N(9)	1.4125(17)	C(50)-C(82)	1.358(2)	N(69)-C(70)	1.4452(19)
N(9)-C(22)	1.3532(17)	C(50)-N(51)	1.4150(18)	C(70)-C(71)	1.392(2)
N(9)-C(10)	1.4433(17)	C(50)-B(43)	1.641(3)	C(70)-C(78)	1.392(2)
C(10)-C(18)	1.395(2)	C(50)-B(43')	1.723(13)	C(71)-C(75)	1.391(2)
C(10)-C(11)	1.403(2)	B(43)-C(46)	1.645(3)	C(71)-C(72)	1.514(3)
C(11)-C(15)	1.392(2)	B(43)-C(44)	1.647(4)	C(72)-C(74)	1.526(4)
C(11)-C(12)	1.521(2)	B(43)-C(48)	1.654(3)	C(72)-C(73)	1.536(3)
C(12)-C(13)	1.533(2)	C(44)-C(45)	1.541(4)	C(75)-C(76)	1.370(3)
C(12)-C(14)	1.533(2)	C(46)-C(47)	1.533(3)	C(76)-C(77)	1.374(3)
C(15)-C(16)	1.382(2)	C(48)-C(49)	1.534(3)	C(77)-C(78)	1.396(2)
C(16)-C(17)	1.380(2)	B(43')-C(44')	1.638(14)	C(78)-C(79')	1.511(3)
C(17)-C(18)	1.396(2)	B(43')-C(48')	1.654(13)	C(78)-C(79)	1.511(3)
C(18)-C(19)	1.522(2)	B(43')-C(46')	1.661(13)	C(79)-C(80)	1.502(3)
C(19)-C(20)	1.5306(19)	C(44')-C(45')	1.530(15)	C(79)-C(81)	1.532(3)
C(19)-C(21)	1.532(2)	C(46')-C(47')	1.545(13)	C(79')-C(81')	1.560(9)
C(02)-C(54)	1.531(2)	C(48')-C(49')	1.516(13)	C(79')-C(80')	1.661(9)
C(22)-N(29)	1.3435(17)	N(51)-C(63)	1.3497(19)		
C(22)-C(23)	1.4727(19)	N(51)-C(52)	1.4518(18)	Cl(2A)-C(1A)-Cl(1A)	111.1(3)
C(23)-C(24)	1.396(2)	C(52)-C(59)	1.3923(19)	Cl(2B)-C(1B)-Cl(1B)	113.7(14)
C(23)-C(28)	1.398(2)	C(52)-C(53)	1.405(2)	Cl(2C)-C(1C)-Cl(1C)	112.6(14)
C(24)-C(25)	1.384(2)	C(53)-C(56)	1.389(2)	Cl(1D)-C(1D)-Cl(2D)	120.6(18)
C(25)-C(26)	1.382(2)	C(53)-C(54)	1.523(2)	C(6)-B(1)-C(2)	110.68(11)
C(26)-C(27)	1.383(2)	C(54)-C(55)	1.528(2)	C(6)-B(1)-C(4)	109.62(11)
C(27)-C(28)	1.384(2)	C(56)-C(57)	1.382(2)	C(2)-B(1)-C(4)	108.93(11)
N(29)-C(42)	1.3807(17)	C(57)-C(58)	1.378(2)	C(6)-B(1)-C(8)	113.86(11)
N(29)-C(30)	1.4465(17)	C(58)-C(59)	1.397(2)	C(2)-B(1)-C(8)	104.20(11)
C(30)-C(31)	1.3963(19)	C(59)-C(60)	1.520(2)	C(4)-B(1)-C(8)	109.35(11)
C(30)-C(38)	1.397(2)	C(60)-C(61)	1.530(2)	C(3)-C(2)-B(1)	115.68(12)
C(31)-C(35)	1.3952(19)	C(60)-C(62)	1.534(2)	C(5)-C(4)-B(1)	118.66(12)
C(31)-C(32)	1.517(2)	C(63)-N(69)	1.3426(18)	C(7)-C(6)-B(1)	113.92(12)
C(32)-C(34)	1.522(2)	C(63)-C(64)	1.470(2)	C(42)-C(8)-N(9)	102.61(11)
C(32)-C(33)	1.528(2)	C(64)-C(65)	1.396(2)	C(42)-C(8)-B(1)	125.70(12)
C(35)-C(36)	1.380(2)	C(64)-C(69)	1.397(2)	N(9)-C(8)-B(1)	131.64(12)
C(36)-C(37)	1.382(2)	C(65)-C(66)	1.382(2)	C(22)-N(9)-C(8)	111.85(11)
C(37)-C(38)	1.3933(19)	C(66)-C(67)	1.379(3)	C(22)-N(9)-C(10)	121.74(11)
C(38)-C(39)	1.522(2)	C(67)-C(68)	1.382(2)	C(8)-N(9)-C(10)	126.34(11)
C(39)-C(40)	1.527(2)	C(68)-C(69)	1.384(2)	C(18)-C(10)-C(11)	123.91(13)

C(18)-C(10)-N(9)	117.95(12)	C(31)-C(32)-C(33)	109.89(12)	C(59)-C(52)-C(53)	123.44(13)
C(11)-C(10)-N(9)	118.07(12)	C(34)-C(32)-C(33)	111.56(13)	C(59)-C(52)-N(51)	118.50(12)
C(15)-C(11)-C(10)	116.56(13)	C(36)-C(35)-C(31)	120.95(13)	C(53)-C(52)-N(51)	118.06(12)
C(15)-C(11)-C(12)	121.16(13)	C(35)-C(36)-C(37)	120.63(13)	C(56)-C(53)-C(52)	116.71(13)
C(10)-C(11)-C(12)	122.27(13)	C(36)-C(37)-C(38)	121.19(14)	C(56)-C(53)-C(54)	120.96(13)
C(11)-C(12)-C(13)	111.65(13)	C(37)-C(38)-C(30)	116.48(13)	C(52)-C(53)-C(54)	122.33(13)
C(11)-C(12)-C(14)	112.71(13)	C(37)-C(38)-C(39)	121.13(13)	C(53)-C(54)-C(55)	112.19(13)
C(13)-C(12)-C(14)	110.04(13)	C(30)-C(38)-C(39)	122.38(12)	C(53)-C(54)-C(02)	112.81(13)
C(16)-C(15)-C(11)	121.17(14)	C(38)-C(39)-C(40)	112.11(12)	C(55)-C(54)-C(02)	109.43(14)
C(17)-C(16)-C(15)	120.62(14)	C(38)-C(39)-C(41)	112.11(12)	C(57)-C(56)-C(53)	121.25(14)
C(16)-C(17)-C(18)	121.05(14)	C(40)-C(39)-C(41)	109.82(13)	C(58)-C(57)-C(56)	120.64(14)
C(10)-C(18)-C(17)	116.67(13)	C(8)-C(42)-N(29)	110.63(12)	C(57)-C(58)-C(59)	120.80(14)
C(10)-C(18)-C(19)	123.08(12)	C(82)-C(50)-N(51)	102.42(13)	C(52)-C(59)-C(58)	117.16(13)
C(17)-C(18)-C(19)	120.25(13)	C(82)-C(50)-B(43)	124.23(15)	C(52)-C(59)-C(60)	123.91(12)
C(18)-C(19)-C(20)	110.72(12)	N(51)-C(50)-B(43)	133.35(15)	C(58)-C(59)-C(60)	118.94(12)
C(18)-C(19)-C(21)	112.16(12)	C(82)-C(50)-B(43')	125.0(5)	C(59)-C(60)-C(61)	111.19(12)
C(20)-C(19)-C(21)	109.82(12)	N(51)-C(50)-B(43')	129.7(5)	C(59)-C(60)-C(62)	111.25(12)
N(29)-C(22)-N(9)	106.17(11)	C(50)-B(43)-C(46)	103.96(18)	C(61)-C(60)-C(62)	110.64(12)
N(29)-C(22)-C(23)	125.20(12)	C(50)-B(43)-C(44)	112.50(18)	N(69)-C(63)-N(51)	106.33(12)
N(9)-C(22)-C(23)	128.59(12)	C(46)-B(43)-C(44)	111.0(2)	N(69)-C(63)-C(64)	124.77(13)
C(24)-C(23)-C(28)	118.37(13)	C(50)-B(43)-C(48)	111.19(17)	N(51)-C(63)-C(64)	128.79(12)
C(24)-C(23)-C(22)	119.56(12)	C(46)-B(43)-C(48)	107.85(18)	C(65)-C(64)-C(69)	118.90(14)
C(28)-C(23)-C(22)	122.07(12)	C(44)-B(43)-C(48)	110.1(2)	C(65)-C(64)-C(63)	118.89(13)
C(25)-C(24)-C(23)	120.74(13)	C(45)-C(44)-B(43)	112.4(3)	C(69)-C(64)-C(63)	122.21(13)
C(26)-C(25)-C(24)	120.31(14)	C(47)-C(46)-B(43)	117.04(17)	C(66)-C(65)-C(64)	120.48(15)
C(25)-C(26)-C(27)	119.59(13)	C(49)-C(48)-B(43)	118.2(2)	C(67)-C(66)-C(65)	120.22(16)
C(26)-C(27)-C(28)	120.52(14)	C(44')-B(43')-C(48')	107.5(12)	C(66)-C(67)-C(68)	119.89(16)
C(27)-C(28)-C(23)	120.46(13)	C(44')-B(43')-C(46')	105.8(12)	C(67)-C(68)-C(69)	120.55(15)
C(22)-N(29)-C(42)	108.72(11)	C(48')-B(43')-C(46')	108.8(10)	C(63)-N(69)-C(82)	108.63(12)
C(22)-N(29)-C(30)	126.23(11)	C(44')-B(43')-C(50)	115.8(10)	C(63)-N(69)-C(70)	128.14(13)
C(42)-N(29)-C(30)	124.14(11)	C(48')-B(43')-C(50)	106.0(8)	C(82)-N(69)-C(70)	122.94(13)
C(31)-C(30)-C(38)	124.05(12)	C(46')-B(43')-C(50)	112.7(9)	C(68)-C(69)-C(64)	119.94(15)
C(31)-C(30)-N(29)	117.32(12)	C(45')-C(44')-B(43')	114.8(16)	C(71)-C(70)-C(78)	123.93(15)
C(38)-C(30)-N(29)	118.63(12)	C(47')-C(46')-B(43')	119.4(11)	C(71)-C(70)-N(69)	118.09(14)
C(35)-C(31)-C(30)	116.68(13)	C(49')-C(48')-B(43')	116.6(10)	C(78)-C(70)-N(69)	117.84(15)
C(35)-C(31)-C(32)	120.42(13)	C(63)-N(51)-C(50)	111.72(12)	C(75)-C(71)-C(70)	117.02(17)
C(30)-C(31)-C(32)	122.89(12)	C(63)-N(51)-C(52)	122.82(11)	C(75)-C(71)-C(72)	119.93(17)
C(31)-C(32)-C(34)	112.29(12)	C(50)-N(51)-C(52)	125.35(12)	C(70)-C(71)-C(72)	123.04(15)

C(71)-C(72)-C(74)	112.7(2)
C(71)-C(72)-C(73)	110.24(19)
C(74)-C(72)-C(73)	110.83(19)
C(76)-C(75)-C(71)	120.80(19)
C(75)-C(76)-C(77)	120.75(17)
C(76)-C(77)-C(78)	121.39(17)
C(70)-C(78)-C(77)	116.10(17)
C(70)-C(78)-C(79')	123.12(15)
C(77)-C(78)-C(79')	120.78(16)
C(70)-C(78)-C(79)	123.12(15)
C(77)-C(78)-C(79)	120.78(16)
C(80)-C(79)-C(78)	109.52(17)
C(80)-C(79)-C(81)	111.80(19)
C(78)-C(79)-C(81)	110.10(18)
C(78)-C(79')-C(81')	121.0(5)
C(78)-C(79')-C(80')	117.1(4)
C(81')-C(79')-C(80')	101.5(6)
C(50)-C(82)-N(69)	110.89(13)

Compound **4**

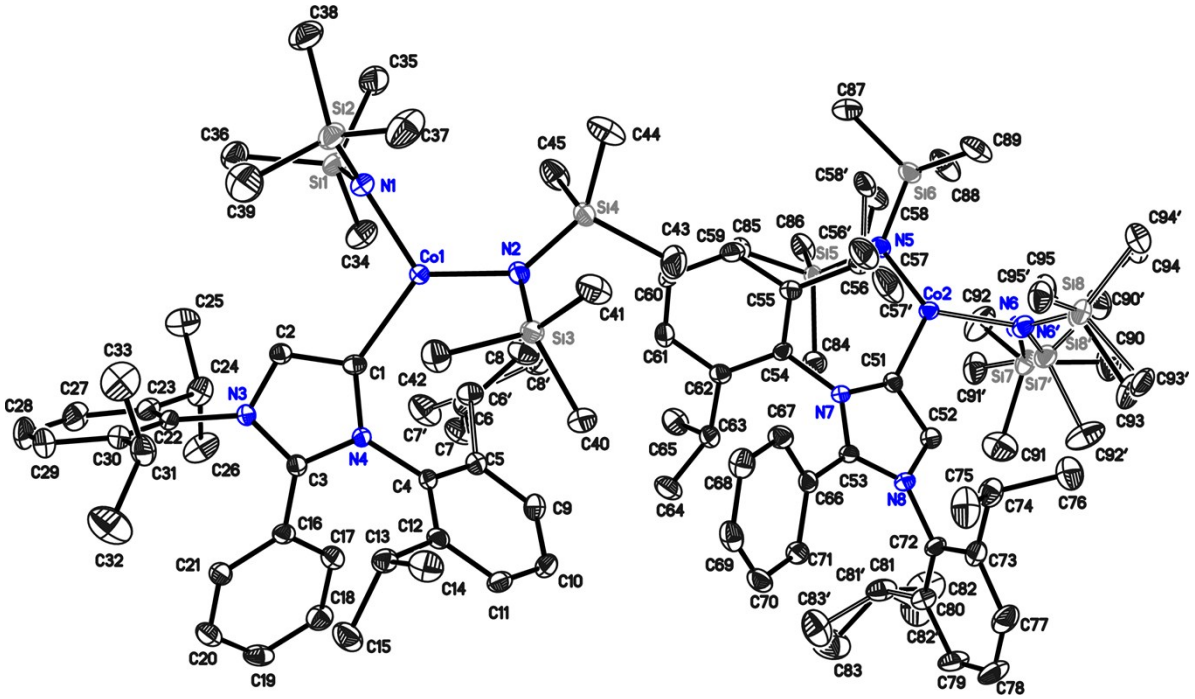


Figure S12. Molecular structure **4**. Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity.

Bond lengths [Å] and angles [°] for Compound 4

Co(1)-N(2)	1.9342(14)
Co(1)-N(1)	1.9484(15)
Co(1)-C(1)	2.0748(16)
Si(1)-N(1)	1.7138(15)
Si(1)-C(34)	1.873(2)
Si(1)-C(35)	1.880(2)
Si(1)-C(36)	1.8844(19)
Si(2)-N(1)	1.7132(15)
Si(2)-C(37)	1.874(2)
Si(2)-C(39)	1.874(2)
Si(2)-C(38)	1.880(2)
Si(3)-N(2)	1.7115(14)
Si(3)-C(40)	1.8727(19)
Si(3)-C(41)	1.8750(19)
Si(3)-C(42)	1.8794(18)
Si(4)-N(2)	1.7110(14)
Si(4)-C(45)	1.8665(19)
Si(4)-C(43)	1.878(2)

Si(4)-C(44)	1.879(2)
Si(5)-N(5)	1.7108(14)
Si(5)-C(85)	1.8731(18)
Si(5)-C(84)	1.8752(19)
Si(5)-C(86)	1.8767(18)
Si(6)-N(5)	1.7091(14)
Si(6)-C(89)	1.870(2)
Si(6)-C(87)	1.876(2)
Si(6)-C(88)	1.879(2)
N(3)-C(3)	1.343(2)
N(3)-C(2)	1.385(2)
N(3)-C(22)	1.447(2)
N(4)-C(3)	1.355(2)
N(4)-C(1)	1.417(2)
N(4)-C(4)	1.457(2)
N(5)-Co(2)	1.9368(14)
N(7)-C(53)	1.359(2)
N(7)-C(51)	1.420(2)
N(7)-C(54)	1.453(2)
N(8)-C(53)	1.343(2)
N(8)-C(52)	1.384(2)
N(8)-C(72)	1.450(2)
C(1)-C(2)	1.366(2)
C(3)-C(16)	1.475(2)
C(4)-C(12)	1.401(2)
C(4)-C(5)	1.402(2)
C(5)-C(9)	1.391(2)
C(5)-C(6)	1.524(4)
C(5)-C(6')	1.547(15)
C(6)-C(8)	1.528(6)
C(6)-C(7)	1.540(4)
C(6')-C(8')	1.47(3)
C(6')-C(7')	1.532(14)
C(9)-C(10)	1.377(3)
C(10)-C(11)	1.377(2)
C(11)-C(12)	1.396(2)
C(12)-C(13)	1.520(2)
C(13)-C(14)	1.533(3)

C(13)-C(15)	1.537(2)
C(16)-C(17)	1.397(2)
C(16)-C(21)	1.399(2)
C(17)-C(18)	1.385(2)
C(18)-C(19)	1.379(3)
C(19)-C(20)	1.381(3)
C(20)-C(21)	1.387(2)
C(22)-C(23)	1.394(2)
C(22)-C(30)	1.402(2)
C(23)-C(27)	1.396(2)
C(23)-C(24)	1.517(2)
C(24)-C(25)	1.531(3)
C(24)-C(26)	1.533(3)
C(27)-C(28)	1.379(3)
C(28)-C(29)	1.377(3)
C(29)-C(30)	1.391(2)
C(30)-C(31)	1.520(2)
C(31)-C(33)	1.526(3)
C(31)-C(32)	1.531(3)
C(51)-C(52)	1.366(2)
C(51)-Co(2)	2.0689(16)
C(53)-C(66)	1.476(2)
C(54)-C(55)	1.400(2)
C(54)-C(62)	1.402(2)
C(55)-C(59)	1.393(2)
C(55)-C(56)	1.523(4)
C(55)-C(56')	1.541(16)
C(56)-C(58)	1.525(4)
C(56)-C(57)	1.533(5)
C(56')-C(58')	1.515(15)
C(56')-C(57')	1.519(15)
C(59)-C(60)	1.379(2)
C(60)-C(61)	1.376(2)
C(61)-C(62)	1.397(2)
C(62)-C(63)	1.521(2)
C(63)-C(65)	1.533(2)
C(63)-C(64)	1.538(2)
C(66)-C(67)	1.393(2)

C(66)-C(71)	1.398(2)
C(67)-C(68)	1.386(2)
C(68)-C(69)	1.381(3)
C(69)-C(70)	1.378(3)
C(70)-C(71)	1.386(2)
C(72)-C(73)	1.391(2)
C(72)-C(80)	1.401(2)
C(73)-C(77)	1.394(3)
C(73)-C(74)	1.520(3)
C(74)-C(75)	1.530(3)
C(74)-C(76)	1.531(3)
C(77)-C(78)	1.382(3)
C(78)-C(79)	1.377(3)
C(79)-C(80)	1.392(2)
C(80)-C(81')	1.520(3)
C(80)-C(81)	1.520(3)
C(81)-C(83)	1.528(8)
C(81)-C(82)	1.542(8)
C(81')-C(82')	1.517(9)
C(81')-C(83')	1.539(8)
Co(2)-N(6)	1.927(7)
Co(2)-N(6')	1.982(8)
N(6)-Si(7)	1.704(7)
N(6)-Si(8)	1.710(7)
Si(7)-C(92)	1.873(5)
Si(7)-C(91)	1.876(5)
Si(7)-C(90)	1.878(4)
Si(8)-C(95)	1.865(8)
Si(8)-C(94)	1.878(8)
Si(8)-C(93)	1.878(8)
N(6')-Si(8')	1.706(8)
N(6')-Si(7')	1.727(7)
Si(7')-C(91')	1.869(4)
Si(7')-C(90')	1.874(5)
Si(7')-C(92')	1.877(5)
Si(8')-C(95')	1.866(9)
Si(8')-C(93')	1.886(9)
Si(8')-C(94')	1.891(9)

N(2)-Co(1)-N(1)	121.81(6)
N(2)-Co(1)-C(1)	127.70(6)
N(1)-Co(1)-C(1)	109.94(6)
N(1)-Si(1)-C(34)	111.32(8)
N(1)-Si(1)-C(35)	114.09(9)
C(34)-Si(1)-C(35)	105.44(10)
N(1)-Si(1)-C(36)	112.80(8)
C(34)-Si(1)-C(36)	105.77(9)
C(35)-Si(1)-C(36)	106.79(9)
N(1)-Si(2)-C(37)	113.68(9)
N(1)-Si(2)-C(39)	110.18(9)
C(37)-Si(2)-C(39)	106.89(12)
N(1)-Si(2)-C(38)	113.59(9)
C(37)-Si(2)-C(38)	104.43(10)
C(39)-Si(2)-C(38)	107.61(10)
N(2)-Si(3)-C(40)	111.78(8)
N(2)-Si(3)-C(41)	113.94(8)
C(40)-Si(3)-C(41)	105.00(9)
N(2)-Si(3)-C(42)	109.83(8)
C(40)-Si(3)-C(42)	110.11(9)
C(41)-Si(3)-C(42)	105.93(9)
N(2)-Si(4)-C(45)	111.66(8)
N(2)-Si(4)-C(43)	112.23(8)
C(45)-Si(4)-C(43)	107.20(10)
N(2)-Si(4)-C(44)	113.92(8)
C(45)-Si(4)-C(44)	104.71(9)
C(43)-Si(4)-C(44)	106.58(10)
N(5)-Si(5)-C(85)	111.63(8)
N(5)-Si(5)-C(84)	110.86(8)
C(85)-Si(5)-C(84)	109.43(9)
N(5)-Si(5)-C(86)	113.60(8)
C(85)-Si(5)-C(86)	105.59(9)
C(84)-Si(5)-C(86)	105.40(9)
N(5)-Si(6)-C(89)	111.75(8)
N(5)-Si(6)-C(87)	112.70(9)
C(89)-Si(6)-C(87)	106.54(11)
N(5)-Si(6)-C(88)	113.12(9)

C(89)-Si(6)-C(88)	105.09(10)
C(87)-Si(6)-C(88)	107.11(11)
Si(2)-N(1)-Si(1)	122.78(8)
Si(2)-N(1)-Co(1)	117.23(8)
Si(1)-N(1)-Co(1)	119.42(8)
Si(4)-N(2)-Si(3)	123.97(8)
Si(4)-N(2)-Co(1)	122.47(8)
Si(3)-N(2)-Co(1)	113.30(7)
C(3)-N(3)-C(2)	108.41(13)
C(3)-N(3)-C(22)	126.91(13)
C(2)-N(3)-C(22)	124.62(13)
C(3)-N(4)-C(1)	111.74(13)
C(3)-N(4)-C(4)	121.89(13)
C(1)-N(4)-C(4)	126.26(13)
Si(6)-N(5)-Si(5)	123.62(8)
Si(6)-N(5)-Co(2)	121.46(8)
Si(5)-N(5)-Co(2)	114.57(7)
C(53)-N(7)-C(51)	111.57(13)
C(53)-N(7)-C(54)	122.28(13)
C(51)-N(7)-C(54)	126.10(13)
C(53)-N(8)-C(52)	108.51(13)
C(53)-N(8)-C(72)	127.48(13)
C(52)-N(8)-C(72)	123.98(13)
C(2)-C(1)-N(4)	102.38(13)
C(2)-C(1)-Co(1)	116.86(12)
N(4)-C(1)-Co(1)	140.30(11)
C(1)-C(2)-N(3)	110.81(14)
N(3)-C(3)-N(4)	106.62(13)
N(3)-C(3)-C(16)	125.60(14)
N(4)-C(3)-C(16)	127.60(14)
C(12)-C(4)-C(5)	122.53(15)
C(12)-C(4)-N(4)	118.86(14)
C(5)-C(4)-N(4)	118.46(14)
C(9)-C(5)-C(4)	117.58(15)
C(9)-C(5)-C(6)	119.0(3)
C(4)-C(5)-C(6)	123.3(3)
C(9)-C(5)-C(6')	121.4(13)
C(4)-C(5)-C(6')	120.1(12)

C(5)-C(6)-C(8)	108.1(3)
C(5)-C(6)-C(7)	113.5(3)
C(8)-C(6)-C(7)	110.0(4)
C(8')-C(6')-C(7')	112.3(19)
C(8')-C(6')-C(5)	115(2)
C(7')-C(6')-C(5)	105.9(11)
C(10)-C(9)-C(5)	121.14(16)
C(9)-C(10)-C(11)	120.20(16)
C(10)-C(11)-C(12)	121.57(16)
C(11)-C(12)-C(4)	116.94(15)
C(11)-C(12)-C(13)	118.25(15)
C(4)-C(12)-C(13)	124.80(15)
C(12)-C(13)-C(14)	111.23(14)
C(12)-C(13)-C(15)	111.17(15)
C(14)-C(13)-C(15)	108.69(15)
C(17)-C(16)-C(21)	118.66(15)
C(17)-C(16)-C(3)	120.08(15)
C(21)-C(16)-C(3)	121.22(15)
C(18)-C(17)-C(16)	120.61(16)
C(19)-C(18)-C(17)	120.25(17)
C(18)-C(19)-C(20)	119.84(16)
C(19)-C(20)-C(21)	120.58(16)
C(20)-C(21)-C(16)	120.05(16)
C(23)-C(22)-C(30)	123.62(15)
C(23)-C(22)-N(3)	118.56(14)
C(30)-C(22)-N(3)	117.82(14)
C(22)-C(23)-C(27)	116.63(16)
C(22)-C(23)-C(24)	123.09(15)
C(27)-C(23)-C(24)	120.28(16)
C(23)-C(24)-C(25)	111.32(15)
C(23)-C(24)-C(26)	111.09(16)
C(25)-C(24)-C(26)	110.84(15)
C(28)-C(27)-C(23)	121.19(17)
C(29)-C(28)-C(27)	120.63(17)
C(28)-C(29)-C(30)	121.05(17)
C(29)-C(30)-C(22)	116.86(16)
C(29)-C(30)-C(31)	120.33(15)
C(22)-C(30)-C(31)	122.81(15)

C(30)-C(31)-C(33)	110.16(15)
C(30)-C(31)-C(32)	112.10(16)
C(33)-C(31)-C(32)	110.98(17)
C(52)-C(51)-N(7)	102.39(13)
C(52)-C(51)-Co(2)	116.40(12)
N(7)-C(51)-Co(2)	140.82(12)
C(51)-C(52)-N(8)	110.89(14)
N(8)-C(53)-N(7)	106.61(13)
N(8)-C(53)-C(66)	125.57(14)
N(7)-C(53)-C(66)	127.55(14)
C(55)-C(54)-C(62)	122.34(15)
C(55)-C(54)-N(7)	118.30(14)
C(62)-C(54)-N(7)	119.20(14)
C(59)-C(55)-C(54)	117.70(15)
C(59)-C(55)-C(56)	118.6(3)
C(54)-C(55)-C(56)	123.6(3)
C(59)-C(55)-C(56')	121.2(11)
C(54)-C(55)-C(56')	120.6(11)
C(55)-C(56)-C(58)	108.6(3)
C(55)-C(56)-C(57)	113.3(3)
C(58)-C(56)-C(57)	110.5(4)
C(58')-C(56')-C(57')	112.4(19)
C(58')-C(56')-C(55)	112.2(17)
C(57')-C(56')-C(55)	108.0(13)
C(60)-C(59)-C(55)	121.11(16)
C(61)-C(60)-C(59)	120.12(16)
C(60)-C(61)-C(62)	121.48(16)
C(61)-C(62)-C(54)	117.19(15)
C(61)-C(62)-C(63)	117.93(15)
C(54)-C(62)-C(63)	124.87(15)
C(62)-C(63)-C(65)	111.23(14)
C(62)-C(63)-C(64)	111.41(14)
C(65)-C(63)-C(64)	108.52(14)
C(67)-C(66)-C(71)	118.76(15)
C(67)-C(66)-C(53)	120.00(15)
C(71)-C(66)-C(53)	121.20(15)
C(68)-C(67)-C(66)	120.61(16)
C(69)-C(68)-C(67)	120.13(17)

C(70)-C(69)-C(68)	119.85(16)
C(69)-C(70)-C(71)	120.62(17)
C(70)-C(71)-C(66)	120.02(17)
C(73)-C(72)-C(80)	123.71(16)
C(73)-C(72)-N(8)	118.64(15)
C(80)-C(72)-N(8)	117.65(15)
C(72)-C(73)-C(77)	116.81(17)
C(72)-C(73)-C(74)	122.85(16)
C(77)-C(73)-C(74)	120.34(16)
C(73)-C(74)-C(75)	111.70(16)
C(73)-C(74)-C(76)	110.73(15)
C(75)-C(74)-C(76)	111.05(16)
C(78)-C(77)-C(73)	121.13(18)
C(79)-C(78)-C(77)	120.42(17)
C(78)-C(79)-C(80)	121.22(18)
C(79)-C(80)-C(72)	116.70(17)
C(79)-C(80)-C(81')	120.34(16)
C(72)-C(80)-C(81')	122.95(15)
C(79)-C(80)-C(81)	120.34(16)
C(72)-C(80)-C(81)	122.95(15)
C(80)-C(81)-C(83)	110.9(5)
C(80)-C(81)-C(82)	109.6(6)
C(83)-C(81)-C(82)	110.9(6)
C(82')-C(81')-C(80)	113.0(7)
C(82')-C(81')-C(83')	109.8(7)
C(80)-C(81')-C(83')	112.0(5)
N(6)-Co(2)-N(5)	119.4(4)
N(5)-Co(2)-N(6')	125.4(5)
N(6)-Co(2)-C(51)	111.8(4)
N(5)-Co(2)-C(51)	127.50(6)
N(6')-Co(2)-C(51)	106.9(5)
Si(7)-N(6)-Si(8)	126.9(5)
Si(7)-N(6)-Co(2)	115.1(4)
Si(8)-N(6)-Co(2)	116.9(4)
N(6)-Si(7)-C(92)	113.0(4)
N(6)-Si(7)-C(91)	110.8(5)
C(92)-Si(7)-C(91)	108.1(3)
N(6)-Si(7)-C(90)	113.2(3)

C(92)-Si(7)-C(90)	104.4(2)
C(91)-Si(7)-C(90)	107.0(2)
N(6)-Si(8)-C(95)	112.2(7)
N(6)-Si(8)-C(94)	112.8(6)
C(95)-Si(8)-C(94)	106.0(6)
N(6)-Si(8)-C(93)	111.8(6)
C(95)-Si(8)-C(93)	106.5(6)
C(94)-Si(8)-C(93)	107.0(6)
Si(8')-N(6')-Si(7')	120.7(5)
Si(8')-N(6')-Co(2)	122.7(5)
Si(7')-N(6')-Co(2)	116.6(4)
N(6')-Si(7')-C(91')	110.8(3)
N(6')-Si(7')-C(90')	114.4(6)
C(91')-Si(7')-C(90')	105.4(3)
N(6')-Si(7')-C(92')	111.9(5)
C(91')-Si(7')-C(92')	105.9(3)
C(90')-Si(7')-C(92')	108.0(3)
N(6')-Si(8')-C(95')	110.1(8)
N(6')-Si(8')-C(93')	115.4(6)
C(95')-Si(8')-C(93')	104.0(7)
N(6')-Si(8')-C(94')	116.4(7)
C(95')-Si(8')-C(94')	106.3(7)

REFERENCES

(1) Ghadwal, R. S.; Reichmann, S. O.; Herbst-Irmer, R., *Chem. Eur. J.* **2015,** *21*, 4247–4251.
(2) Bryan, A. M.; Long, G. J.; Grandjean, F.; Power, P. P., *Inorg. Chem.* **2013,** *52*, 12152–12160.
(3) Kahn, O., *Molecular magnetism*. VCH-Verlag, Weinheim: New York, 1993.
(4) a) Stalke, D., *Chem Soc Rev* **1998,** *27*, 171–178; b) Kottke, T.; Stalke, D., *J. Appl. Crystallogr.* **1993,** *26*, 615–619.
(5) Bruker AXS Inc. *SAINT v8.30C*, WI, USA: Madison, 2013.
(6) Krause, L.; Herbst-Irmer, R.; Sheldrick, G. M.; Stalke, D., *J. Appl. Crystallogr.* **2015,** *48*, 3–10.
(7) Sheldrick, G. M., *Acta Cryst. A* **2015,** *71*, 3–8.
(8) Sheldrick, G., *Acta Cryst. C* **2015,** *71*, 3–8.
(9) Huebschle, C. B.; Sheldrick, G. M.; Dittrich, B., *Acta Cryst. A* **2011,** *67*, C592.