Supporting Information for

Three-Coordinate and Four-Coordinate Cobalt Hydride Complexes That React with Dinitrogen

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General Considerations. All manipulations were performed under argon atmosphere in an M. Braun glove box maintained at or below 1 ppm of O_2, or by Schlenk techniques. Glassware was dried at 150 °C overnight. NMR data were recorded on a Bruker Avance 400 or 500 MHz spectrometer. All peaks in the NMR spectra are singlets, referenced to residual C_6D_5H at δ 7.16 ppm. In some cases, it was not possible to determine integrations because of peak overlap. IR spectra were recorded on a Mattson Instruments 6020 Galaxy Series FTIR, with a resolution of 4 cm^{-1}. UV-vis spectra were measured on a Cary 50 spectrophotometer, using screw-cap cuvettes. Solution magnetic susceptibilities were determined by the Evans method.[1] Elemental analyses were determined by Columbia Analytical Services, Tucson, AZ. The nitrogen and carbon analysis on the extremely sensitive compounds reported here was often low, probably from some decomposition during transport and/or handling. Sample purity was verified by integrating the NMR resonances against an internal integration standard of a capillary of LFeCl,[2] which typically indicated > 90% of the expected integration (except **1**, as described below).

Pentane, diethyl ether and toluene were purified by passage through activated alumina and "deoxygenizer" columns from Glass Contour Co. Deuterated benzene was first dried over CaH_2, then over Na/benzophenone, and then vacuum transferred into a storage container. Before use, an aliquot of each solvent was tested with a drop of sodium benzophenone ketyl in THF solution. Celite was dried overnight at 200 °C under vacuum. The preparation of LCoCl has been reported.[3] Cyclohexene (Aldrich) was degassed, vacuum transferred to a new container and stored over molecular sieves in the glovebox at -35 °C. $KHBEt_3$ was synthesized by a literature procedure from KH and BEt_3,[4] and $KDBEt_3$ was synthesized in an analogous fashion using KD. KD was purchased from AECR. Naphthalene was purified by vacuum sublimation.

Synthesis and Characterization of $[LCoH]_2$ (1). In an argon-filled glove box, a resealable flask was charged with LCoCl (169 mg, 0.283 mmol) and $KHBEt_3$ (39.0 mg, 0.283 mmol). The headspace was evacuated, and toluene (18 mL) was vacuum transferred into the flask at 77 K. The flask was warmed to room temperature and the mixture was stirred while allowing it to slowly warm. After 15 min, the volatile materials were removed under vacuum. In an argon-filled glovebox, the residue was extracted with 10 mL pentane, and filtered through Celite to give a yellow solution which was concentrated to 6 mL. Toluene (4 mL) was added, and the solution was cooled to –35 °C to give dark yellow crystals (114 mg, 72%). ^{1}H NMR (C_6D_6, 295 K): δ 22.9, 18.2, 3.2, 1.6, -9.8, -17.6 ppm. (See Figure S-1 for the room-temperature ^{1}H NMR spectrum, demonstrating the presence of impurities; see Figure S-2 for variable-temperature ^{1}H NMR spectra.) μ_{eff} (Evans, C_6D_6, 295 K) = 6.4(4) μ_B. UV-vis (pentane): 920 (ε = 4400 $M^{-1}cm^{-1}$), 519 (ε = 11300 $M^{-1}cm^{-1}$) nm. Anal. Calcd. for $C_{70}H_{108}N_4Co_2$: C 74.83, H 9.69, N 4.99. Found: C 74.25, H 8.98, N 4.02. The synthesis of **1-D** used an analogous procedure with $KDBEt_3$. The ^{1}H NMR and IR spectra of **1** and of **1-D** were identical (Figures S-3 and S-4).

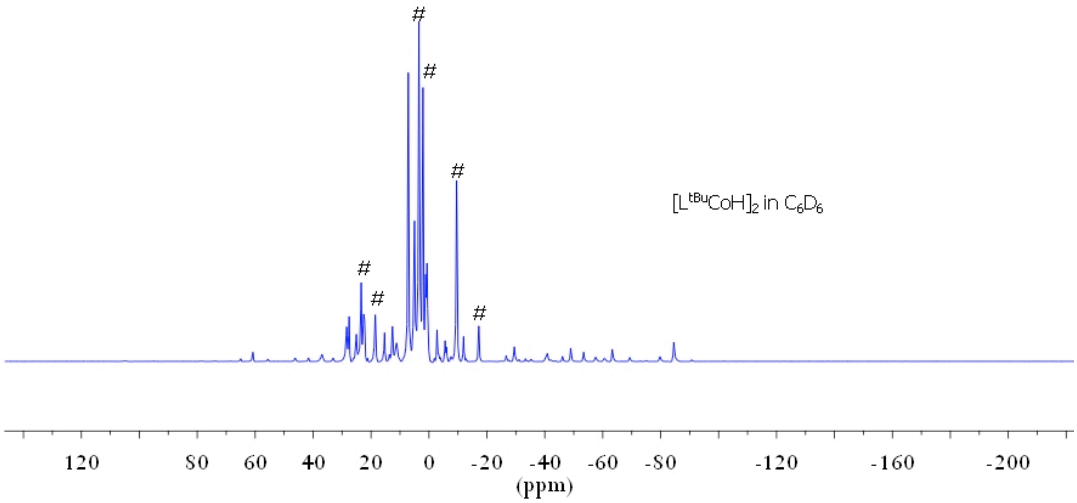


Figure S-1. ^{1}H NMR spectrum of **1** in C_6D_6. Peaks labeled # are assigned to **1**, because these are the only peaks that change upon addition of N_2.

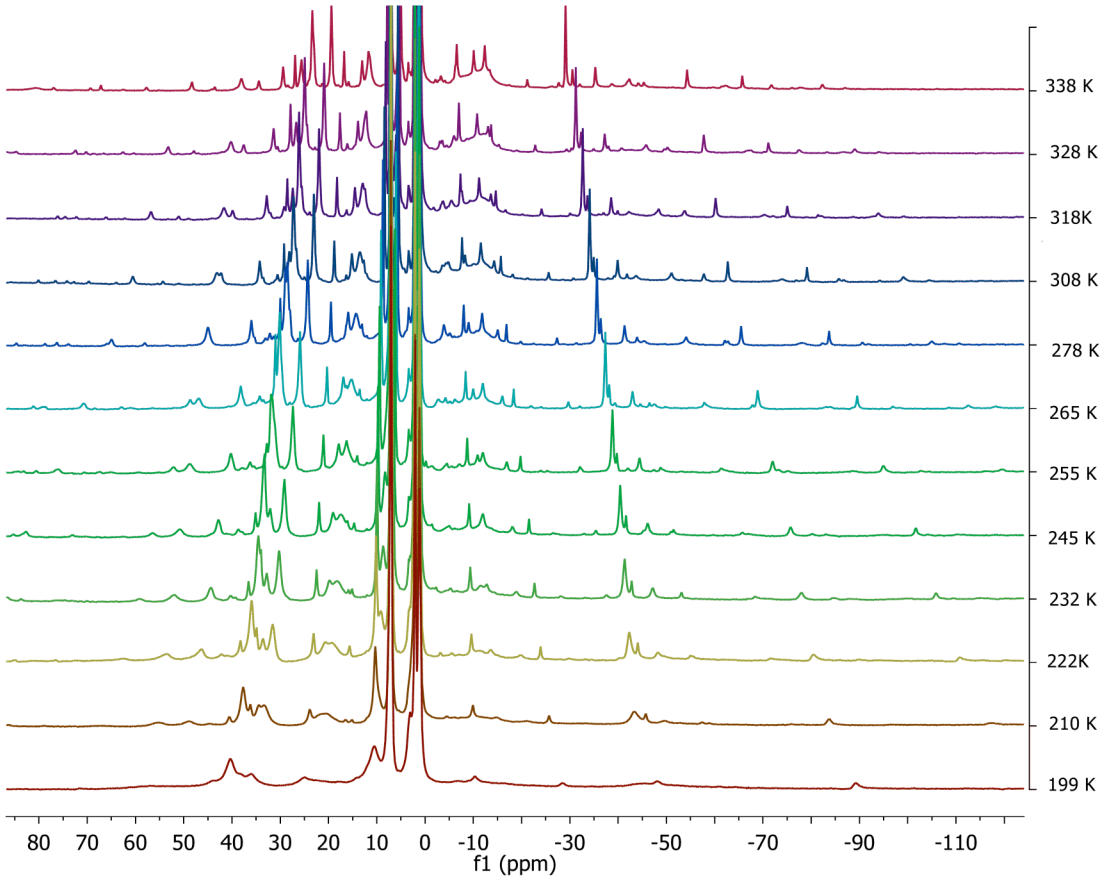


Figure S-2. Variable-temperature ^{1}H NMR spectra of a solution of **1** in toluene-d_8. The only major change is greater broadening and shifting at low temperature because of the higher magnetism (as expected from the Curie Law).

The FTIR spectra of **1** and **1-D** were identical, and showed no obvious Co-H stretching band. KBr: 2954 (s), 2929 (m), 1523 (w), 1460 (m), 1378 (s), 1356 (s), 1310 (s), 1218 (m), 1153 (w), 1089 (s), 798 (m), 756 (s) cm^{-1}.

Figure S-3. IR spectrum of **1**.

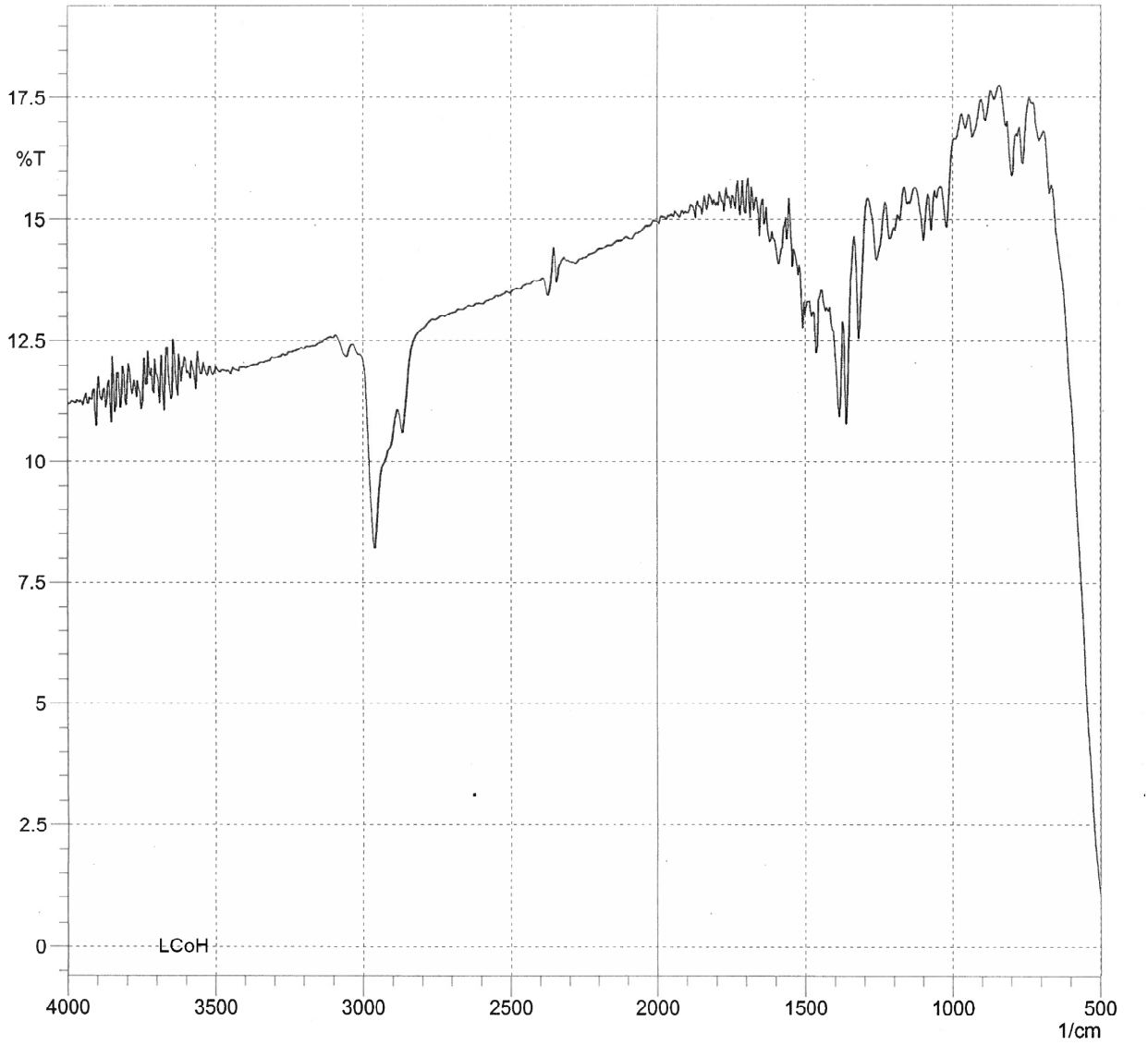
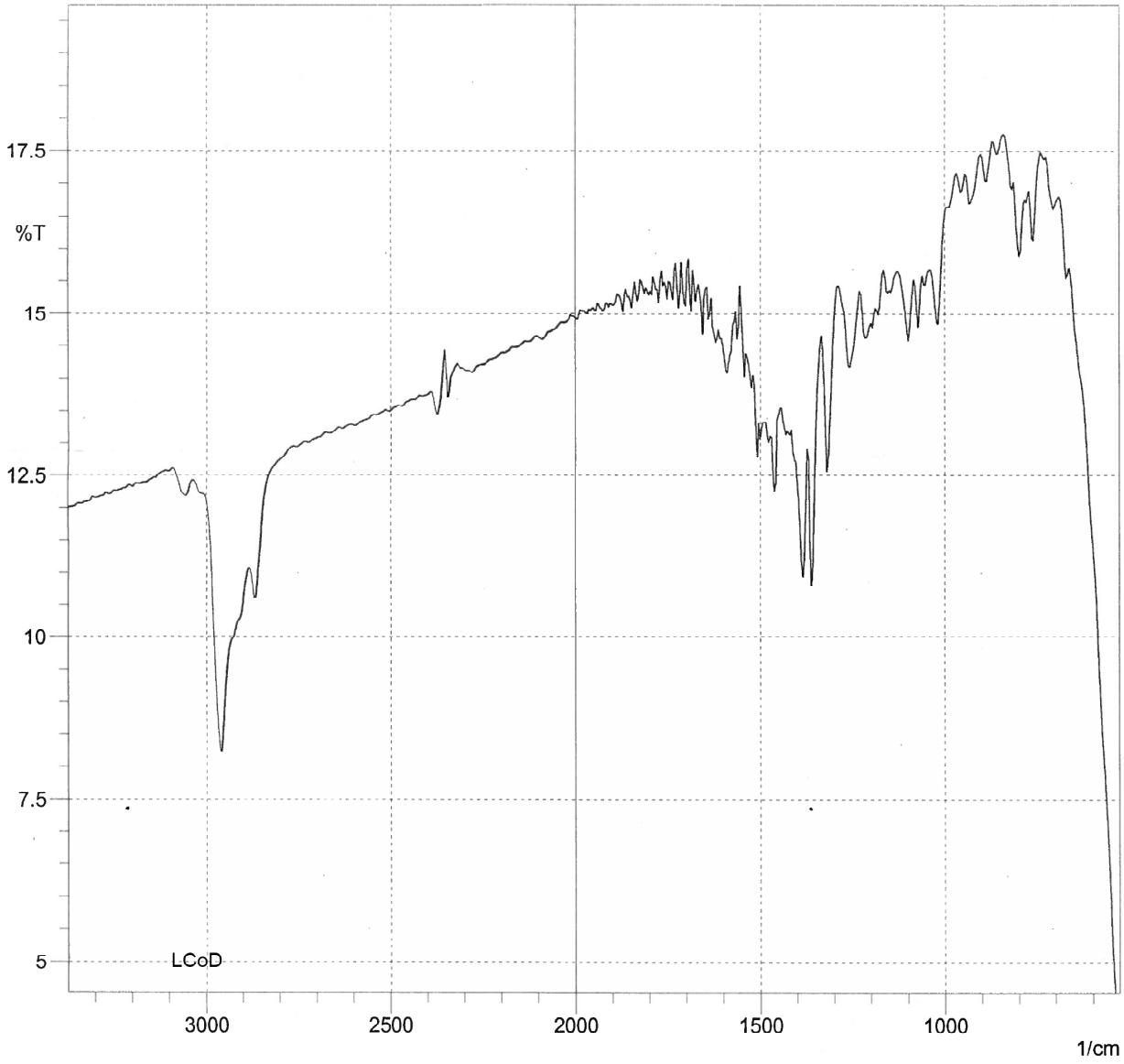


Figure S-4. IR spectrum of **1-D**.



Synthesis and Characterization of [KLCoH]$_2$ (2). Under argon atmosphere, a solution of $KHBEt_3$ (106 mg, 0.769 mmol) in cold toluene (5 mL, -35 °C) was added to a stirred red-brown solution of LCoCl (231 mg, 0.387 mmol) in cold toluene (10 mL, -35 °C). The color changed to yellow-brown, then red-brown with the formation of white precipitate in a few minutes. The mixture was stirred for 15 minutes, followed by removal of volatile materials under vacuum to give a red-brown solid. The solid was extracted with pentane (10 mL) and filtered through Celite. Removal of volatile materials gave a red-brown solid which was then rinsed with cold pentane (2 mL) and was used without further purification (162 mg, 70%). Single crystals came from cooling a pentane/toluene solution. ^{1}H NMR (500 MHz, C_6D_6): δ 53.7 (8H, *m*-*H* or C*H*$(CH_3)_2$), 28.6 (8H, *m*-*H* or C*H*$(CH_3)_2$), 9.5 (24H, CH(C*H*$_3)_2$), -9.4 (36H, C(C*H*$_3)_3$), -13.7 (24H, CH(C*H*$_3)_2$), -50.7 (4H, p-*H*), -114.3 (2H, backbone C-*H*) ppm. The spectrum was similar in THF-d_8 and in cyclohexane-d_{12} (Figure S-5), and showed little change with temperature (Figure S-6). μ_{eff} (Evans, C_6D_6, 295 K): 5.6(2) μ_B. Anal. Calcd. for $K_2C_{70}H_{108}N_4Co_2$: C 69.96, H 9.06, N 4.66. Found C 70.02, H 9.20, N 4.28. UV-vis (pentane): 824 (ε = 600 $M^{-1}cm^{-1}$), 707 (ε = 2100 $M^{-1}cm^{-1}$), 560 (ε = 200 $M^{-1}cm^{-1}$), 422 (ε = 11100 $M^{-1}cm^{-1}$), 311 (ε = 28900 $M^{-1}cm^{-1}$) nm. The synthesis of **2-D** used an analogous procedure with $KDBEt_3$. The ^{1}H NMR and IR spectra of **2** and of **2-D** were identical (Figures S-7 and S-8).

Solution Molecular Weight of 2. A Schlenk flask was charged with **2** (11.9 mg) and naphthalene (92.7 mg) under argon. The mixture was warmed and melted until the cobalt complex completely dissolved. After cooling the waxy solid, a small portion was placed in three melting-point capillaries, each of which was sealed. This procedure was done with two different concentrations of **2**. Melting point depressions, compared to that of authentic naphthalene, were measured on a Thomas Hoover melting point apparatus, using a VWR Precision 0.01 Thermometer equipped with a Pt-100Ω sensor. Molecular weights were determined using the formula: molecular weight = $K \cdot w \cdot 1000/\Delta T \cdot W$, where K = 4.9 for naphthalene, w = weight of **2**, W = weight of naphthalene and ΔT = temperature depression.[5]

Table S-1. Molecular-weight measurements for **2**.

Mass of **2** (mg)	Mass of naph. (mg)	Melting point (°C)	ΔT (° C)	Calcd. MW
11.9	92.7	79.88	0.52	1210
11.9	92.7	79.82	0.58	1084
11.9	92.7	79.81	0.59	1068
16.2	80.1	79.51	0.89	1113
16.2	80.1	79.60	0.80	1232
16.2	80.1	79.53	0.87	1139

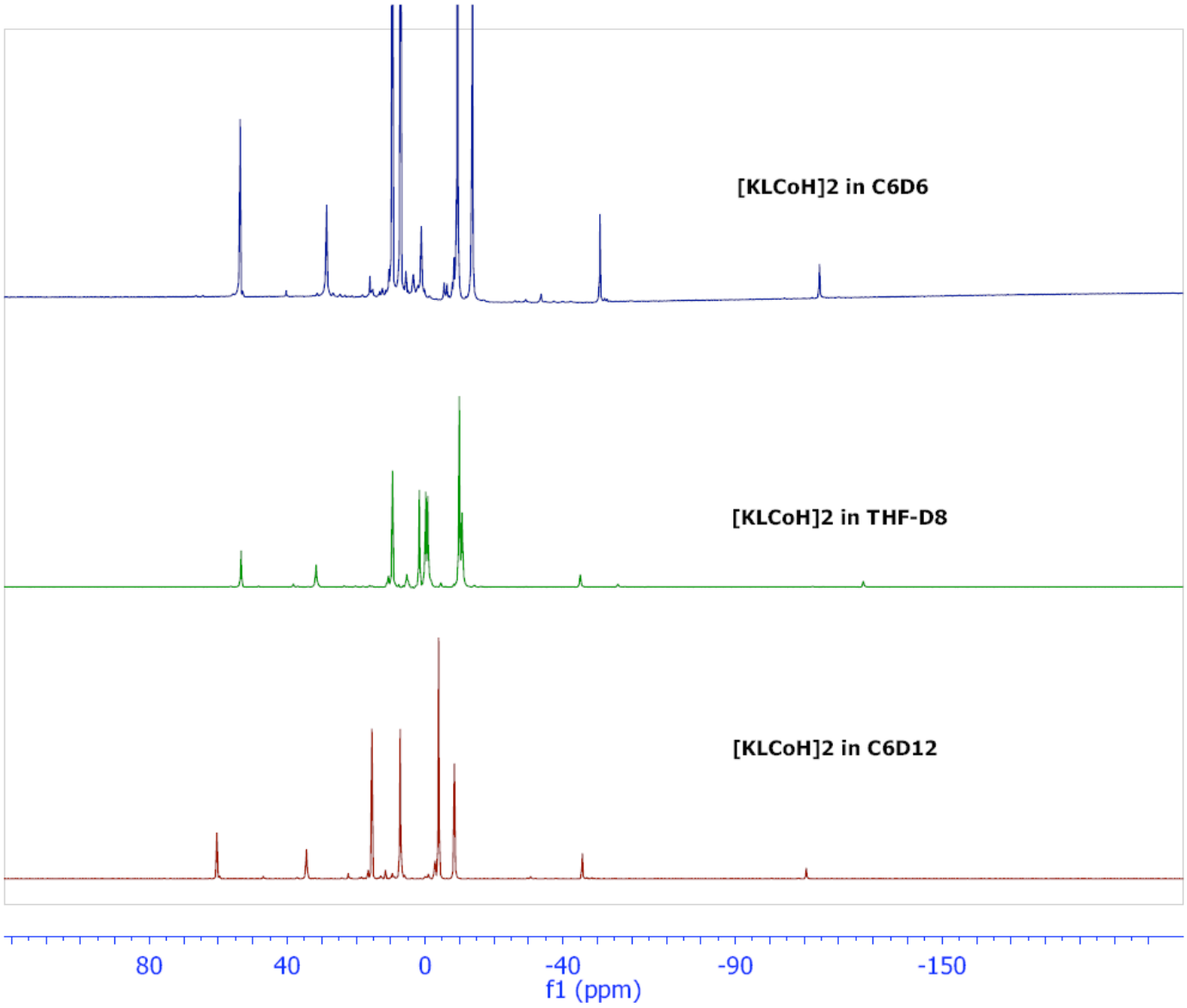


Figure S-5. ^{1}H NMR spectra of $[KLCoH]_2$ (2) in C_6D_6, THF-d_8, and C_6D_{12}.

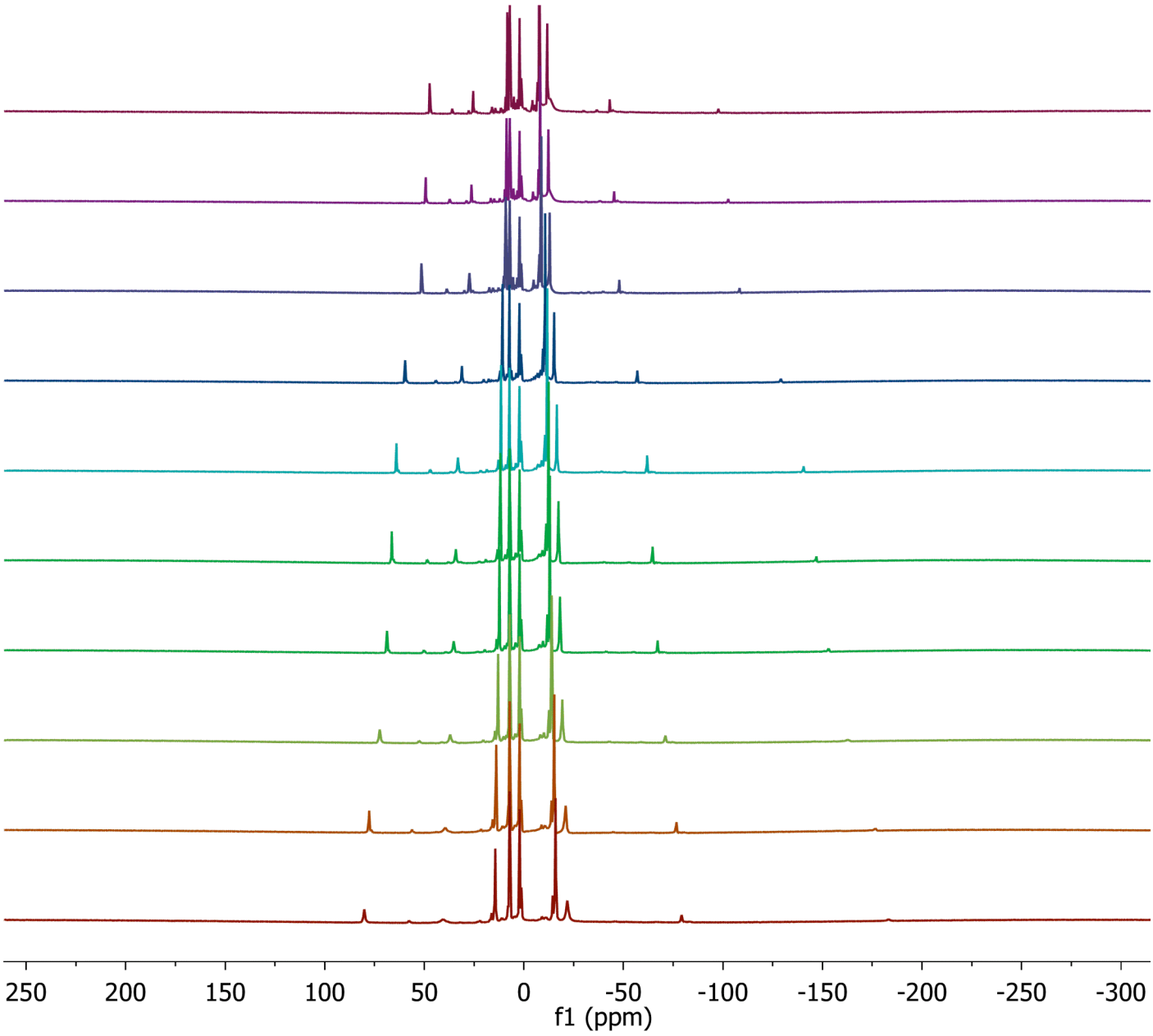


Figure S-6. Variable-temperature ^{1}H NMR spectra of a solution of **2** in toluene-d_8. The only major change is greater broadening and shifting at low temperature because of the higher magnetism (as expected from the Curie Law).

The FTIR spectra of **2** and **2-D** were identical, and showed no obvious Co-H stretching band. KBr: 2953 (s), 2930 (m), 1520 (w), 1504 (m), 1452 (m), 1421 (s), 1378 (s), 1375 (s), 1352 (s), 1313 (s), 1208 (m), 1150 (w), 1092 (s), 789 (m), 745 (s) cm^{-1}.

Figure S-7. IR spectrum of **2**.

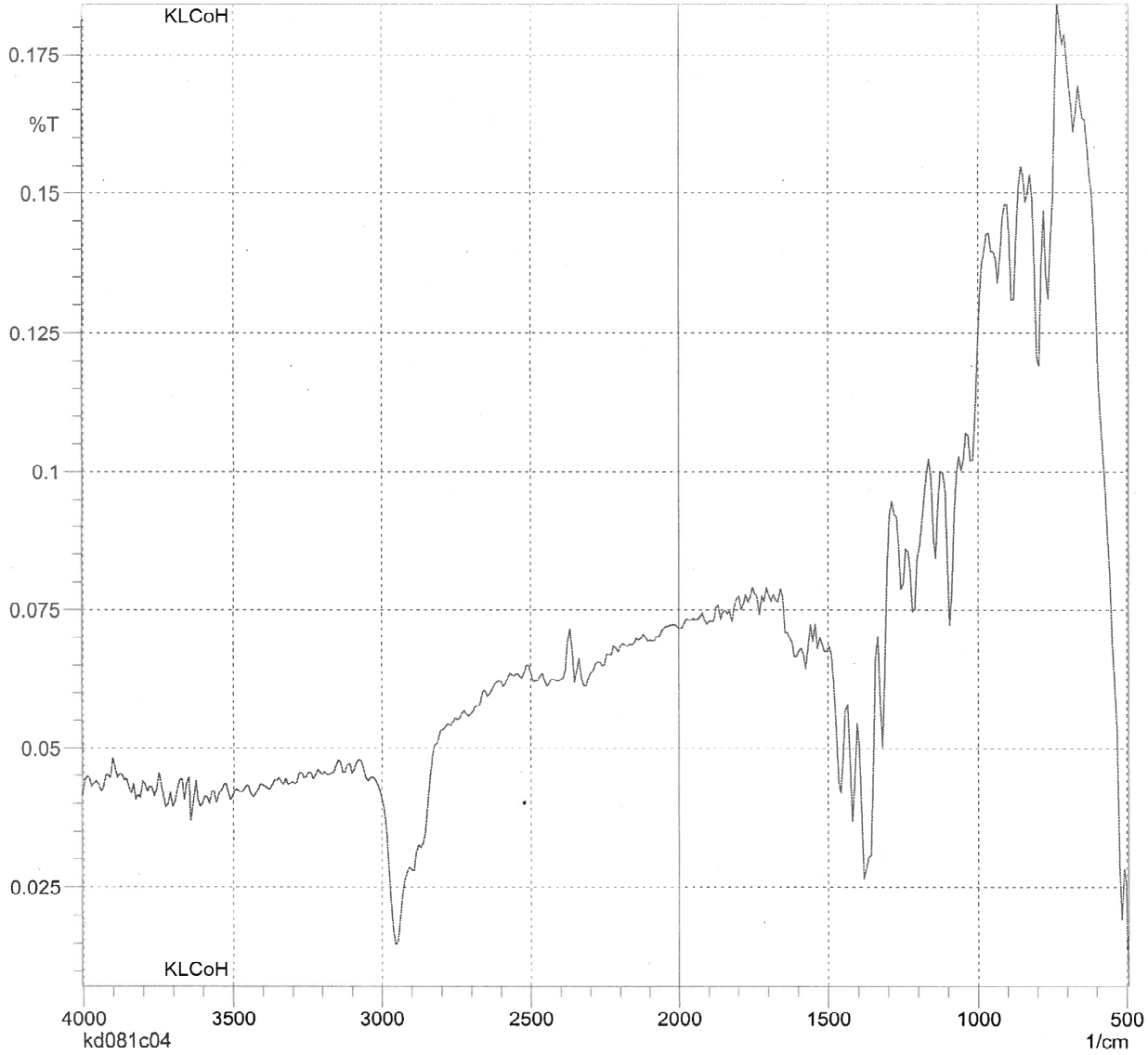
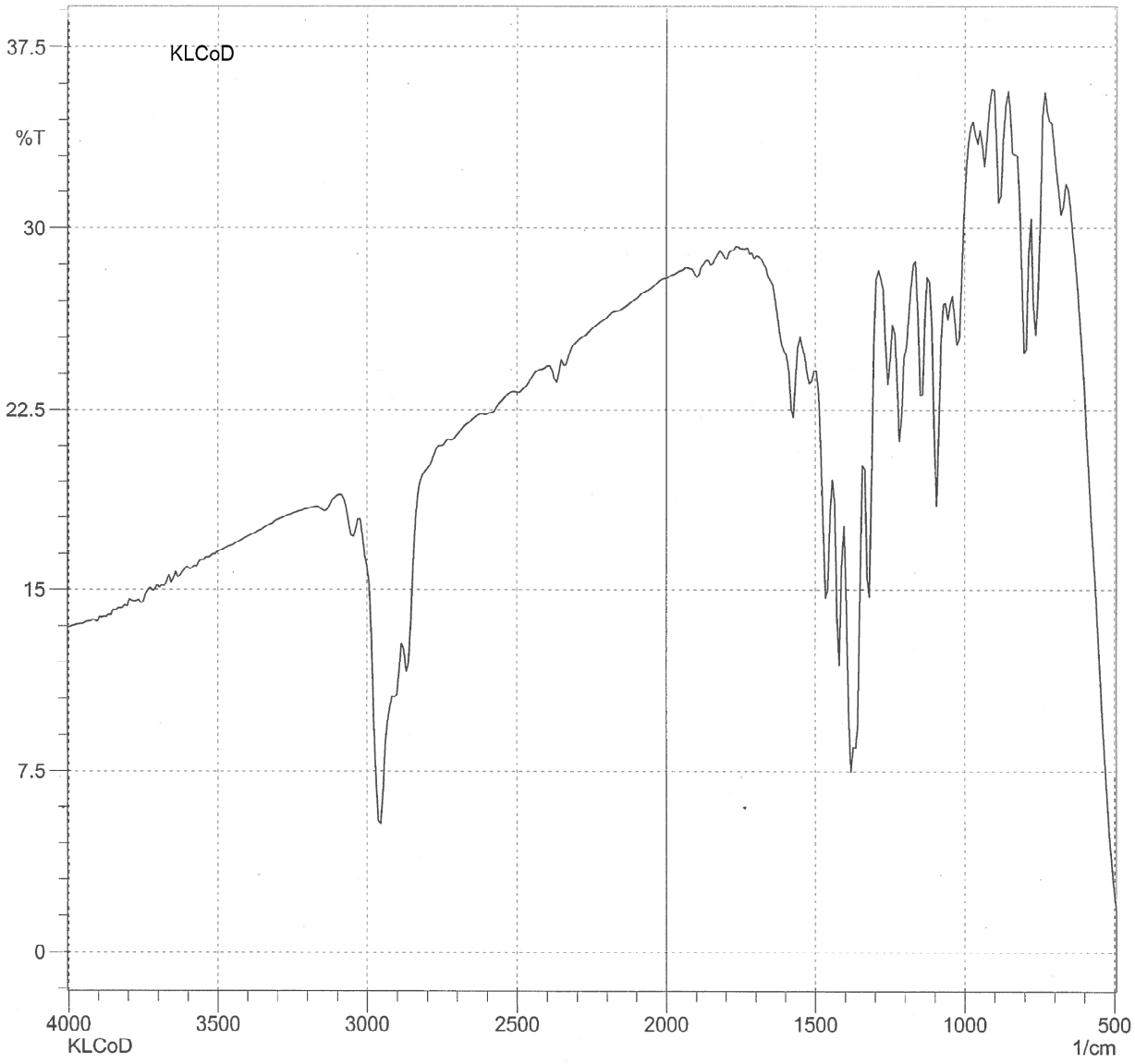
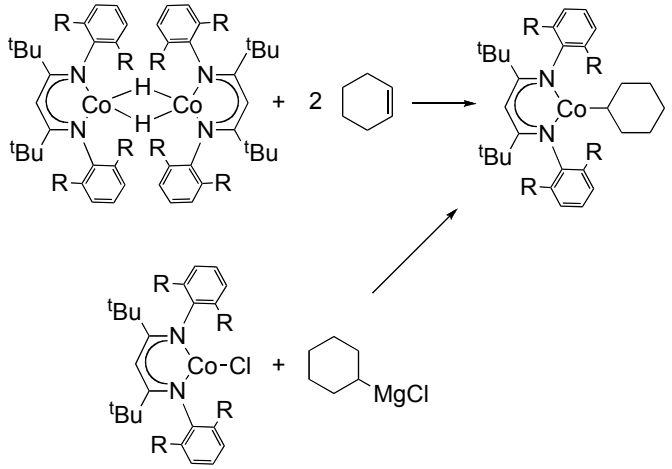


Figure S-8. IR spectrum of **2-D**.



Reaction of 1 with cyclohexene to give LCoCy. Cyclohexene (16.5 μL, 161 μmol) was added via a syringe to a solution of **1** (91 mg, 83 μmol) in Et_2O (15 mL). Over the course of 1 h, the brown solution became yellow in color. The volatiles were removed in vacuum. The yellow solid was extracted with diethyl ether (12 mL), reduced to 8 mL and cooled at -35 °C to give yellow crystals (71 mg, 68%). The ^{1}H NMR spectrum was identical to a that of L^{tBu}CoCy, as prepared below.



Scheme S-1. Two routes to LCoCy.

Independent preparation of LCoCy. To a stirred red brown slurry of LCoCl (93 mg, 0.16 mmol) in Et_2O (15 mL) was added cyclohexylmagnesium chloride (0.08 mL, 2.0 M in Et_2O, 0.16 mmol), giving an immediate color change to yellow with formation of a white precipitate. The mixture was stirred for 2 h, filtered through Celite, concentrated to 8 mL and cooled at -35 °C to give yellow crystals (91.4 mg, 91%). ^{1}H NMR (500 MHz, C_6D_6): δ 132.7 (2H, Cy-γ-CH_2), 113.1 (1H, backbone C-H), 68.2 (4H, *m*-H or C*H*$(CH_3)_2$), 27.9 (18H, C$(CH_3)_3$), -2.4 (12H, CH(C*H*$_3)_2$), -28.3 (2H, *p*-H), -52.9 (4H, *m*-H or C*H*$(CH_3)_2$), -125.3 (12H, CH(C*H*$_3)_2$) ppm. μ_{eff} (Evans, C_6D_6, 295 K) = 4.8(2) μ_B. Anal. Calcd. for $C_{41}H_{58}N_2Co$: C 77.20, H 9.16, N 4.39. Found C 76.02, H 9.23, N 4.27. UV-vis (Et_2O): 886 (ε = 5400 $M^{-1}cm^{-1}$), 486 (ε = 12260 $M^{-1}cm^{-1}$), 358 (ε = 21600

$M^{-1}cm^{-1}$) nm. IR (KBr): 2952 (s), 1519 (w), 1443 (m), 1401 (s), 1382 (s), 1375 (s), 1354 (s), 1311 (s), 1201 (m), 1153(w), 1094 (s), 793 (m), 753 (s) cm^{-1}.

Activation of N_2 by 1. In an argon filled glove box, a J. Young resealable NMR tube was charged with **1** (9.5 mg, 8.7 μmol) and C_6D_6 (0.4 mL). An internal reference consisting of a capillary containing a solution of $L^{tBu}FeCl$ (22.5 mM) in C_6D_6 was added. The sample was degassed, taken into a N_2-filled box and briefly opened. The tube was then shaken on a vortex mixer. ^1H NMR spectra were recorded after 1 h, showing the formation of a product with an ^1H NMR spectrum identical to LCoNNCoL with a yield of 89%. (The unknown impurities present in **1** did not change, indicating that they do not react with dinitrogen. See Figure S-9.) ^1H NMR (500 MHz, C_6D_6, 295 K): δ 92.0 (2H, backbone C-H), 40.8 (36H, $C(CH_3)_3$), 8.2 (8H, *m*-H or $CH(CH_3)_2$), -12.4 (24H, $CH(CH_3)_2$), -45.3 (8H, $CH(CH_3)_2$ or *m*-H), -67.8 (24H, $CH(CH_3)_2$), -73.6 (4H, *p*-H) ppm.

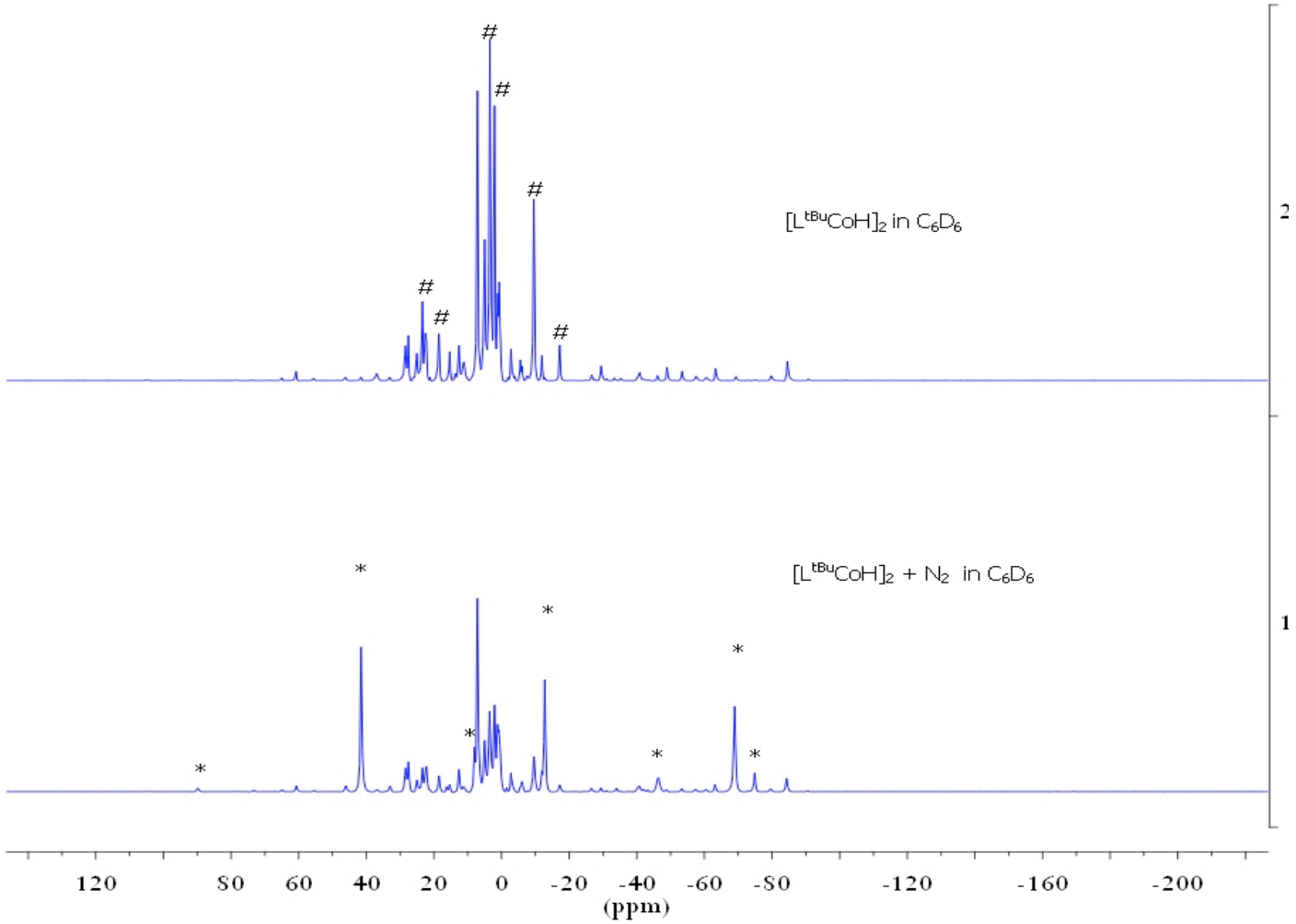


Figure S-9. ^{1}H NMR spectra of the reaction of 1 with dinitrogen (C_6D_6). Peaks labeled # are from complex 1, peaks labeled * are from LCoNNCoL.

Crossover Experiment with 1 and 1-D. A 25 mL Schlenk tube was charged with **1** (256 mg) and **1-D** (256 mg) under argon, evacuated, and brought into an N_2-filled glove box. Toluene (35 mL) was added to the flask under nitrogen, and the mixture was stirred for 2 h. A septum was attached to the branch of the tube. 2.5 mL gas was removed by syringe and injected to a NMR tube containing C_6D_6. H_2 and HD were detected by ^1H NMR (Figure S-10).

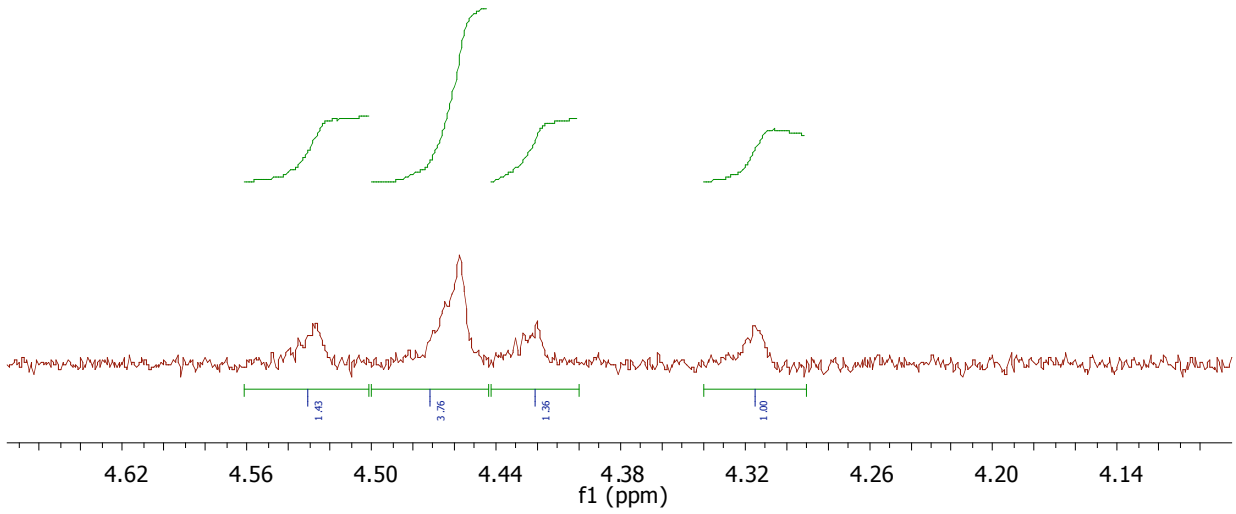


Figure S-10.

Activation of N_2 by 2. In an argon-filled glove box, a resealable NMR tube was charged with **2** (4.1 mg, 3.5 μmol) and C_6D_6 (0.3 mL). An internal reference consisting of a capillary containing a solution of LFeCl (22.5 mM) in C_6D_6 was added. After the sample was degassed, the tube was taken into an N_2-filled glove box and opened to let N_2 in. The tube was then shaken on a vortex mixer. ^{1}H NMR spectra were recorded every 20 to 40 minutes (Figure S-11). After about 7 h, ^{1}H NMR spectra showed full conversion to K_2LCoNNCoL with a yield of 91%. ^{1}H NMR (500 MHz, C_6D_6, 295 K): δ 24.9 (8H, *m*-H or C*H*$(CH_3)_2$), 18.6 (8H, C*H*$(CH_3)_2$ or *m*-H), 10.6 (24H, CH(C*H*$_3)_2$), 3.3 (24H, CH(C*H*$_3)_2$), -5.4 (36H, C(C*H*$_3)_3$), -25.1 (4H, *p*-H), -72.4 (2H, backbone C-H) ppm.

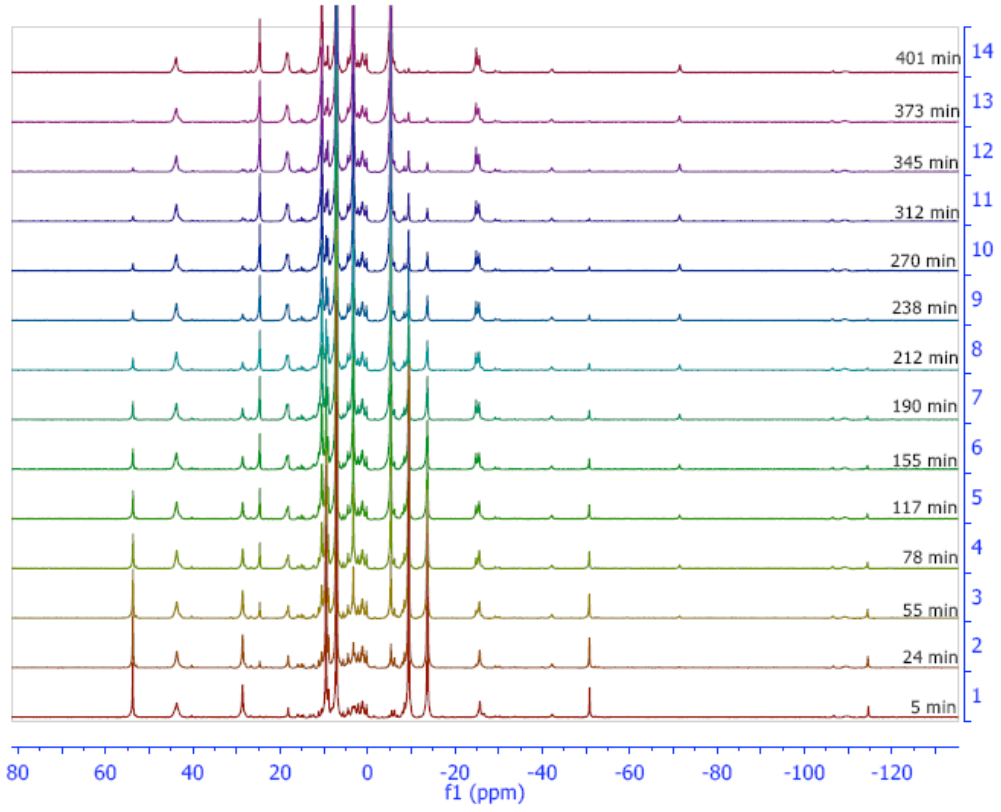


Figure S-11. ^{1}H NMR spectra of the reaction of **2** with N_2 (C_6D_6). LFeCl was used as an internal integration standard.

Crossover Experiment with 2 and 2-D. A 25 mL Schlenk tube was charged with **1** (202 mg) and **1-D** (202 mg) under argon, evacuated, and brought into an N_2-filled glove box. Toluene (30 mL) was added to the flask under nitrogen, and the mixture was stirred for 24 h. A septum was attached to the branch of the tube. 2.5 mL of the headspace was removed by syringe and injected to a NMR tube containing C_6D_6. Only H_2 was detected by ^1H NMR, with no HD detectable (Figure S-12).

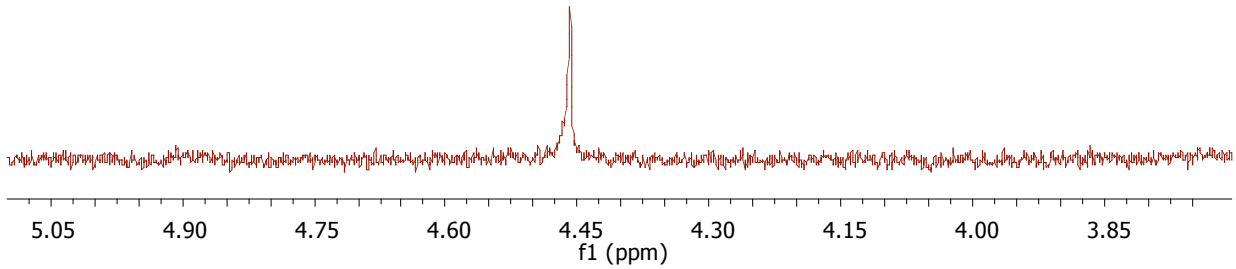


Figure S-12.

GC quantification of H_2.

Calibration Plot: A 25 mL round bottom flask was charged with toluene (10 mL) and a magnetic stir bar. A vacuum adaptor was attached with a septum on top. 8.0 mL of gas from the headspace was removed using a syringe, and 8.0 mL of CH_4 was injected into the closed system as an internal standard. A sample of H_2 was injected to the flask (0.20 mL, 0.60 mL, 1.0 mL, 1.4 mL, 1.8 mL, at 1051 mbar). An aliquot of the headspace was then injected into a GC-17A gas chromatograph (Shimadzu) with a 5 Å molecular sieve column (30 m × 0.25 mm, oven temperature 26 °C, carrier gas N_2, 600 kPa). A calibration plot was obtained by plotting the ratio of GC peak integrations H_2/CH_4 versus the amount of hydrogen added to the flask.

Table S-2. GC calibration plot data.

V_{H2}/ mL	Integration of H_2 peak	Integration of CH_4 peak	Integration Ratio of H_2:CH_4
0.2	8.011	91.899	0.087
0.6	21.432	78.543	0.273
1	31.078	68.902	0.451
1.4	39.831	60.121	0.663
1.8	45.232	54.732	0.826

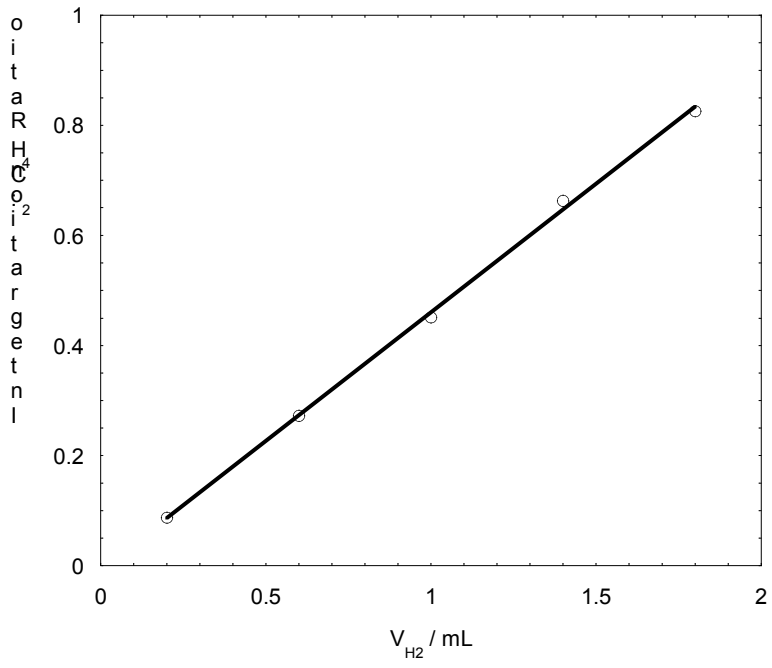


Figure S-13. GC calibration plot.

Detection of evolved H_2 from 1 + N_2. In an argon-filled box, the same round bottom flask used for the H_2 calibration was charged with **1** (43 mg, 38 μmol) and a stir bar. The flask was then closed at the vacuum adaptor, taken into a N_2 box and 8 mL of gas was taken out. 10 mL of toluene was injected and the mixture was stirred at room temperature for 2 h. The whole set-up was then taken out of the glove box, 8 mL CH_4 was added and the headspace was subjected to GC analysis as described above. The integration ratio was compared to the calibration plot to quantify the amount of free hydrogen released from the reaction. The solution was analyzed by ^{1}H NMR spectroscopy to determine the yield of **3**. The above reaction was repeated and the results were shown in Table S-2.

Table S-3. Hydrogen detection data. **1** = LCo(μ-H)$_2$CoL, **3** = LCoNNCoL.

1 / μmol	**3** / μmol	H_2 detected / μmol	yields	
			3	H_2
38.3	24.2	21.8	89%	80%
24.5	21.8	19.8	90%	81%
25.2	21.9	19.9	87%	78%

Detection of evolved H_2 from 2 + N_2. In an argon-filled box, the same round bottom flask used for the H_2 calibration was charged with **2** (32 mg, 27 μmol) and a stir bar. The flask was then closed at the vacuum adaptor, taken into a N_2 box and 8 mL gas was taken out. 10 mL of toluene was injected and the mixture was stirred at room temperature for 10 h until the solution color turned to dark purple. The whole set-up was then taken out of the glove box, 8 mL CH_4 was added and the headspace was subjected to GC analysis as described above. The integration ratio was compared to the calibration plot to quantify the amount of free hydrogen released from the reaction. The solution was analyzed by ^{1}H NMR spectroscopy to determine the yield of **4**. The reaction was repeated and the results are shown in Table S-3.

Table S-4. Hydrogen detection data. **2** = $[KLCoH]_2$, **4** = $K_2LCoNNCoL$.

2 / μmol	**4** / μmol	H_2 detected / μmol	yield	
			4	H_2
26.6	24.2	21.8	91%	82%
24.5	21.8	20.8	89%	85%
24.7	22.5	20	91%	81%

References

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REFERENCE NUMBER: holkd15

CRYSTAL STRUCTURE REPORT

$C_{77}\,H_{116}\,Co_2\,N_4$

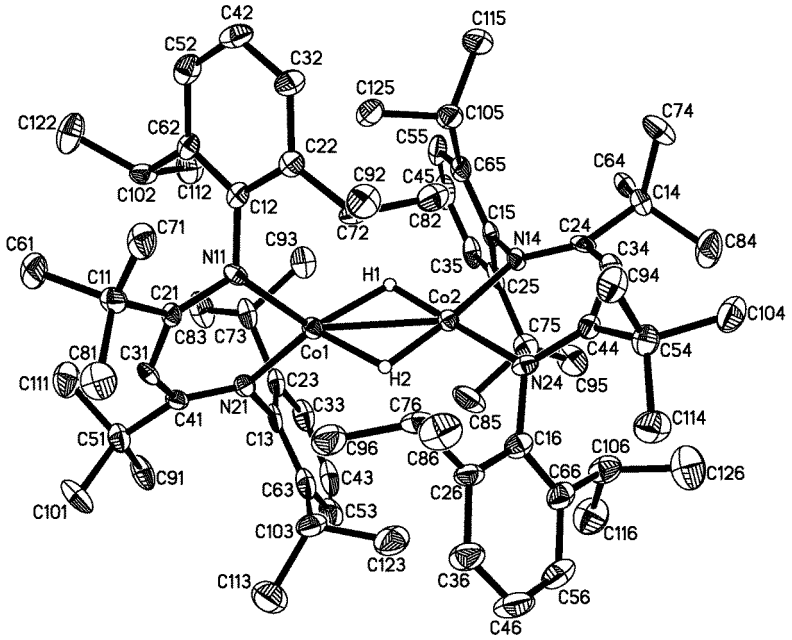
or

$[LCo(\mu\text{-}H)]_2 \cdot$ toluene

Report prepared for:

K. Ding, Prof. P. Holland

June 23, 2008



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Data collection

A crystal (0.36 x 0.28 x 0.10 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART APEX II CCD Platform diffractometer for a data collection at 100.0(1) K.[1] A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 120 seconds and a detector distance of 5.02 cm. A randomly oriented region of reciprocal space was surveyed: three major sections of frames were collected with 0.75º steps in ω at three different ϕ settings and a detector position of -33º in 2θ. The intensity data were corrected for absorption.[2] Final cell constants were calculated from the xyz centroids of 4096 strong reflections from the actual data collection after integration.[3] See Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97[4] and refined using SHELXL-97.[5] The space group *P*-1 was determined based on the lack of systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. Bridging hydride atoms were assigned from the difference Fourier map; their positions were refined independently of all heavier atoms and their isotropic displacement parameters were refined relative to those of the cobalt atoms (U_{iso}[H] = 2.0U_{eq}[Co]). All other hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

The refinement stalled at $R1 = 0.103$, at which point twin modeling was required. After the non-merohedral twin law, [-0.665 0 0.335 / 0.274 -1 0.274 / 1.665 0 0.665], a 180º rotation about direct lattice [1 0 1], was determined,[6] the data were re-integrated,[3] and a new absorption correction was applied.[7] There were 84812 unique reflections associated solely with the first component, 84580 reflections associated solely with the second component, and 16736 overlapping reflections. The mass ratio of the two components refined to 63:37. The final full matrix least squares refinement converged to $R1 = 0.0732$ (F^2, $I > 2\sigma(I)$) and $wR2 = 0.1699$ (F^2, all data).

Structure description

The structure is the one suggested. There are three unique di-cobalt species in the asymmetric unit with all atoms in general positions. Additionally there are three co-crystallized toluene solvent molecules in the asymmetric unit: two are in general positions and the third is divided between two crystallographic inversion centers. There are a variety of disorders among the alkyl groups and solvent molecules, all modeled over two positions (ratio in parentheses): ^{t}Bu group C211 (81:19), ^{t}Bu group C451 (52:48), ^{i}Pr group C473 (79:21), ^{i}Pr group C503 (78:22), and four toluene solvent molecules (50:50 [inversion], 50:50 [inversion], 72:28, 61:39). Similar ratios may suggest related disorders.

Intramolecular angles between N-Co-N planes of each dinuclear molecule are 84.87(15), 89.82(16), and 89.21(16) degrees, respectively, for Co1/Co2, Co3/Co4, and Co5/Co6. The angles between N-Co-N and H-Co-H planes are 85.6(18) degrees for N11-Co1-N21 and H1-Co1-H2, and 9.3(38) degrees for N14-Co2-N24 and H1-Co2-H2. Similarly defined angles are 75.0(18), 14.5(37), 68.7(22), and 20.9(34) degrees for the remaining molecules.

Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility, B51 Hutchison Hall, Department of Chemistry, University of Rochester. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel and the X-ray Crystallographic Facility of the Department of Chemistry at the University of Rochester.

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[1] *APEX2*, version 2.2-0; Bruker AXS: Madison, WI, 2007.

[2] Sheldrick, G. M. *SADABS*, version 2007/4; University of Göttingen: Göttingen, Germany, 2007.

[3] *SAINT*, version 7.46A; Bruker AXS: Madison, WI, 2007.

[4] Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G. L.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *SIR97: A new program for solving and refining crystal structures*; Istituto di Cristallografia, CNR: Bari, Italy, 1999.

[5] Sheldrick, G. M. *Acta. Cryst.* **2008**, *A64*, 112-122.

Some equations of interest:

$$R_{int} = \Sigma|F_o^2 - \langle F_o^2 \rangle| \,/\, \Sigma|F_o^2|$$

$$R1 = \Sigma||F_o| - |F_c|| \,/\, \Sigma|F_o|$$

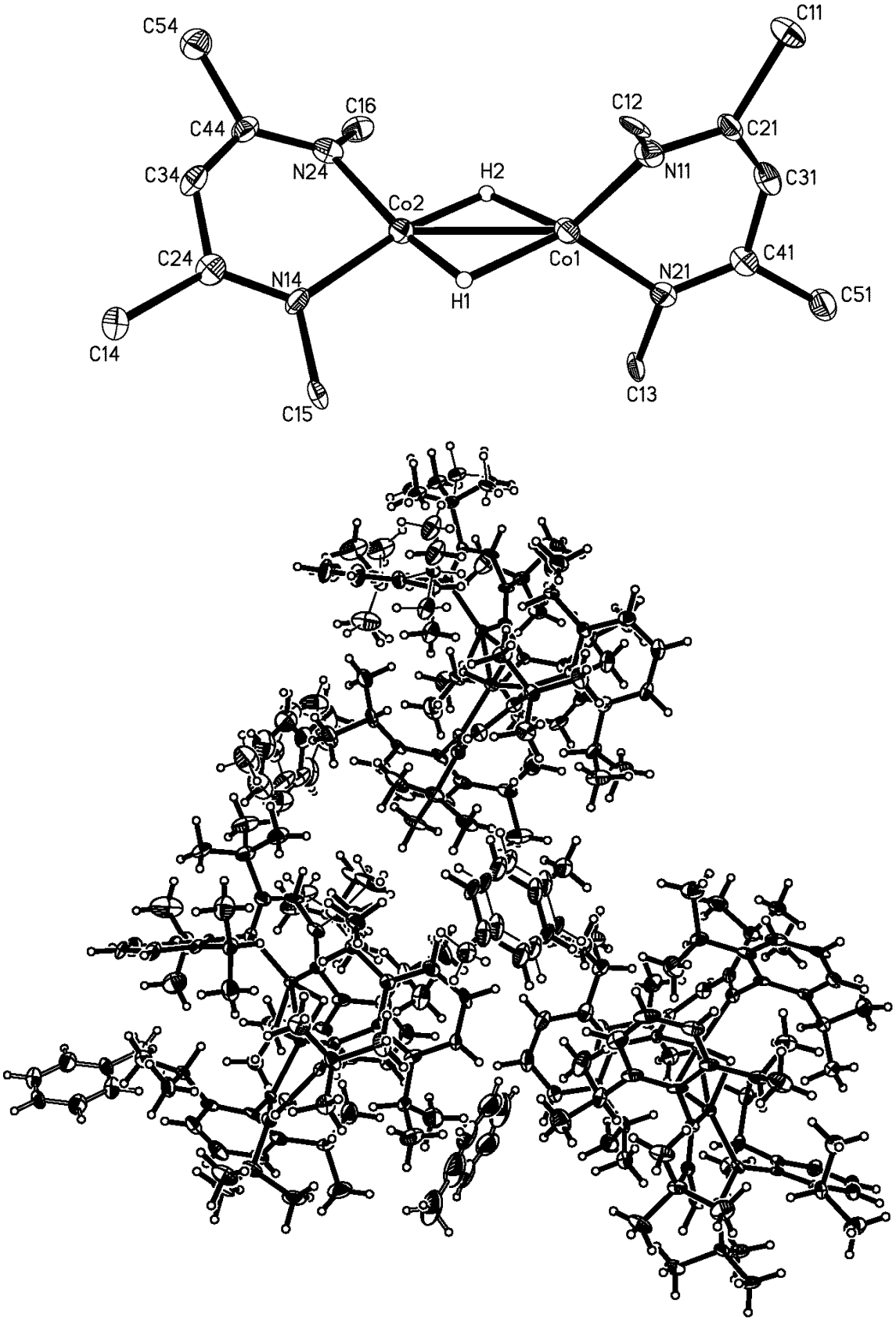
$$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] \,/\, \Sigma[w(F_o^2)^2]]^{1/2}$$

where $w = 1 \,/\, [\sigma^2(F_o^2) + (aP)^2 + bP]$ and

$$P = 1/3 \max(0, F_o^2) + 2/3\, F_c^2$$

$$\text{GOF} = S = [\Sigma[w(F_o^2 - F_c^2)^2] \,/\, (m-n)]^{1/2}$$

where m = number of reflections and n = number of parameters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H2
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Co2
Co1
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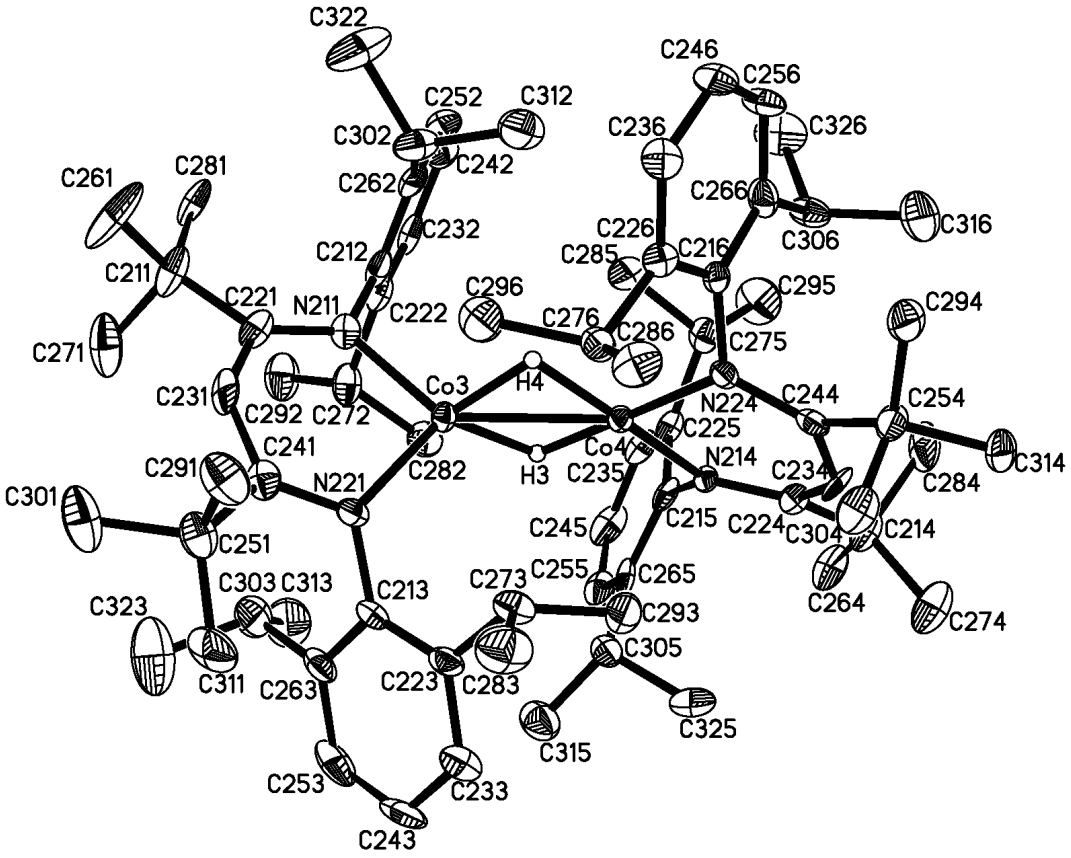
N21
H1
C51
C14
C15
C13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C306
C212
C285
C216
C211
C221
N211
C222
C296
C295
C294
C276
C286
C275
C271
C231
C292
C272
Co3
H4
N224
C244
C254
C225
C241
Co4
C314
C291
C282
H3
C235
N214
C234
C284
C301
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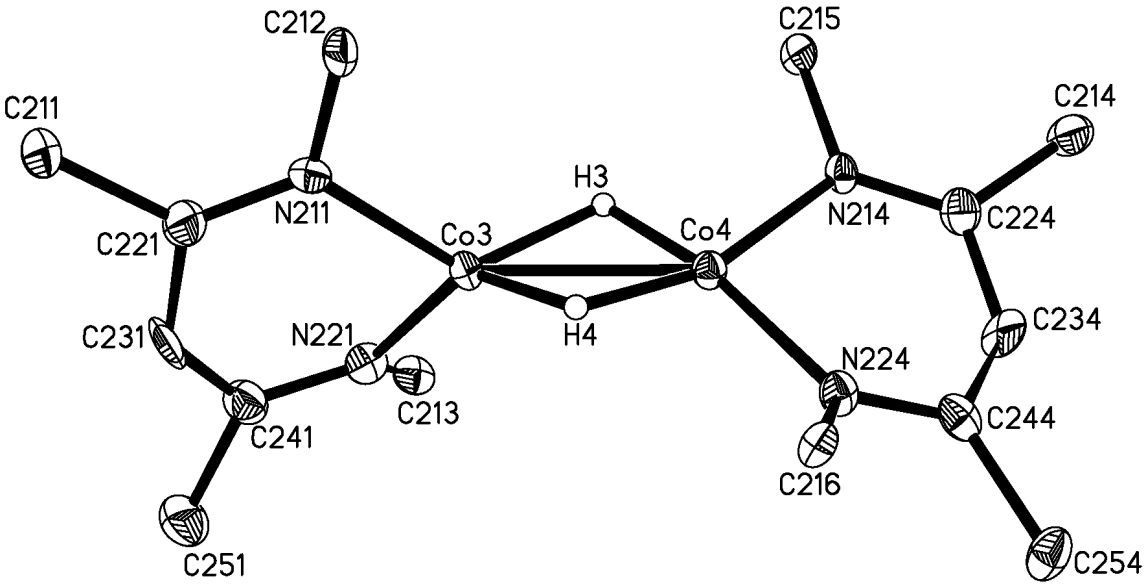
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C213
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C241
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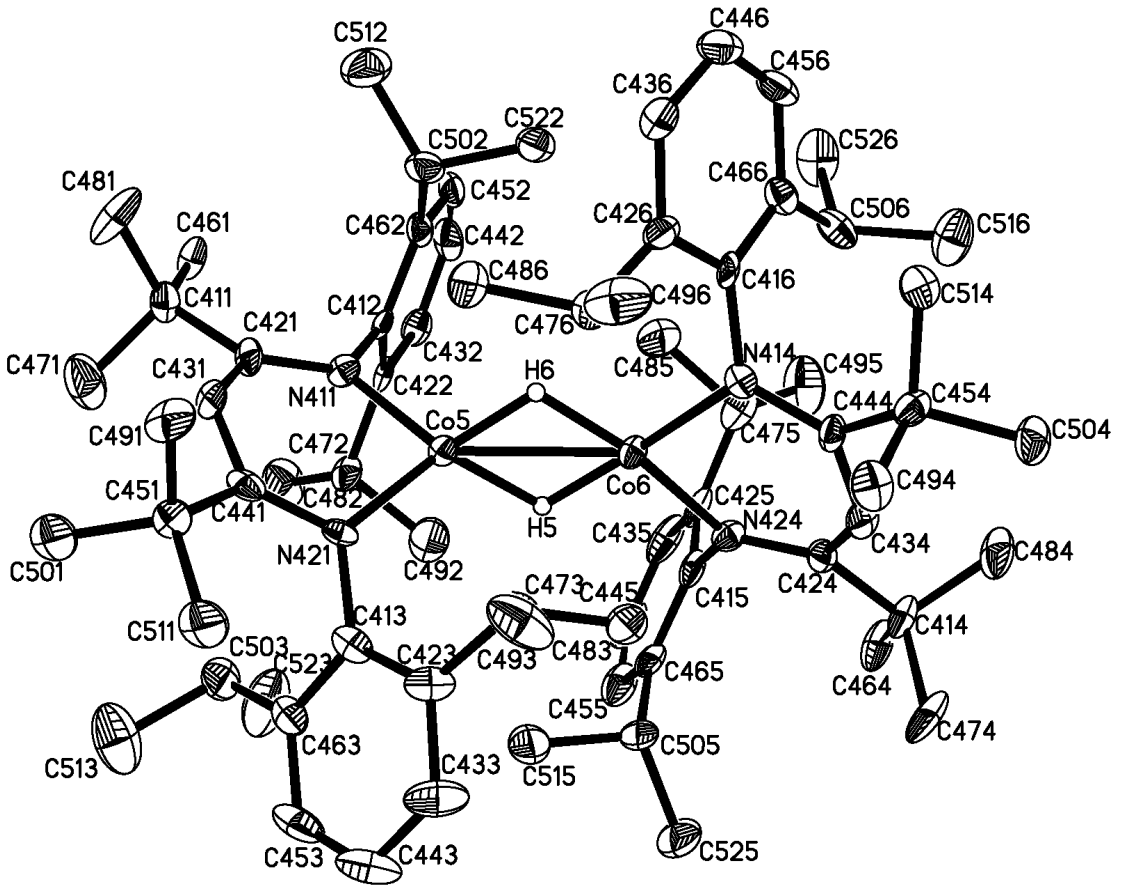
C251
C254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C516
C486
C416
C411
C412
C496
C476
C514
C421
C432
C471
C431
C485
N414
C495
H6
N411
C422
C444
C454
Co5
C475
C504
C491
C472
C494
C451
C482
Co6
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C441
H5
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C414
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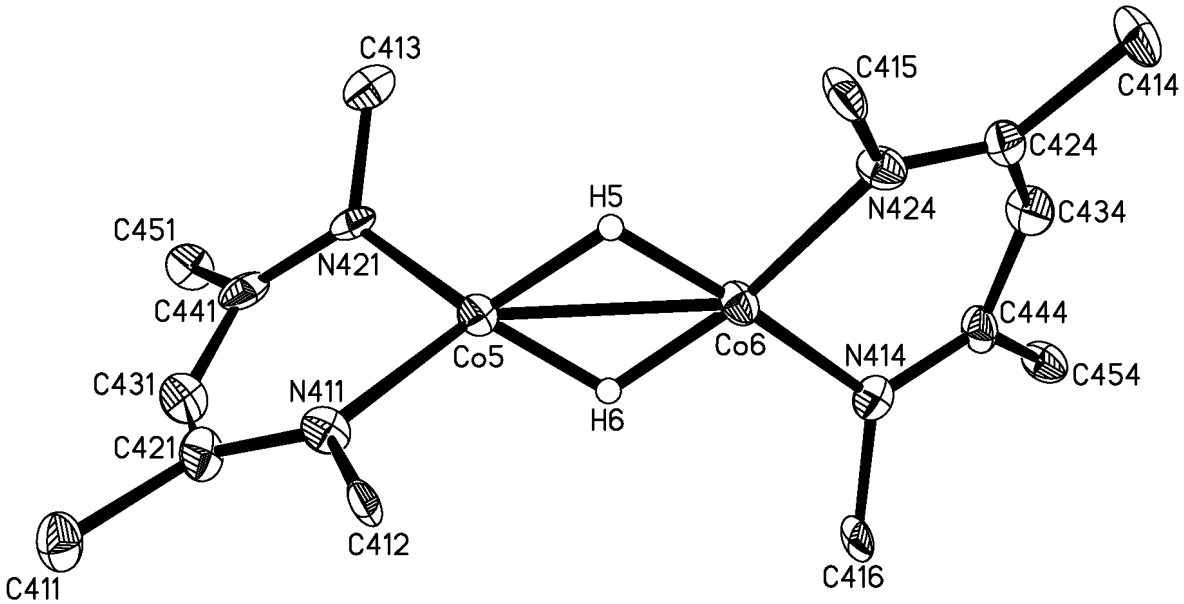
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C451
N424
C434
N421
C441
C444
Co5
Co6
N414
C431
C454
N411
H6
C421
C412
C416
C411

Table 1. Crystal data and structure refinement for holkd15.

Identification code	holkd15	
Empirical formula	C77 H116 Co2 N4	
Formula weight	1215.60	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 13.283(4) Å	α = 80.537(5)°
	b = 24.629(8) Å	β = 83.396(4)°
	c = 32.790(10) Å	γ = 80.793(5)°
Volume	10401(6) Å^3	
Z	6	
Density (calculated)	1.164 Mg/m^3	
Absorption coefficient	0.522 mm^{-1}	
F(000)	3960	
Crystal color, morphology	dark orange, block	
Crystal size	0.36 x 0.28 x 0.10 mm^3	
Theta range for data collection	1.41 to 25.03°	
Index ranges	$-15 \le h \le 15, -28 \le k \le 29, 0 \le l \le 39$	
Reflections collected	36503	
Independent reflections	36503 [R(int) = 0.0000]	
Observed reflections	18717	
Completeness to theta = 25.03°	99.3%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9496 and 0.8342	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	36503 / 40 / 2356	
Goodness-of-fit on F^2	1.007	
Final R indices [I>2sigma(I)]	R1 = 0.0732, wR2 = 0.1358	
R indices (all data)	R1 = 0.1656, wR2 = 0.1699	
Largest diff. peak and hole	0.881 and -0.671 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for holkd15. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	4925(1)	7984(1)	1577(1)	16(1)
Co2	3662(1)	7391(1)	1941(1)	15(1)
N11	4765(3)	8589(2)	1103(1)	16(1)
N21	6393(3)	8014(2)	1632(1)	17(1)
N14	2640(3)	7463(2)	2422(1)	15(1)
N24	3183(3)	6744(2)	1786(1)	17(1)
C11	5553(4)	8873(2)	350(2)	21(1)
C21	5597(4)	8629(2)	824(2)	16(1)
C31	6595(4)	8445(2)	929(2)	20(1)
C41	6993(4)	8231(2)	1313(2)	18(1)
C51	8134(4)	8319(2)	1317(2)	24(2)
C61	6031(5)	9417(2)	251(2)	32(2)
C71	4497(4)	8990(3)	191(2)	30(2)
C81	6194(5)	8448(3)	93(2)	34(2)
C91	8718(4)	8054(3)	1696(2)	30(2)
C101	8786(4)	8118(3)	938(2)	35(2)
C111	8107(5)	8952(3)	1281(2)	37(2)
C12	3884(4)	9007(2)	1054(2)	16(1)
C22	2936(4)	8875(2)	974(2)	19(1)
C32	2116(5)	9300(2)	911(2)	23(1)
C42	2208(5)	9842(2)	926(2)	26(2)
C52	3123(5)	9967(2)	1021(2)	26(2)
C62	3965(4)	9561(2)	1097(2)	18(1)
C72	2774(4)	8286(2)	961(2)	19(1)
C82	2136(5)	8072(2)	1359(2)	28(2)
C92	2262(5)	8219(3)	578(2)	29(2)
C102	4903(4)	9715(2)	1250(2)	21(1)
C112	4756(5)	9654(3)	1727(2)	32(2)
C122	5137(5)	10307(2)	1080(2)	39(2)
C13	6797(4)	7716(2)	2009(2)	19(1)
C23	6760(4)	7987(2)	2358(2)	21(1)

C33	7168(4)	7678(3)	2712(2)	29(2)
C43	7585(5)	7125(3)	2721(2)	33(2)
C53	7585(4)	6867(3)	2382(2)	32(2)
C63	7168(4)	7149(3)	2022(2)	27(2)
C73	6324(4)	8591(2)	2355(2)	24(1)
C83	7029(5)	8926(3)	2516(2)	40(2)
C93	5281(4)	8647(3)	2608(2)	29(2)
C103	7137(5)	6839(2)	1664(2)	29(2)
C113	8196(5)	6605(3)	1474(2)	44(2)
C123	6503(5)	6361(3)	1802(2)	42(2)
C14	982(4)	7212(2)	2861(2)	21(1)
C24	1807(4)	7220(2)	2478(2)	18(1)
C34	1569(4)	6926(2)	2176(2)	20(1)
C44	2199(4)	6667(2)	1875(2)	17(1)
C54	1615(5)	6328(2)	1633(2)	25(1)
C64	1166(4)	7441(2)	3245(2)	23(1)
C74	-31(4)	7535(3)	2710(2)	33(2)
C84	854(5)	6602(3)	3018(2)	42(2)
C94	1180(5)	6757(2)	1274(2)	28(2)
C104	707(5)	6096(2)	1896(2)	34(2)
C114	2245(5)	5831(3)	1440(2)	34(2)
C15	2858(4)	7790(2)	2720(2)	17(1)
C25	3499(4)	7543(2)	3034(2)	20(1)
C35	3700(4)	7865(3)	3310(2)	25(2)
C45	3306(5)	8414(3)	3288(2)	27(2)
C55	2696(5)	8662(2)	2980(2)	28(2)
C65	2455(4)	8353(2)	2689(2)	21(1)
C75	3962(4)	6936(2)	3068(2)	23(1)
C85	5076(5)	6889(3)	2874(2)	50(2)
C95	3913(5)	6621(3)	3510(2)	39(2)
C105	1794(4)	8657(2)	2353(2)	25(1)
C115	797(5)	8989(3)	2521(2)	36(2)
C125	2400(5)	9042(2)	2042(2)	28(2)
C16	3931(4)	6313(2)	1635(2)	22(1)
C26	4368(4)	6361(2)	1219(2)	23(1)
C36	5067(5)	5925(2)	1095(2)	33(2)

C46	5322(5)	5442(3)	1368(2)	41(2)
C56	4932(5)	5401(3)	1775(2)	35(2)
C66	4238(5)	5833(2)	1918(2)	26(2)
C76	4077(5)	6855(2)	891(2)	26(2)
C86	3597(5)	6686(3)	533(2)	36(2)
C96	4994(5)	7152(3)	710(2)	38(2)
C106	3875(5)	5771(3)	2379(2)	31(2)
C116	4757(5)	5545(3)	2654(2)	44(2)
C126	3051(5)	5396(3)	2499(2)	47(2)
Co3	8287(1)	2379(1)	1710(1)	16(1)
Co4	9492(1)	3033(1)	1399(1)	14(1)
N211	6808(3)	2362(2)	1690(1)	19(1)
N221	8554(3)	1660(2)	2068(1)	19(1)
N214	10436(3)	3069(2)	889(1)	14(1)
N224	9986(3)	3626(2)	1619(1)	16(1)
C231	6780(5)	1717(2)	2314(2)	27(2)
C241	7797(5)	1503(2)	2358(2)	24(1)
C251	8004(5)	1117(3)	2785(2)	32(2)
C221	6281(4)	2052(3)	1981(2)	25(2)
C211	5136(6)	1969(5)	1993(3)	33(2)
C261	4579(8)	2050(14)	2420(3)	62(5)
C271	5150(12)	1354(4)	1933(9)	48(4)
C281	4464(4)	2322(3)	1666(2)	32(2)
C21"	5101(13)	2037(16)	2026(8)	33(2)
C26"	4590(30)	2270(40)	2417(11)	62(5)
C27"	5000(40)	1407(18)	2080(30)	48(4)
C28"	4464(4)	2322(3)	1666(2)	32(2)
C291	7969(5)	1521(3)	3096(2)	38(2)
C301	7121(6)	766(3)	2933(2)	49(2)
C311	8985(5)	716(3)	2811(2)	40(2)
C212	6331(4)	2743(3)	1364(2)	24(2)
C222	6289(4)	2595(2)	970(2)	21(1)
C232	5822(4)	2981(3)	669(2)	26(2)
C242	5431(4)	3514(3)	745(2)	29(2)
C252	5476(4)	3660(3)	1130(2)	30(2)
C262	5931(4)	3284(3)	1439(2)	24(2)

C272	6747(5)	2014(3)	877(2)	27(2)
C282	7719(5)	2049(2)	581(2)	29(2)
C292	5999(5)	1734(3)	689(2)	40(2)
C302	5971(4)	3471(3)	1860(2)	31(2)
C312	6631(5)	3931(3)	1809(2)	40(2)
C322	4904(5)	3677(3)	2064(2)	54(2)
C213	9479(4)	1287(2)	1997(2)	19(1)
C223	10413(4)	1401(2)	2082(2)	21(1)
C233	11286(5)	1015(2)	2015(2)	31(2)
C243	11236(5)	527(2)	1874(2)	37(2)
C253	10303(6)	430(2)	1769(2)	37(2)
C263	9415(5)	808(2)	1821(2)	26(2)
C273	10535(5)	1924(2)	2251(2)	22(1)
C283	10929(5)	1792(3)	2682(2)	44(2)
C293	11239(5)	2268(3)	1955(2)	35(2)
C303	8432(5)	700(3)	1675(2)	39(2)
C313	8524(6)	701(3)	1212(2)	50(2)
C323	8094(7)	154(3)	1896(2)	69(3)
C214	11957(4)	3450(3)	417(2)	26(2)
C224	11248(4)	3325(2)	832(2)	21(1)
C234	11519(4)	3566(2)	1159(2)	23(1)
C244	10953(4)	3744(2)	1506(2)	18(1)
C254	11572(4)	4026(2)	1778(2)	24(1)
C264	11930(5)	3119(3)	58(2)	32(2)
C274	13092(5)	3364(3)	501(2)	42(2)
C284	11645(5)	4073(3)	251(2)	41(2)
C294	10975(5)	4480(2)	2024(2)	32(2)
C304	12068(5)	3550(3)	2088(2)	30(2)
C314	12460(4)	4298(2)	1518(2)	27(2)
C215	10152(4)	2812(2)	560(2)	19(1)
C225	9493(4)	3129(2)	277(2)	21(1)
C235	9308(4)	2889(3)	-57(2)	26(2)
C245	9732(5)	2357(3)	-100(2)	33(2)
C255	10332(5)	2039(3)	189(2)	29(2)
C265	10539(4)	2252(2)	534(2)	21(1)
C275	8984(4)	3712(2)	325(2)	24(1)

C285	7911(5)	3690(3)	533(2)	50(2)
C295	8952(6)	4104(3)	-92(2)	47(2)
C305	11125(4)	1877(2)	873(2)	24(1)
C315	11201(5)	1266(2)	844(2)	39(2)
C325	12199(4)	2006(3)	906(2)	32(2)
C216	9269(4)	4008(2)	1840(2)	17(1)
C226	8936(4)	3879(2)	2259(2)	19(1)
C236	8306(4)	4285(2)	2456(2)	24(1)
C246	7972(5)	4803(2)	2240(2)	28(2)
C256	8252(4)	4910(2)	1820(2)	25(1)
C266	8883(4)	4521(2)	1613(2)	23(1)
C276	9262(4)	3325(2)	2523(2)	21(1)
C286	9839(5)	3395(3)	2887(2)	31(2)
C296	8351(5)	3025(3)	2688(2)	33(2)
C306	9128(5)	4658(2)	1147(2)	25(1)
C316	9931(5)	5049(3)	1026(2)	43(2)
C326	8158(5)	4919(3)	931(2)	41(2)
Co5	1779(1)	2193(1)	5060(1)	16(1)
Co6	2987(1)	2823(1)	4697(1)	16(1)
N411	287(3)	2194(2)	5050(1)	18(1)
N421	1999(3)	1526(2)	5478(1)	17(1)
N414	3486(3)	3460(2)	4865(1)	17(1)
C411	-1417(4)	1878(2)	5396(2)	24(1)
C421	-255(4)	1935(2)	5366(2)	20(1)
C431	214(5)	1651(2)	5718(2)	23(2)
C441	1228(5)	1427(2)	5777(2)	21(1)
C461	-2053(4)	2153(3)	5033(2)	28(2)
C471	-1473(5)	1245(3)	5431(2)	47(2)
C481	-1965(5)	2095(3)	5789(2)	45(2)
C451	1435(15)	1103(8)	6228(4)	21(2)
C491	1130(30)	1512(13)	6532(15)	31(5)
C501	724(13)	642(7)	6324(5)	35(2)
C511	2521(13)	821(8)	6308(5)	35(2)
C45"	1296(16)	1103(9)	6238(4)	21(2)
C49"	1360(30)	1550(14)	6495(17)	31(5)
C50"	339(14)	819(8)	6429(5)	35(2)

C51"	2224(15)	651(8)	6315(6)	35(2)
C412	-173(4)	2533(2)	4700(2)	15(1)
C422	-206(4)	2307(2)	4330(2)	18(1)
C432	-676(4)	2648(2)	4009(2)	23(1)
C442	-1089(4)	3185(3)	4034(2)	28(2)
C452	-1024(4)	3405(2)	4389(2)	26(2)
C462	-562(4)	3090(2)	4724(2)	19(1)
C472	231(4)	1708(2)	4295(2)	23(1)
C482	-491(5)	1400(3)	4121(2)	47(2)
C492	1229(5)	1696(3)	4014(2)	50(2)
C502	-507(4)	3355(2)	5107(2)	26(2)
C512	-1567(5)	3587(3)	5297(2)	43(2)
C522	154(4)	3821(2)	4996(2)	30(2)
C413	2895(5)	1113(2)	5458(2)	21(1)
C423	3855(5)	1230(2)	5531(2)	25(2)
C433	4700(5)	806(3)	5530(2)	40(2)
C443	4607(6)	290(3)	5459(2)	45(2)
C453	3672(5)	186(2)	5365(2)	34(2)
C463	2811(5)	586(2)	5361(2)	23(1)
C473	4035(7)	1807(3)	5586(3)	22(2)
C483	4638(6)	2091(4)	5210(3)	30(2)
C493	4533(8)	1805(4)	5986(3)	44(3)
C47'	3970(30)	1717(10)	5744(8)	22(2)
C48'	4790(20)	1961(14)	5444(11)	30(2)
C49'	4280(30)	1584(17)	6188(10)	44(3)
C503	1823(5)	458(3)	5233(2)	34(2)
C513	1634(11)	-135(4)	5446(3)	57(4)
C523	1892(6)	437(3)	4770(2)	57(2)
C50Z	1823(5)	458(3)	5233(2)	34(2)
C51Z	990(30)	127(19)	5476(11)	57(4)
C52Z	1892(6)	437(3)	4770(2)	57(2)
C414	5608(4)	3042(3)	3746(2)	26(2)
C424	4796(4)	3022(2)	4138(2)	19(1)
C434	5073(4)	3288(2)	4449(2)	21(1)
C444	4474(4)	3532(2)	4763(2)	19(1)
C454	5098(4)	3841(2)	5017(2)	21(1)

C464	5369(5)	2841(3)	3354(2)	33(2)
C474	6613(4)	2681(3)	3881(2)	39(2)
C484	5780(5)	3648(3)	3612(2)	37(2)
C494	5583(4)	3382(2)	5343(2)	26(2)
C504	5980(4)	4095(2)	4740(2)	28(2)
C514	4516(4)	4313(2)	5243(2)	26(2)
C415	3630(4)	2528(3)	3869(2)	21(1)
C425	2951(4)	2836(3)	3588(2)	23(2)
C435	2668(5)	2571(3)	3290(2)	35(2)
C445	3018(5)	2024(3)	3271(2)	37(2)
C455	3667(5)	1720(3)	3547(2)	33(2)
C465	3982(4)	1964(2)	3857(2)	20(1)
C475	2545(4)	3438(3)	3617(2)	26(2)
C485	1467(5)	3476(3)	3835(2)	43(2)
C495	2556(6)	3817(3)	3195(2)	49(2)
C505	4696(4)	1610(2)	4152(2)	29(2)
C515	4117(5)	1200(2)	4451(2)	37(2)
C525	5640(5)	1289(3)	3938(2)	40(2)
C416	2778(4)	3864(2)	5065(2)	17(1)
N424	3938(3)	2795(2)	4187(1)	18(1)
C426	2429(4)	3765(2)	5489(2)	21(1)
C436	1812(4)	4195(2)	5669(2)	24(2)
C446	1520(4)	4704(2)	5439(2)	28(2)
C456	1802(5)	4787(2)	5020(2)	28(2)
C466	2419(4)	4375(2)	4824(2)	21(1)
C476	2724(5)	3221(2)	5769(2)	23(1)
C486	1785(5)	2946(3)	5936(2)	47(2)
C496	3275(5)	3301(3)	6140(2)	42(2)
C506	2650(5)	4484(2)	4353(2)	27(2)
C516	3535(5)	4820(3)	4222(2)	39(2)
C526	1725(5)	4789(3)	4132(2)	41(2)
C17	6359(13)	4974(9)	-429(6)	90(3)
C27	5456(9)	4966(7)	-105(5)	90(3)
C37	5404(9)	4971(5)	320(5)	54(2)
C47	4462(11)	4991(5)	555(4)	65(3)
C57	3573(9)	5006(6)	365(4)	90(3)

C67	3626(9)	5001(5)	-60(4)	65(3)
C77	4567(11)	4981(6)	-295(4)	54(2)
C87	8027(8)	335(5)	213(4)	37(3)
C97	9159(9)	146(12)	94(9)	28(3)
C107	9860(10)	517(12)	59(10)	36(4)
C117	10891(10)	346(12)	-51(10)	39(4)
C127	11220(9)	-196(12)	-125(10)	28(3)
C137	10519(10)	-568(12)	-89(10)	36(4)
C147	9488(10)	-397(12)	20(10)	39(4)
C157	1587(10)	129(7)	3585(4)	86(5)
C167	2630(5)	143(3)	3386(2)	43(3)
C177	3474(6)	10(3)	3616(2)	52(3)
C187	4455(5)	21(4)	3418(3)	69(4)
C197	4592(5)	167(3)	2990(3)	78(5)
C207	3748(7)	301(3)	2759(2)	77(4)
C217	2767(6)	289(3)	2957(2)	46(3)
C15'	4883(19)	-80(15)	3258(11)	78(5)
C16'	3756(12)	40(8)	3290(7)	43(3)
C17'	3249(16)	180(9)	2931(5)	46(3)
C18'	2185(16)	248(11)	2958(6)	69(4)
C19'	1629(12)	175(11)	3344(7)	86(5)
C20'	2135(17)	35(11)	3703(6)	77(4)
C21'	3199(17)	-32(10)	3676(5)	52(3)
C227	6291(8)	5223(5)	3613(4)	45(3)
C237	7420(6)	5159(5)	3461(4)	38(3)
C247	8074(8)	4705(5)	3639(5)	42(3)
C257	9118(7)	4650(5)	3515(4)	39(3)
C267	9507(6)	5049(5)	3214(4)	38(3)
C277	8853(7)	5502(5)	3036(4)	42(3)
C287	7809(7)	5557(5)	3160(4)	39(3)
C22'	10229(11)	5051(7)	3096(6)	45(3)
C23'	9101(10)	5111(9)	3253(7)	38(3)
C24'	8415(11)	5545(8)	3072(7)	42(3)
C25'	7374(11)	5577(9)	3198(7)	39(3)
C26'	7020(10)	5175(9)	3505(8)	38(3)
C27'	7706(13)	4740(9)	3686(8)	42(3)

C28'	8746(12)	4708(9)	3560(7)	39(3)

Table 3. Bond lengths [Å] and angles [°] for holkd15.

Co(1)-N(11)	1.972(4)	C(81)-H(81A)	0.9800
Co(1)-N(21)	1.993(4)	C(81)-H(81B)	0.9800
Co(1)-Co(2)	2.4750(12)	C(81)-H(81C)	0.9800
Co(1)-H(1)	1.75(5)	C(91)-H(91A)	0.9800
Co(1)-H(2)	1.59(5)	C(91)-H(91B)	0.9800
Co(2)-N(24)	1.967(4)	C(91)-H(91C)	0.9800
Co(2)-N(14)	1.971(4)	C(101)-H(10A)	0.9800
Co(2)-H(1)	1.43(5)	C(101)-H(10B)	0.9800
Co(2)-H(2)	1.52(5)	C(101)-H(10C)	0.9800
N(11)-C(21)	1.356(6)	C(111)-H(11A)	0.9800
N(11)-C(12)	1.434(7)	C(111)-H(11B)	0.9800
N(21)-C(41)	1.331(6)	C(111)-H(11C)	0.9800
N(21)-C(13)	1.445(7)	C(12)-C(22)	1.413(7)
N(14)-C(24)	1.321(6)	C(12)-C(62)	1.417(7)
N(14)-C(15)	1.444(7)	C(22)-C(32)	1.394(8)
N(24)-C(44)	1.342(7)	C(22)-C(72)	1.509(7)
N(24)-C(16)	1.441(7)	C(32)-C(42)	1.370(7)
C(11)-C(71)	1.521(8)	C(32)-H(32A)	0.9500
C(11)-C(81)	1.540(8)	C(42)-C(52)	1.381(8)
C(11)-C(61)	1.544(8)	C(42)-H(42A)	0.9500
C(11)-C(21)	1.578(7)	C(52)-C(62)	1.391(8)
C(21)-C(31)	1.392(7)	C(52)-H(52A)	0.9500
C(31)-C(41)	1.412(7)	C(62)-C(102)	1.519(8)
C(31)-H(31A)	0.9500	C(72)-C(82)	1.537(8)
C(41)-C(51)	1.566(8)	C(72)-C(92)	1.539(7)
C(51)-C(101)	1.534(8)	C(72)-H(72A)	1.0000
C(51)-C(91)	1.537(8)	C(82)-H(82A)	0.9800
C(51)-C(111)	1.540(8)	C(82)-H(82B)	0.9800
C(61)-H(61A)	0.9800	C(82)-H(82C)	0.9800
C(61)-H(61B)	0.9800	C(92)-H(92A)	0.9800
C(61)-H(61C)	0.9800	C(92)-H(92B)	0.9800
C(71)-H(71A)	0.9800	C(92)-H(92C)	0.9800
C(71)-H(71B)	0.9800	C(102)-C(112)	1.539(8)
C(71)-H(71C)	0.9800	C(102)-C(122)	1.540(7)

C(102)-H(10D)	1.0000	C(14)-C(64)	1.523(7)
C(112)-H(11D)	0.9800	C(14)-C(84)	1.536(8)
C(112)-H(11E)	0.9800	C(14)-C(74)	1.539(8)
C(112)-H(11F)	0.9800	C(14)-C(24)	1.568(7)
C(122)-H(12A)	0.9800	C(24)-C(34)	1.409(7)
C(122)-H(12B)	0.9800	C(34)-C(44)	1.389(7)
C(122)-H(12C)	0.9800	C(34)-H(34A)	0.9500
C(13)-C(63)	1.400(8)	C(44)-C(54)	1.579(8)
C(13)-C(23)	1.407(8)	C(54)-C(104)	1.531(8)
C(23)-C(33)	1.394(8)	C(54)-C(94)	1.545(8)
C(23)-C(73)	1.508(8)	C(54)-C(114)	1.549(8)
C(33)-C(43)	1.381(8)	C(64)-H(64A)	0.9800
C(33)-H(33A)	0.9500	C(64)-H(64B)	0.9800
C(43)-C(53)	1.371(9)	C(64)-H(64C)	0.9800
C(43)-H(43A)	0.9500	C(74)-H(74A)	0.9800
C(53)-C(63)	1.391(8)	C(74)-H(74B)	0.9800
C(53)-H(53A)	0.9500	C(74)-H(74C)	0.9800
C(63)-C(103)	1.511(8)	C(84)-H(84A)	0.9800
C(73)-C(93)	1.529(8)	C(84)-H(84B)	0.9800
C(73)-C(83)	1.529(8)	C(84)-H(84C)	0.9800
C(73)-H(73A)	1.0000	C(94)-H(94A)	0.9800
C(83)-H(83A)	0.9800	C(94)-H(94B)	0.9800
C(83)-H(83B)	0.9800	C(94)-H(94C)	0.9800
C(83)-H(83C)	0.9800	C(104)-H(10F)	0.9800
C(93)-H(93A)	0.9800	C(104)-H(10G)	0.9800
C(93)-H(93B)	0.9800	C(104)-H(10H)	0.9800
C(93)-H(93C)	0.9800	C(114)-H(11J)	0.9800
C(103)-C(123)	1.534(8)	C(114)-H(11K)	0.9800
C(103)-C(113)	1.535(8)	C(114)-H(11L)	0.9800
C(103)-H(10E)	1.0000	C(15)-C(65)	1.396(7)
C(113)-H(11G)	0.9800	C(15)-C(25)	1.409(8)
C(113)-H(11H)	0.9800	C(25)-C(35)	1.369(8)
C(113)-H(11I)	0.9800	C(25)-C(75)	1.514(8)
C(123)-H(12D)	0.9800	C(35)-C(45)	1.362(8)
C(123)-H(12E)	0.9800	C(35)-H(35A)	0.9500
C(123)-H(12F)	0.9800	C(45)-C(55)	1.370(8)

C(45)-H(45A)	0.9500	C(86)-H(86A)	0.9800
C(55)-C(65)	1.406(8)	C(86)-H(86B)	0.9800
C(55)-H(55A)	0.9500	C(86)-H(86C)	0.9800
C(65)-C(105)	1.514(8)	C(96)-H(96A)	0.9800
C(75)-C(95)	1.530(8)	C(96)-H(96B)	0.9800
C(75)-C(85)	1.536(8)	C(96)-H(96C)	0.9800
C(75)-H(75A)	1.0000	C(106)-C(126)	1.521(8)
C(85)-H(85A)	0.9800	C(106)-C(116)	1.537(8)
C(85)-H(85B)	0.9800	C(106)-H(10J)	1.0000
C(85)-H(85C)	0.9800	C(116)-H(11P)	0.9800
C(95)-H(95A)	0.9800	C(116)-H(11Q)	0.9800
C(95)-H(95B)	0.9800	C(116)-H(11R)	0.9800
C(95)-H(95C)	0.9800	C(126)-H(12J)	0.9800
C(105)-C(125)	1.524(7)	C(126)-H(12K)	0.9800
C(105)-C(115)	1.537(8)	C(126)-H(12L)	0.9800
C(105)-H(10I)	1.0000	Co(3)-N(221)	1.962(4)
C(115)-H(11M)	0.9800	Co(3)-N(211)	1.980(5)
C(115)-H(11N)	0.9800	Co(3)-Co(4)	2.4716(11)
C(115)-H(11O)	0.9800	Co(3)-H(3)	1.64(5)
C(125)-H(12G)	0.9800	Co(3)-H(4)	1.54(5)
C(125)-H(12H)	0.9800	Co(4)-N(224)	1.962(4)
C(125)-H(12I)	0.9800	Co(4)-N(214)	1.970(4)
C(16)-C(66)	1.414(8)	Co(4)-H(3)	1.46(5)
C(16)-C(26)	1.415(8)	Co(4)-H(4)	1.58(5)
C(26)-C(36)	1.385(8)	N(211)-C(221)	1.326(7)
C(26)-C(76)	1.516(8)	N(211)-C(212)	1.436(7)
C(36)-C(46)	1.387(8)	N(221)-C(241)	1.360(7)
C(36)-H(36A)	0.9500	N(221)-C(213)	1.432(7)
C(46)-C(56)	1.366(9)	N(214)-C(224)	1.314(7)
C(46)-H(46A)	0.9500	N(214)-C(215)	1.449(7)
C(56)-C(66)	1.398(8)	N(224)-C(244)	1.360(7)
C(56)-H(56A)	0.9500	N(224)-C(216)	1.447(6)
C(66)-C(106)	1.523(8)	C(231)-C(241)	1.384(8)
C(76)-C(96)	1.532(8)	C(231)-C(221)	1.416(8)
C(76)-C(86)	1.541(8)	C(231)-H(23A)	0.9500
C(76)-H(76A)	1.0000	C(241)-C(251)	1.584(8)

C(251)-C(311)	1.506(9)	C(222)-C(232)	1.382(8)
C(251)-C(291)	1.529(8)	C(222)-C(272)	1.528(8)
C(251)-C(301)	1.555(8)	C(232)-C(242)	1.384(8)
C(221)-C(211)	1.562(9)	C(232)-H(23B)	0.9500
C(221)-C(21")	1.563(17)	C(242)-C(252)	1.380(8)
C(211)-C(261)	1.533(10)	C(242)-H(24A)	0.9500
C(211)-C(281)	1.540(9)	C(252)-C(262)	1.379(8)
C(211)-C(271)	1.558(10)	C(252)-H(25A)	0.9500
C(261)-H(26A)	0.9800	C(262)-C(302)	1.535(8)
C(261)-H(26B)	0.9800	C(272)-C(282)	1.528(8)
C(261)-H(26C)	0.9800	C(272)-C(292)	1.532(8)
C(271)-H(27A)	0.9800	C(272)-H(27G)	1.0000
C(271)-H(27B)	0.9800	C(282)-H(28G)	0.9800
C(271)-H(27C)	0.9800	C(282)-H(28H)	0.9800
C(281)-H(28A)	0.9800	C(282)-H(28I)	0.9800
C(281)-H(28B)	0.9800	C(292)-H(29D)	0.9800
C(281)-H(28C)	0.9800	C(292)-H(29E)	0.9800
C(21")-C(26")	1.533(18)	C(292)-H(29F)	0.9800
C(21")-C(27")	1.559(19)	C(302)-C(312)	1.518(8)
C(26")-H(26D)	0.9800	C(302)-C(322)	1.542(8)
C(26")-H(26E)	0.9800	C(302)-H(30D)	1.0000
C(26")-H(26F)	0.9800	C(312)-H(31E)	0.9800
C(27")-H(27D)	0.9800	C(312)-H(31F)	0.9800
C(27")-H(27E)	0.9800	C(312)-H(31G)	0.9800
C(27")-H(27F)	0.9800	C(322)-H(32B)	0.9800
C(291)-H(29A)	0.9800	C(322)-H(32C)	0.9800
C(291)-H(29B)	0.9800	C(322)-H(32D)	0.9800
C(291)-H(29C)	0.9800	C(213)-C(223)	1.385(8)
C(301)-H(30A)	0.9800	C(213)-C(263)	1.414(7)
C(301)-H(30B)	0.9800	C(223)-C(233)	1.398(8)
C(301)-H(30C)	0.9800	C(223)-C(273)	1.519(7)
C(311)-H(31B)	0.9800	C(233)-C(243)	1.371(8)
C(311)-H(31C)	0.9800	C(233)-H(23C)	0.9500
C(311)-H(31D)	0.9800	C(243)-C(253)	1.389(9)
C(212)-C(262)	1.405(8)	C(243)-H(24B)	0.9500
C(212)-C(222)	1.406(8)	C(253)-C(263)	1.392(8)

C(253)-H(25B)	0.9500	C(274)-H(27L)	0.9800
C(263)-C(303)	1.516(9)	C(284)-H(28M)	0.9800
C(273)-C(293)	1.520(8)	C(284)-H(28N)	0.9800
C(273)-C(283)	1.532(8)	C(284)-H(28O)	0.9800
C(273)-H(27H)	1.0000	C(294)-H(29J)	0.9800
C(283)-H(28J)	0.9800	C(294)-H(29K)	0.9800
C(283)-H(28K)	0.9800	C(294)-H(29L)	0.9800
C(283)-H(28L)	0.9800	C(304)-H(30F)	0.9800
C(293)-H(29G)	0.9800	C(304)-H(30G)	0.9800
C(293)-H(29H)	0.9800	C(304)-H(30H)	0.9800
C(293)-H(29I)	0.9800	C(314)-H(31K)	0.9800
C(303)-C(313)	1.508(9)	C(314)-H(31L)	0.9800
C(303)-C(323)	1.529(9)	C(314)-H(31M)	0.9800
C(303)-H(30E)	1.0000	C(215)-C(225)	1.402(8)
C(313)-H(31H)	0.9800	C(215)-C(265)	1.406(8)
C(313)-H(31I)	0.9800	C(225)-C(235)	1.391(8)
C(313)-H(31J)	0.9800	C(225)-C(275)	1.509(8)
C(323)-H(32E)	0.9800	C(235)-C(245)	1.363(8)
C(323)-H(32F)	0.9800	C(235)-H(23E)	0.9500
C(323)-H(32G)	0.9800	C(245)-C(255)	1.370(9)
C(214)-C(274)	1.540(8)	C(245)-H(24C)	0.9500
C(214)-C(264)	1.544(8)	C(255)-C(265)	1.393(8)
C(214)-C(284)	1.548(8)	C(255)-H(25C)	0.9500
C(214)-C(224)	1.581(7)	C(265)-C(305)	1.527(8)
C(224)-C(234)	1.413(8)	C(275)-C(285)	1.514(8)
C(234)-C(244)	1.383(7)	C(275)-C(295)	1.541(8)
C(234)-H(23D)	0.9500	C(275)-H(27M)	1.0000
C(244)-C(254)	1.584(8)	C(285)-H(28P)	0.9800
C(254)-C(304)	1.537(8)	C(285)-H(28Q)	0.9800
C(254)-C(314)	1.549(7)	C(285)-H(28R)	0.9800
C(254)-C(294)	1.548(8)	C(295)-H(29M)	0.9800
C(264)-H(26H)	0.9800	C(295)-H(29N)	0.9800
C(264)-H(26I)	0.9800	C(295)-H(29O)	0.9800
C(264)-H(26J)	0.9800	C(305)-C(315)	1.511(7)
C(274)-H(27I)	0.9800	C(305)-C(325)	1.529(8)
C(274)-H(27J)	0.9800	C(305)-H(30I)	1.0000

C(315)-H(31N)	0.9800	Co(5)-N(411)	1.985(5)
C(315)-H(31O)	0.9800	Co(5)-Co(6)	2.4808(12)
C(315)-H(31P)	0.9800	Co(5)-H(5)	1.59(5)
C(325)-H(32H)	0.9800	Co(5)-H(6)	1.44(5)
C(325)-H(32I)	0.9800	Co(6)-N(414)	1.975(4)
C(325)-H(32J)	0.9800	Co(6)-N(424)	1.981(4)
C(216)-C(226)	1.395(7)	Co(6)-H(5)	1.48(5)
C(216)-C(266)	1.408(7)	Co(6)-H(6)	1.49(5)
C(226)-C(236)	1.392(7)	N(411)-C(421)	1.326(6)
C(226)-C(276)	1.519(8)	N(411)-C(412)	1.438(7)
C(236)-C(246)	1.384(8)	N(421)-C(441)	1.356(7)
C(236)-H(23F)	0.9500	N(421)-C(413)	1.439(7)
C(246)-C(256)	1.378(8)	N(414)-C(444)	1.348(6)
C(246)-H(24D)	0.9500	N(414)-C(416)	1.443(7)
C(256)-C(266)	1.381(8)	C(411)-C(481)	1.538(8)
C(256)-H(25D)	0.9500	C(411)-C(461)	1.540(8)
C(266)-C(306)	1.521(8)	C(411)-C(471)	1.555(8)
C(276)-C(296)	1.519(8)	C(411)-C(421)	1.563(8)
C(276)-C(286)	1.536(8)	C(421)-C(431)	1.404(8)
C(276)-H(27N)	1.0000	C(431)-C(441)	1.394(8)
C(286)-H(28T)	0.9800	C(431)-H(43B)	0.9500
C(286)-H(28U)	0.9800	C(441)-C(451)	1.592(9)
C(286)-H(28V)	0.9800	C(441)-C(45")	1.594(9)
C(296)-H(29P)	0.9800	C(461)-H(46B)	0.9800
C(296)-H(29Q)	0.9800	C(461)-H(46C)	0.9800
C(296)-H(29R)	0.9800	C(461)-H(46D)	0.9800
C(306)-C(316)	1.526(8)	C(471)-H(47A)	0.9800
C(306)-C(326)	1.538(8)	C(471)-H(47B)	0.9800
C(306)-H(30J)	1.0000	C(471)-H(47C)	0.9800
C(316)-H(31Q)	0.9800	C(481)-H(48A)	0.9800
C(316)-H(31R)	0.9800	C(481)-H(48B)	0.9800
C(316)-H(31S)	0.9800	C(481)-H(48C)	0.9800
C(326)-H(32K)	0.9800	C(451)-C(491)	1.509(14)
C(326)-H(32L)	0.9800	C(451)-C(511)	1.530(13)
C(326)-H(32M)	0.9800	C(451)-C(501)	1.562(15)
Co(5)-N(421)	1.965(4)	C(491)-H(49A)	0.9800

C(491)-H(49B)	0.9800	C(482)-H(48F)	0.9800
C(491)-H(49C)	0.9800	C(492)-H(49G)	0.9800
C(501)-H(50A)	0.9800	C(492)-H(49H)	0.9800
C(501)-H(50B)	0.9800	C(492)-H(49I)	0.9800
C(501)-H(50C)	0.9800	C(502)-C(522)	1.527(8)
C(511)-H(51A)	0.9800	C(502)-C(512)	1.534(8)
C(511)-H(51B)	0.9800	C(502)-H(50G)	1.0000
C(511)-H(51C)	0.9800	C(512)-H(51G)	0.9800
C(45")-C(49")	1.514(14)	C(512)-H(51H)	0.9800
C(45")-C(51")	1.536(15)	C(512)-H(51I)	0.9800
C(45")-C(50")	1.566(14)	C(522)-H(52B)	0.9800
C(49")-H(49D)	0.9800	C(522)-H(52C)	0.9800
C(49")-H(49E)	0.9800	C(522)-H(52D)	0.9800
C(49")-H(49F)	0.9800	C(413)-C(423)	1.407(8)
C(50")-H(50D)	0.9800	C(413)-C(463)	1.410(7)
C(50")-H(50E)	0.9800	C(423)-C(433)	1.405(8)
C(50")-H(50F)	0.9800	C(423)-C(47')	1.518(12)
C(51")-H(51D)	0.9800	C(423)-C(473)	1.519(8)
C(51")-H(51E)	0.9800	C(433)-C(443)	1.356(9)
C(51")-H(51F)	0.9800	C(433)-H(43D)	0.9500
C(412)-C(462)	1.399(7)	C(443)-C(453)	1.385(9)
C(412)-C(422)	1.423(7)	C(443)-H(44B)	0.9500
C(422)-C(432)	1.378(8)	C(453)-C(463)	1.384(8)
C(422)-C(472)	1.513(7)	C(453)-H(45C)	0.9500
C(432)-C(442)	1.360(8)	C(463)-C(503)	1.517(8)
C(432)-H(43C)	0.9500	C(473)-C(483)	1.525(10)
C(442)-C(452)	1.379(8)	C(473)-C(493)	1.536(10)
C(442)-H(44A)	0.9500	C(473)-H(47E)	1.0000
C(452)-C(462)	1.381(8)	C(483)-H(48G)	0.9800
C(452)-H(45B)	0.9500	C(483)-H(48H)	0.9800
C(462)-C(502)	1.521(8)	C(483)-H(48I)	0.9800
C(472)-C(482)	1.523(8)	C(493)-H(49J)	0.9800
C(472)-C(492)	1.524(8)	C(493)-H(49K)	0.9800
C(472)-H(47D)	1.0000	C(493)-H(49L)	0.9800
C(482)-H(48D)	0.9800	C(47')-C(48')	1.52(2)
C(482)-H(48E)	0.9800	C(47')-C(49')	1.527(19)

C(47')-H(47F)	1.0000	C(474)-H(47I)	0.9800
C(48')-H(48J)	0.9800	C(484)-H(48M)	0.9800
C(48')-H(48K)	0.9800	C(484)-H(48N)	0.9800
C(48')-H(48L)	0.9800	C(484)-H(48O)	0.9800
C(49')-H(49M)	0.9800	C(494)-H(49P)	0.9800
C(49')-H(49N)	0.9800	C(494)-H(49Q)	0.9800
C(49')-H(49O)	0.9800	C(494)-H(49R)	0.9800
C(503)-C(523)	1.517(9)	C(504)-H(50I)	0.9800
C(503)-C(513)	1.557(9)	C(504)-H(50J)	0.9800
C(503)-H(50H)	1.0000	C(504)-H(50K)	0.9800
C(513)-H(51J)	0.9800	C(514)-H(51P)	0.9800
C(513)-H(51K)	0.9800	C(514)-H(51Q)	0.9800
C(513)-H(51L)	0.9800	C(514)-H(51R)	0.9800
C(523)-H(52E)	0.9800	C(415)-C(465)	1.400(8)
C(523)-H(52F)	0.9800	C(415)-C(425)	1.406(8)
C(523)-H(52G)	0.9800	C(415)-N(424)	1.447(7)
C(51Z)-H(51M)	0.9800	C(425)-C(435)	1.377(8)
C(51Z)-H(51N)	0.9800	C(425)-C(475)	1.510(8)
C(51Z)-H(51O)	0.9800	C(435)-C(445)	1.363(9)
C(414)-C(484)	1.531(8)	C(435)-H(43F)	0.9500
C(414)-C(464)	1.533(8)	C(445)-C(455)	1.369(9)
C(414)-C(474)	1.547(8)	C(445)-H(44C)	0.9500
C(414)-C(424)	1.578(7)	C(455)-C(465)	1.395(8)
C(424)-N(424)	1.330(7)	C(455)-H(45D)	0.9500
C(424)-C(434)	1.413(7)	C(465)-C(505)	1.504(8)
C(434)-C(444)	1.384(7)	C(475)-C(485)	1.522(8)
C(434)-H(43E)	0.9500	C(475)-C(495)	1.535(8)
C(444)-C(454)	1.589(8)	C(475)-H(47J)	1.0000
C(454)-C(494)	1.537(8)	C(485)-H(48P)	0.9800
C(454)-C(514)	1.537(7)	C(485)-H(48Q)	0.9800
C(454)-C(504)	1.546(7)	C(485)-H(48R)	0.9800
C(464)-H(46E)	0.9800	C(495)-H(49S)	0.9800
C(464)-H(46F)	0.9800	C(495)-H(49T)	0.9800
C(464)-H(46G)	0.9800	C(495)-H(49U)	0.9800
C(474)-H(47G)	0.9800	C(505)-C(515)	1.524(8)
C(474)-H(47H)	0.9800	C(505)-C(525)	1.534(8)

C(505)-H(50L)	1.0000	C(17)-C(27)	1.509(9)
C(515)-H(51S)	0.9800	C(17)-H(17A)	0.9800
C(515)-H(51T)	0.9800	C(17)-H(17B)	0.9800
C(515)-H(51U)	0.9800	C(17)-H(17C)	0.9800
C(525)-H(52K)	0.9800	C(27)-C(37)	1.3900
C(525)-H(52L)	0.9800	C(27)-C(77)	1.3900
C(525)-H(52M)	0.9800	C(37)-C(47)	1.3900
C(416)-C(426)	1.407(7)	C(37)-H(37A)	0.9500
C(416)-C(466)	1.416(8)	C(47)-C(57)	1.3900
C(426)-C(436)	1.399(7)	C(47)-H(47N)	0.9500
C(426)-C(476)	1.519(8)	C(57)-C(67)	1.3900
C(436)-C(446)	1.376(8)	C(57)-H(57A)	0.9500
C(436)-H(43G)	0.9500	C(67)-C(77)	1.3900
C(446)-C(456)	1.372(8)	C(67)-H(67A)	0.9500
C(446)-H(44D)	0.9500	C(77)-H(77A)	0.9500
C(456)-C(466)	1.394(8)	C(87)-C(97)	1.526(9)
C(456)-H(45E)	0.9500	C(87)-H(87A)	0.9800
C(466)-C(506)	1.525(8)	C(87)-H(87B)	0.9800
C(476)-C(486)	1.517(8)	C(87)-H(87C)	0.9800
C(476)-C(496)	1.545(8)	C(97)-C(107)	1.3900
C(476)-H(47K)	1.0000	C(97)-C(147)	1.3900
C(486)-H(48S)	0.9800	C(107)-C(117)	1.3900
C(486)-H(48T)	0.9800	C(107)-H(107)	0.9500
C(486)-H(48U)	0.9800	C(117)-C(127)	1.3900
C(496)-H(49V)	0.9800	C(117)-H(117)	0.9500
C(496)-H(49W)	0.9800	C(127)-C(137)	1.3900
C(496)-H(49X)	0.9800	C(127)-H(127)	0.9500
C(506)-C(526)	1.525(8)	C(137)-C(147)	1.3900
C(506)-C(516)	1.526(8)	C(137)-H(137)	0.9500
C(506)-H(50M)	1.0000	C(147)-H(147)	0.9500
C(516)-H(51V)	0.9800	C(157)-C(167)	1.465(13)
C(516)-H(51W)	0.9800	C(157)-H(15A)	0.9800
C(516)-H(51X)	0.9800	C(157)-H(15B)	0.9800
C(526)-H(52N)	0.9800	C(157)-H(15C)	0.9800
C(526)-H(52O)	0.9800	C(167)-C(177)	1.3900
C(526)-H(52P)	0.9800	C(167)-C(217)	1.3900

C(177)-C(187)	1.3900	C(277)-C(287)	1.3900
C(177)-H(17D)	0.9500	C(277)-H(277)	0.9500
C(187)-C(197)	1.3900	C(287)-H(287)	0.9500
C(187)-H(18A)	0.9500	C(22')-C(23')	1.519(14)
C(197)-C(207)	1.3900	C(22')-H(22D)	0.9800
C(197)-H(19A)	0.9500	C(22')-H(22E)	0.9800
C(207)-C(217)	1.3900	C(22')-H(22F)	0.9800
C(207)-H(20A)	0.9500	C(23')-C(24')	1.3900
C(217)-H(21A)	0.9500	C(23')-C(28')	1.3900
C(15')-C(16')	1.474(19)	C(24')-C(25')	1.3900
C(15')-H(15D)	0.9800	C(24')-H(24')	0.9500
C(15')-H(15E)	0.9800	C(25')-C(26')	1.3900
C(15')-H(15F)	0.9800	C(25')-H(25')	0.9500
C(16')-C(17')	1.3900	C(26')-C(27')	1.3900
C(16')-C(21')	1.3900	C(26')-H(26')	0.9500
C(17')-C(18')	1.3900	C(27')-C(28')	1.3900
C(17')-H(17E)	0.9500	C(27')-H(27')	0.9500
C(18')-C(19')	1.3900	C(28')-H(28')	0.9500
C(18')-H(18B)	0.9500	N(11)-Co(1)-N(21)	96.53(18)
C(19')-C(20')	1.3900	N(11)-Co(1)-Co(2)	129.27(13)
C(19')-H(19B)	0.9500	N(21)-Co(1)-Co(2)	134.17(13)
C(20')-C(21')	1.3900	N(11)-Co(1)-H(1)	121.9(17)
C(20')-H(20B)	0.9500	N(21)-Co(1)-H(1)	125.7(17)
C(21')-H(21B)	0.9500	Co(2)-Co(1)-H(1)	34.5(17)
C(227)-C(237)	1.516(12)	N(11)-Co(1)-H(2)	124.7(18)
C(227)-H(22A)	0.9800	N(21)-Co(1)-H(2)	119.4(18)
C(227)-H(22B)	0.9800	Co(2)-Co(1)-H(2)	36.2(18)
C(227)-H(22C)	0.9800	H(1)-Co(1)-H(2)	70(2)
C(237)-C(247)	1.3900	N(24)-Co(2)-N(14)	95.32(18)
C(237)-C(287)	1.3900	N(24)-Co(2)-Co(1)	130.89(13)
C(247)-C(257)	1.3900	N(14)-Co(2)-Co(1)	133.12(13)
C(247)-H(247)	0.9500	N(24)-Co(2)-H(1)	170(2)
C(257)-C(267)	1.3900	N(14)-Co(2)-H(1)	89(2)
C(257)-H(257)	0.9500	Co(1)-Co(2)-H(1)	44(2)
C(267)-C(277)	1.3900	N(24)-Co(2)-H(2)	94.1(19)
C(267)-H(267)	0.9500	N(14)-Co(2)-H(2)	170.1(19)

Co(1)-Co(2)-H(2)	38.2(19)	C(11)-C(61)-H(61B)	109.5
H(1)-Co(2)-H(2)	82(3)	H(61A)-C(61)-H(61B)	109.5
C(21)-N(11)-C(12)	118.7(4)	C(11)-C(61)-H(61C)	109.5
C(21)-N(11)-Co(1)	115.8(4)	H(61A)-C(61)-H(61C)	109.5
C(12)-N(11)-Co(1)	125.2(3)	H(61B)-C(61)-H(61C)	109.5
C(41)-N(21)-C(13)	122.0(5)	C(11)-C(71)-H(71A)	109.5
C(41)-N(21)-Co(1)	121.0(4)	C(11)-C(71)-H(71B)	109.5
C(13)-N(21)-Co(1)	116.3(3)	H(71A)-C(71)-H(71B)	109.5
C(24)-N(14)-C(15)	121.0(4)	C(11)-C(71)-H(71C)	109.5
C(24)-N(14)-Co(2)	122.6(4)	H(71A)-C(71)-H(71C)	109.5
C(15)-N(14)-Co(2)	116.4(3)	H(71B)-C(71)-H(71C)	109.5
C(44)-N(24)-C(16)	120.4(4)	C(11)-C(81)-H(81A)	109.5
C(44)-N(24)-Co(2)	120.3(3)	C(11)-C(81)-H(81B)	109.5
C(16)-N(24)-Co(2)	118.6(4)	H(81A)-C(81)-H(81B)	109.5
C(71)-C(11)-C(81)	106.0(5)	C(11)-C(81)-H(81C)	109.5
C(71)-C(11)-C(61)	108.0(5)	H(81A)-C(81)-H(81C)	109.5
C(81)-C(11)-C(61)	108.1(5)	H(81B)-C(81)-H(81C)	109.5
C(71)-C(11)-C(21)	116.2(5)	C(51)-C(91)-H(91A)	109.5
C(81)-C(11)-C(21)	108.2(4)	C(51)-C(91)-H(91B)	109.5
C(61)-C(11)-C(21)	110.1(5)	H(91A)-C(91)-H(91B)	109.5
N(11)-C(21)-C(31)	122.9(5)	C(51)-C(91)-H(91C)	109.5
N(11)-C(21)-C(11)	124.6(5)	H(91A)-C(91)-H(91C)	109.5
C(31)-C(21)-C(11)	112.5(4)	H(91B)-C(91)-H(91C)	109.5
C(21)-C(31)-C(41)	131.8(5)	C(51)-C(101)-H(10A)	109.5
C(21)-C(31)-H(31A)	114.1	C(51)-C(101)-H(10B)	109.5
C(41)-C(31)-H(31A)	114.1	H(10A)-C(101)-H(10B)	109.5
N(21)-C(41)-C(31)	120.2(5)	C(51)-C(101)-H(10C)	109.5
N(21)-C(41)-C(51)	126.9(5)	H(10A)-C(101)-H(10C)	109.5
C(31)-C(41)-C(51)	112.8(5)	H(10B)-C(101)-H(10C)	109.5
C(101)-C(51)-C(91)	106.1(5)	C(51)-C(111)-H(11A)	109.5
C(101)-C(51)-C(111)	108.6(5)	C(51)-C(111)-H(11B)	109.5
C(91)-C(51)-C(111)	106.6(5)	H(11A)-C(111)-H(11B)	109.5
C(101)-C(51)-C(41)	110.5(5)	C(51)-C(111)-H(11C)	109.5
C(91)-C(51)-C(41)	119.3(5)	H(11A)-C(111)-H(11C)	109.5
C(111)-C(51)-C(41)	105.3(5)	H(11B)-C(111)-H(11C)	109.5
C(11)-C(61)-H(61A)	109.5	C(22)-C(12)-C(62)	119.6(5)

C(22)-C(12)-N(11)	121.4(5)	C(62)-C(102)-C(122)	115.0(5)
C(62)-C(12)-N(11)	119.0(5)	C(112)-C(102)-C(122)	108.5(5)
C(32)-C(22)-C(12)	119.2(5)	C(62)-C(102)-H(10D)	108.2
C(32)-C(22)-C(72)	118.6(5)	C(112)-C(102)-H(10D)	108.2
C(12)-C(22)-C(72)	122.2(5)	C(122)-C(102)-H(10D)	108.2
C(42)-C(32)-C(22)	121.5(6)	C(102)-C(112)-H(11D)	109.5
C(42)-C(32)-H(32A)	119.3	C(102)-C(112)-H(11E)	109.5
C(22)-C(32)-H(32A)	119.3	H(11D)-C(112)-H(11E)	109.5
C(32)-C(42)-C(52)	119.2(6)	C(102)-C(112)-H(11F)	109.5
C(32)-C(42)-H(42A)	120.4	H(11D)-C(112)-H(11F)	109.5
C(52)-C(42)-H(42A)	120.4	H(11E)-C(112)-H(11F)	109.5
C(42)-C(52)-C(62)	122.2(5)	C(102)-C(122)-H(12A)	109.5
C(42)-C(52)-H(52A)	118.9	C(102)-C(122)-H(12B)	109.5
C(62)-C(52)-H(52A)	118.9	H(12A)-C(122)-H(12B)	109.5
C(52)-C(62)-C(12)	118.1(5)	C(102)-C(122)-H(12C)	109.5
C(52)-C(62)-C(102)	119.5(5)	H(12A)-C(122)-H(12C)	109.5
C(12)-C(62)-C(102)	122.2(5)	H(12B)-C(122)-H(12C)	109.5
C(22)-C(72)-C(82)	109.4(4)	C(63)-C(13)-C(23)	121.7(5)
C(22)-C(72)-C(92)	113.8(5)	C(63)-C(13)-N(21)	118.0(5)
C(82)-C(72)-C(92)	109.9(5)	C(23)-C(13)-N(21)	120.3(5)
C(22)-C(72)-H(72A)	107.8	C(33)-C(23)-C(13)	117.5(6)
C(82)-C(72)-H(72A)	107.8	C(33)-C(23)-C(73)	120.0(5)
C(92)-C(72)-H(72A)	107.8	C(13)-C(23)-C(73)	122.4(5)
C(72)-C(82)-H(82A)	109.5	C(43)-C(33)-C(23)	121.2(6)
C(72)-C(82)-H(82B)	109.5	C(43)-C(33)-H(33A)	119.4
H(82A)-C(82)-H(82B)	109.5	C(23)-C(33)-H(33A)	119.4
C(72)-C(82)-H(82C)	109.5	C(53)-C(43)-C(33)	120.1(6)
H(82A)-C(82)-H(82C)	109.5	C(53)-C(43)-H(43A)	119.9
H(82B)-C(82)-H(82C)	109.5	C(33)-C(43)-H(43A)	119.9
C(72)-C(92)-H(92A)	109.5	C(43)-C(53)-C(63)	121.4(6)
C(72)-C(92)-H(92B)	109.5	C(43)-C(53)-H(53A)	119.3
H(92A)-C(92)-H(92B)	109.5	C(63)-C(53)-H(53A)	119.3
C(72)-C(92)-H(92C)	109.5	C(53)-C(63)-C(13)	117.9(6)
H(92A)-C(92)-H(92C)	109.5	C(53)-C(63)-C(103)	119.4(6)
H(92B)-C(92)-H(92C)	109.5	C(13)-C(63)-C(103)	122.7(5)
C(62)-C(102)-C(112)	108.5(5)	C(23)-C(73)-C(93)	110.4(5)

C(23)-C(73)-C(83)	113.5(5)	C(64)-C(14)-C(74)	107.0(5)
C(93)-C(73)-C(83)	109.4(5)	C(84)-C(14)-C(74)	109.8(5)
C(23)-C(73)-H(73A)	107.8	C(64)-C(14)-C(24)	120.0(5)
C(93)-C(73)-H(73A)	107.8	C(84)-C(14)-C(24)	107.6(5)
C(83)-C(73)-H(73A)	107.8	C(74)-C(14)-C(24)	107.8(5)
C(73)-C(83)-H(83A)	109.5	N(14)-C(24)-C(34)	120.9(5)
C(73)-C(83)-H(83B)	109.5	N(14)-C(24)-C(14)	127.3(5)
H(83A)-C(83)-H(83B)	109.5	C(34)-C(24)-C(14)	111.8(5)
C(73)-C(83)-H(83C)	109.5	C(44)-C(34)-C(24)	130.6(5)
H(83A)-C(83)-H(83C)	109.5	C(44)-C(34)-H(34A)	114.7
H(83B)-C(83)-H(83C)	109.5	C(24)-C(34)-H(34A)	114.7
C(73)-C(93)-H(93A)	109.5	N(24)-C(44)-C(34)	121.6(5)
C(73)-C(93)-H(93B)	109.5	N(24)-C(44)-C(54)	125.0(5)
H(93A)-C(93)-H(93B)	109.5	C(34)-C(44)-C(54)	113.2(5)
C(73)-C(93)-H(93C)	109.5	C(104)-C(54)-C(94)	107.4(5)
H(93A)-C(93)-H(93C)	109.5	C(104)-C(54)-C(114)	105.6(5)
H(93B)-C(93)-H(93C)	109.5	C(94)-C(54)-C(114)	107.5(5)
C(63)-C(103)-C(123)	110.0(5)	C(104)-C(54)-C(44)	113.1(5)
C(63)-C(103)-C(113)	114.1(5)	C(94)-C(54)-C(44)	105.0(4)
C(123)-C(103)-C(113)	109.0(5)	C(114)-C(54)-C(44)	117.7(5)
C(63)-C(103)-H(10E)	107.9	C(14)-C(64)-H(64A)	109.5
C(123)-C(103)-H(10E)	107.9	C(14)-C(64)-H(64B)	109.5
C(113)-C(103)-H(10E)	107.9	H(64A)-C(64)-H(64B)	109.5
C(103)-C(113)-H(11G)	109.5	C(14)-C(64)-H(64C)	109.5
C(103)-C(113)-H(11H)	109.5	H(64A)-C(64)-H(64C)	109.5
H(11G)-C(113)-H(11H)	109.5	H(64B)-C(64)-H(64C)	109.5
C(103)-C(113)-H(11I)	109.5	C(14)-C(74)-H(74A)	109.5
H(11G)-C(113)-H(11I)	109.5	C(14)-C(74)-H(74B)	109.5
H(11H)-C(113)-H(11I)	109.5	H(74A)-C(74)-H(74B)	109.5
C(103)-C(123)-H(12D)	109.5	C(14)-C(74)-H(74C)	109.5
C(103)-C(123)-H(12E)	109.5	H(74A)-C(74)-H(74C)	109.5
H(12D)-C(123)-H(12E)	109.5	H(74B)-C(74)-H(74C)	109.5
C(103)-C(123)-H(12F)	109.5	C(14)-C(84)-H(84A)	109.5
H(12D)-C(123)-H(12F)	109.5	C(14)-C(84)-H(84B)	109.5
H(12E)-C(123)-H(12F)	109.5	H(84A)-C(84)-H(84B)	109.5
C(64)-C(14)-C(84)	104.4(5)	C(14)-C(84)-H(84C)	109.5

H(84A)-C(84)-H(84C)	109.5	C(15)-C(65)-C(105)	123.8(5)
H(84B)-C(84)-H(84C)	109.5	C(55)-C(65)-C(105)	117.7(5)
C(54)-C(94)-H(94A)	109.5	C(25)-C(75)-C(95)	114.2(5)
C(54)-C(94)-H(94B)	109.5	C(25)-C(75)-C(85)	109.5(5)
H(94A)-C(94)-H(94B)	109.5	C(95)-C(75)-C(85)	110.0(5)
C(54)-C(94)-H(94C)	109.5	C(25)-C(75)-H(75A)	107.6
H(94A)-C(94)-H(94C)	109.5	C(95)-C(75)-H(75A)	107.6
H(94B)-C(94)-H(94C)	109.5	C(85)-C(75)-H(75A)	107.6
C(54)-C(104)-H(10F)	109.5	C(75)-C(85)-H(85A)	109.5
C(54)-C(104)-H(10G)	109.5	C(75)-C(85)-H(85B)	109.5
H(10F)-C(104)-H(10G)	109.5	H(85A)-C(85)-H(85B)	109.5
C(54)-C(104)-H(10H)	109.5	C(75)-C(85)-H(85C)	109.5
H(10F)-C(104)-H(10H)	109.5	H(85A)-C(85)-H(85C)	109.5
H(10G)-C(104)-H(10H)	109.5	H(85B)-C(85)-H(85C)	109.5
C(54)-C(114)-H(11J)	109.5	C(75)-C(95)-H(95A)	109.5
C(54)-C(114)-H(11K)	109.5	C(75)-C(95)-H(95B)	109.5
H(11J)-C(114)-H(11K)	109.5	H(95A)-C(95)-H(95B)	109.5
C(54)-C(114)-H(11L)	109.5	C(75)-C(95)-H(95C)	109.5
H(11J)-C(114)-H(11L)	109.5	H(95A)-C(95)-H(95C)	109.5
H(11K)-C(114)-H(11L)	109.5	H(95B)-C(95)-H(95C)	109.5
C(65)-C(15)-C(25)	120.2(5)	C(65)-C(105)-C(125)	110.2(5)
C(65)-C(15)-N(14)	119.8(5)	C(65)-C(105)-C(115)	113.4(5)
C(25)-C(15)-N(14)	120.0(5)	C(125)-C(105)-C(115)	109.8(5)
C(35)-C(25)-C(15)	118.6(6)	C(65)-C(105)-H(10I)	107.7
C(35)-C(25)-C(75)	120.4(5)	C(125)-C(105)-H(10I)	107.7
C(15)-C(25)-C(75)	121.0(5)	C(115)-C(105)-H(10I)	107.7
C(45)-C(35)-C(25)	122.2(6)	C(105)-C(115)-H(11M)	109.5
C(45)-C(35)-H(35A)	118.9	C(105)-C(115)-H(11N)	109.5
C(25)-C(35)-H(35A)	118.9	H(11M)-C(115)-H(11N)	109.5
C(35)-C(45)-C(55)	119.9(5)	C(105)-C(115)-H(11O)	109.5
C(35)-C(45)-H(45A)	120.1	H(11M)-C(115)-H(11O)	109.5
C(55)-C(45)-H(45A)	120.1	H(11N)-C(115)-H(11O)	109.5
C(45)-C(55)-C(65)	120.7(6)	C(105)-C(125)-H(12G)	109.5
C(45)-C(55)-H(55A)	119.7	C(105)-C(125)-H(12H)	109.5
C(65)-C(55)-H(55A)	119.7	H(12G)-C(125)-H(12H)	109.5
C(15)-C(65)-C(55)	118.5(6)	C(105)-C(125)-H(12I)	109.5

H(12G)-C(125)-H(12I)	109.5	H(96A)-C(96)-H(96C)	109.5
H(12H)-C(125)-H(12I)	109.5	H(96B)-C(96)-H(96C)	109.5
C(66)-C(16)-C(26)	119.7(5)	C(66)-C(106)-C(126)	113.0(5)
C(66)-C(16)-N(24)	118.1(5)	C(66)-C(106)-C(116)	112.4(5)
C(26)-C(16)-N(24)	122.2(5)	C(126)-C(106)-C(116)	108.0(5)
C(36)-C(26)-C(16)	118.8(6)	C(66)-C(106)-H(10J)	107.7
C(36)-C(26)-C(76)	117.6(5)	C(126)-C(106)-H(10J)	107.7
C(16)-C(26)-C(76)	123.6(5)	C(116)-C(106)-H(10J)	107.7
C(46)-C(36)-C(26)	121.2(6)	C(106)-C(116)-H(11P)	109.5
C(46)-C(36)-H(36A)	119.4	C(106)-C(116)-H(11Q)	109.5
C(26)-C(36)-H(36A)	119.4	H(11P)-C(116)-H(11Q)	109.5
C(56)-C(46)-C(36)	120.2(6)	C(106)-C(116)-H(11R)	109.5
C(56)-C(46)-H(46A)	119.9	H(11P)-C(116)-H(11R)	109.5
C(36)-C(46)-H(46A)	119.9	H(11Q)-C(116)-H(11R)	109.5
C(46)-C(56)-C(66)	121.0(6)	C(106)-C(126)-H(12J)	109.5
C(46)-C(56)-H(56A)	119.5	C(106)-C(126)-H(12K)	109.5
C(66)-C(56)-H(56A)	119.5	H(12J)-C(126)-H(12K)	109.5
C(56)-C(66)-C(16)	119.0(6)	C(106)-C(126)-H(12L)	109.5
C(56)-C(66)-C(106)	118.1(6)	H(12J)-C(126)-H(12L)	109.5
C(16)-C(66)-C(106)	122.9(5)	H(12K)-C(126)-H(12L)	109.5
C(26)-C(76)-C(96)	112.1(5)	N(221)-Co(3)-N(211)	95.97(19)
C(26)-C(76)-C(86)	111.9(5)	N(221)-Co(3)-Co(4)	129.12(14)
C(96)-C(76)-C(86)	108.9(5)	N(211)-Co(3)-Co(4)	134.90(14)
C(26)-C(76)-H(76A)	107.9	N(221)-Co(3)-H(3)	119.8(18)
C(96)-C(76)-H(76A)	107.9	N(211)-Co(3)-H(3)	126.2(18)
C(86)-C(76)-H(76A)	107.9	Co(4)-Co(3)-H(3)	34.7(18)
C(76)-C(86)-H(86A)	109.5	N(221)-Co(3)-H(4)	135.8(19)
C(76)-C(86)-H(86B)	109.5	N(211)-Co(3)-H(4)	111.3(19)
H(86A)-C(86)-H(86B)	109.5	Co(4)-Co(3)-H(4)	38.2(19)
C(76)-C(86)-H(86C)	109.5	H(3)-Co(3)-H(4)	71(2)
H(86A)-C(86)-H(86C)	109.5	N(224)-Co(4)-N(214)	95.44(18)
H(86B)-C(86)-H(86C)	109.5	N(224)-Co(4)-Co(3)	131.49(13)
C(76)-C(96)-H(96A)	109.5	N(214)-Co(4)-Co(3)	132.49(13)
C(76)-C(96)-H(96B)	109.5	N(224)-Co(4)-H(3)	170(2)
H(96A)-C(96)-H(96B)	109.5	N(214)-Co(4)-H(3)	93(2)
C(76)-C(96)-H(96C)	109.5	Co(3)-Co(4)-H(3)	40(2)

N(224)-Co(4)-H(4)	98.5(18)	C(261)-C(211)-C(221)	110.1(7)
N(214)-Co(4)-H(4)	162.2(19)	C(281)-C(211)-C(221)	119.4(6)
Co(3)-Co(4)-H(4)	37.0(18)	C(271)-C(211)-C(221)	106.1(7)
H(3)-Co(4)-H(4)	75(3)	C(26")-C(21")-C(27")	108(2)
C(221)-N(211)-C(212)	122.5(5)	C(26")-C(21")-C(221)	111(2)
C(221)-N(211)-Co(3)	121.7(4)	C(27")-C(21")-C(221)	105(2)
C(212)-N(211)-Co(3)	115.6(3)	C(21")-C(26")-H(26D)	109.5
C(241)-N(221)-C(213)	120.8(5)	C(21")-C(26")-H(26E)	109.5
C(241)-N(221)-Co(3)	118.1(4)	H(26D)-C(26")-H(26E)	109.5
C(213)-N(221)-Co(3)	120.8(3)	C(21")-C(26")-H(26F)	109.5
C(224)-N(214)-C(215)	120.6(4)	H(26D)-C(26")-H(26F)	109.5
C(224)-N(214)-Co(4)	124.1(4)	H(26E)-C(26")-H(26F)	109.5
C(215)-N(214)-Co(4)	115.2(3)	C(21")-C(27")-H(27D)	109.5
C(244)-N(224)-C(216)	118.7(4)	C(21")-C(27")-H(27E)	109.5
C(244)-N(224)-Co(4)	120.5(3)	H(27D)-C(27")-H(27E)	109.5
C(216)-N(224)-Co(4)	119.8(3)	C(21")-C(27")-H(27F)	109.5
C(241)-C(231)-C(221)	132.3(5)	H(27D)-C(27")-H(27F)	109.5
C(241)-C(231)-H(23A)	113.8	H(27E)-C(27")-H(27F)	109.5
C(221)-C(231)-H(23A)	113.8	C(251)-C(291)-H(29A)	109.5
N(221)-C(241)-C(231)	121.2(5)	C(251)-C(291)-H(29B)	109.5
N(221)-C(241)-C(251)	123.5(5)	H(29A)-C(291)-H(29B)	109.5
C(231)-C(241)-C(251)	114.9(5)	C(251)-C(291)-H(29C)	109.5
C(311)-C(251)-C(291)	108.7(5)	H(29A)-C(291)-H(29C)	109.5
C(311)-C(251)-C(301)	106.3(5)	H(29B)-C(291)-H(29C)	109.5
C(291)-C(251)-C(301)	107.1(5)	C(251)-C(301)-H(30A)	109.5
C(311)-C(251)-C(241)	118.7(5)	C(251)-C(301)-H(30B)	109.5
C(291)-C(251)-C(241)	104.8(5)	H(30A)-C(301)-H(30B)	109.5
C(301)-C(251)-C(241)	110.7(5)	C(251)-C(301)-H(30C)	109.5
N(211)-C(221)-C(231)	119.9(5)	H(30A)-C(301)-H(30C)	109.5
N(211)-C(221)-C(211)	127.5(6)	H(30B)-C(301)-H(30C)	109.5
C(231)-C(221)-C(211)	112.5(5)	C(251)-C(311)-H(31B)	109.5
N(211)-C(221)-C(21")	127.2(9)	C(251)-C(311)-H(31C)	109.5
C(231)-C(221)-C(21")	112.7(9)	H(31B)-C(311)-H(31C)	109.5
C(261)-C(211)-C(281)	106.9(7)	C(251)-C(311)-H(31D)	109.5
C(261)-C(211)-C(271)	108.3(7)	H(31B)-C(311)-H(31D)	109.5
C(281)-C(211)-C(271)	105.6(7)	H(31C)-C(311)-H(31D)	109.5

C(262)-C(212)-C(222)	119.6(6)	C(312)-C(302)-C(262)	110.0(5)
C(262)-C(212)-N(211)	118.4(5)	C(312)-C(302)-C(322)	109.0(5)
C(222)-C(212)-N(211)	122.0(6)	C(262)-C(302)-C(322)	113.0(5)
C(232)-C(222)-C(212)	119.3(6)	C(312)-C(302)-H(30D)	108.2
C(232)-C(222)-C(272)	120.2(5)	C(262)-C(302)-H(30D)	108.2
C(212)-C(222)-C(272)	120.6(5)	C(322)-C(302)-H(30D)	108.2
C(222)-C(232)-C(242)	120.8(6)	C(302)-C(312)-H(31E)	109.5
C(222)-C(232)-H(23B)	119.6	C(302)-C(312)-H(31F)	109.5
C(242)-C(232)-H(23B)	119.6	H(31E)-C(312)-H(31F)	109.5
C(252)-C(242)-C(232)	120.0(6)	C(302)-C(312)-H(31G)	109.5
C(252)-C(242)-H(24A)	120.0	H(31E)-C(312)-H(31G)	109.5
C(232)-C(242)-H(24A)	120.0	H(31F)-C(312)-H(31G)	109.5
C(262)-C(252)-C(242)	120.6(6)	C(302)-C(322)-H(32B)	109.5
C(262)-C(252)-H(25A)	119.7	C(302)-C(322)-H(32C)	109.5
C(242)-C(252)-H(25A)	119.7	H(32B)-C(322)-H(32C)	109.5
C(252)-C(262)-C(212)	119.7(6)	C(302)-C(322)-H(32D)	109.5
C(252)-C(262)-C(302)	118.5(6)	H(32B)-C(322)-H(32D)	109.5
C(212)-C(262)-C(302)	121.8(6)	H(32C)-C(322)-H(32D)	109.5
C(222)-C(272)-C(282)	109.6(5)	C(223)-C(213)-C(263)	120.8(5)
C(222)-C(272)-C(292)	112.7(5)	C(223)-C(213)-N(221)	121.1(5)
C(282)-C(272)-C(292)	109.4(5)	C(263)-C(213)-N(221)	118.0(5)
C(222)-C(272)-H(27G)	108.3	C(213)-C(223)-C(233)	118.6(5)
C(282)-C(272)-H(27G)	108.3	C(213)-C(223)-C(273)	123.2(5)
C(292)-C(272)-H(27G)	108.3	C(233)-C(223)-C(273)	118.3(5)
C(272)-C(282)-H(28G)	109.5	C(243)-C(233)-C(223)	121.8(6)
C(272)-C(282)-H(28H)	109.5	C(243)-C(233)-H(23C)	119.1
H(28G)-C(282)-H(28H)	109.5	C(223)-C(233)-H(23C)	119.1
C(272)-C(282)-H(28I)	109.5	C(233)-C(243)-C(253)	119.1(6)
H(28G)-C(282)-H(28I)	109.5	C(233)-C(243)-H(24B)	120.4
H(28H)-C(282)-H(28I)	109.5	C(253)-C(243)-H(24B)	120.4
C(272)-C(292)-H(29D)	109.5	C(243)-C(253)-C(263)	121.3(6)
C(272)-C(292)-H(29E)	109.5	C(243)-C(253)-H(25B)	119.4
H(29D)-C(292)-H(29E)	109.5	C(263)-C(253)-H(25B)	119.4
C(272)-C(292)-H(29F)	109.5	C(253)-C(263)-C(213)	118.2(6)
H(29D)-C(292)-H(29F)	109.5	C(253)-C(263)-C(303)	119.2(5)
H(29E)-C(292)-H(29F)	109.5	C(213)-C(263)-C(303)	122.6(5)

C(223)-C(273)-C(293)	111.2(5)	C(274)-C(214)-C(264)	104.8(5)
C(223)-C(273)-C(283)	112.2(5)	C(274)-C(214)-C(284)	107.8(5)
C(293)-C(273)-C(283)	109.9(5)	C(264)-C(214)-C(284)	107.5(5)
C(223)-C(273)-H(27H)	107.8	C(274)-C(214)-C(224)	111.1(5)
C(293)-C(273)-H(27H)	107.8	C(264)-C(214)-C(224)	119.3(5)
C(283)-C(273)-H(27H)	107.8	C(284)-C(214)-C(224)	105.8(5)
C(273)-C(283)-H(28J)	109.5	N(214)-C(224)-C(234)	119.7(5)
C(273)-C(283)-H(28K)	109.5	N(214)-C(224)-C(214)	127.8(5)
H(28J)-C(283)-H(28K)	109.5	C(234)-C(224)-C(214)	112.3(5)
C(273)-C(283)-H(28L)	109.5	C(244)-C(234)-C(224)	131.9(5)
H(28J)-C(283)-H(28L)	109.5	C(244)-C(234)-H(23D)	114.1
H(28K)-C(283)-H(28L)	109.5	C(224)-C(234)-H(23D)	114.1
C(273)-C(293)-H(29G)	109.5	N(224)-C(244)-C(234)	121.4(5)
C(273)-C(293)-H(29H)	109.5	N(224)-C(244)-C(254)	124.0(5)
H(29G)-C(293)-H(29H)	109.5	C(234)-C(244)-C(254)	114.2(5)
C(273)-C(293)-H(29I)	109.5	C(304)-C(254)-C(314)	106.5(5)
H(29G)-C(293)-H(29I)	109.5	C(304)-C(254)-C(294)	108.3(5)
H(29H)-C(293)-H(29I)	109.5	C(314)-C(254)-C(294)	105.3(5)
C(313)-C(303)-C(263)	111.7(6)	C(304)-C(254)-C(244)	105.8(5)
C(313)-C(303)-C(323)	109.3(5)	C(314)-C(254)-C(244)	112.4(5)
C(263)-C(303)-C(323)	112.5(6)	C(294)-C(254)-C(244)	118.1(5)
C(313)-C(303)-H(30E)	107.8	C(214)-C(264)-H(26H)	109.5
C(263)-C(303)-H(30E)	107.8	C(214)-C(264)-H(26I)	109.5
C(323)-C(303)-H(30E)	107.8	H(26H)-C(264)-H(26I)	109.5
C(303)-C(313)-H(31H)	109.5	C(214)-C(264)-H(26J)	109.5
C(303)-C(313)-H(31I)	109.5	H(26H)-C(264)-H(26J)	109.5
H(31H)-C(313)-H(31I)	109.5	H(26I)-C(264)-H(26J)	109.5
C(303)-C(313)-H(31J)	109.5	C(214)-C(274)-H(27I)	109.5
H(31H)-C(313)-H(31J)	109.5	C(214)-C(274)-H(27J)	109.5
H(31I)-C(313)-H(31J)	109.5	H(27I)-C(274)-H(27J)	109.5
C(303)-C(323)-H(32E)	109.5	C(214)-C(274)-H(27L)	109.5
C(303)-C(323)-H(32F)	109.5	H(27I)-C(274)-H(27L)	109.5
H(32E)-C(323)-H(32F)	109.5	H(27J)-C(274)-H(27L)	109.5
C(303)-C(323)-H(32G)	109.5	C(214)-C(284)-H(28M)	109.5
H(32E)-C(323)-H(32G)	109.5	C(214)-C(284)-H(28N)	109.5
H(32F)-C(323)-H(32G)	109.5	H(28M)-C(284)-H(28N)	109.5

C(214)-C(284)-H(28O)	109.5	C(255)-C(265)-C(215)	117.3(6)
H(28M)-C(284)-H(28O)	109.5	C(255)-C(265)-C(305)	120.3(6)
H(28N)-C(284)-H(28O)	109.5	C(215)-C(265)-C(305)	122.4(5)
C(254)-C(294)-H(29J)	109.5	C(225)-C(275)-C(285)	109.3(5)
C(254)-C(294)-H(29K)	109.5	C(225)-C(275)-C(295)	112.6(5)
H(29J)-C(294)-H(29K)	109.5	C(285)-C(275)-C(295)	110.1(5)
C(254)-C(294)-H(29L)	109.5	C(225)-C(275)-H(27M)	108.2
H(29J)-C(294)-H(29L)	109.5	C(285)-C(275)-H(27M)	108.2
H(29K)-C(294)-H(29L)	109.5	C(295)-C(275)-H(27M)	108.2
C(254)-C(304)-H(30F)	109.5	C(275)-C(285)-H(28P)	109.5
C(254)-C(304)-H(30G)	109.5	C(275)-C(285)-H(28Q)	109.5
H(30F)-C(304)-H(30G)	109.5	H(28P)-C(285)-H(28Q)	109.5
C(254)-C(304)-H(30H)	109.5	C(275)-C(285)-H(28R)	109.5
H(30F)-C(304)-H(30H)	109.5	H(28P)-C(285)-H(28R)	109.5
H(30G)-C(304)-H(30H)	109.5	H(28Q)-C(285)-H(28R)	109.5
C(254)-C(314)-H(31K)	109.5	C(275)-C(295)-H(29M)	109.5
C(254)-C(314)-H(31L)	109.5	C(275)-C(295)-H(29N)	109.5
H(31K)-C(314)-H(31L)	109.5	H(29M)-C(295)-H(29N)	109.5
C(254)-C(314)-H(31M)	109.5	C(275)-C(295)-H(29O)	109.5
H(31K)-C(314)-H(31M)	109.5	H(29M)-C(295)-H(29O)	109.5
H(31L)-C(314)-H(31M)	109.5	H(29N)-C(295)-H(29O)	109.5
C(225)-C(215)-C(265)	121.7(5)	C(315)-C(305)-C(265)	113.1(5)
C(225)-C(215)-N(214)	119.1(5)	C(315)-C(305)-C(325)	108.4(5)
C(265)-C(215)-N(214)	119.2(5)	C(265)-C(305)-C(325)	115.3(5)
C(235)-C(225)-C(215)	117.8(6)	C(315)-C(305)-H(30I)	106.5
C(235)-C(225)-C(275)	119.7(5)	C(265)-C(305)-H(30I)	106.5
C(215)-C(225)-C(275)	122.5(5)	C(325)-C(305)-H(30I)	106.5
C(245)-C(235)-C(225)	120.8(6)	C(305)-C(315)-H(31N)	109.5
C(245)-C(235)-H(23E)	119.6	C(305)-C(315)-H(31O)	109.5
C(225)-C(235)-H(23E)	119.6	H(31N)-C(315)-H(31O)	109.5
C(235)-C(245)-C(255)	121.1(6)	C(305)-C(315)-H(31P)	109.5
C(235)-C(245)-H(24C)	119.4	H(31N)-C(315)-H(31P)	109.5
C(255)-C(245)-H(24C)	119.4	H(31O)-C(315)-H(31P)	109.5
C(245)-C(255)-C(265)	121.0(6)	C(305)-C(325)-H(32H)	109.5
C(245)-C(255)-H(25C)	119.5	C(305)-C(325)-H(32I)	109.5
C(265)-C(255)-H(25C)	119.5	H(32H)-C(325)-H(32I)	109.5

C(305)-C(325)-H(32J)	109.5	C(276)-C(296)-H(29R)	109.5
H(32H)-C(325)-H(32J)	109.5	H(29P)-C(296)-H(29R)	109.5
H(32I)-C(325)-H(32J)	109.5	H(29Q)-C(296)-H(29R)	109.5
C(226)-C(216)-C(266)	119.9(5)	C(266)-C(306)-C(316)	113.2(5)
C(226)-C(216)-N(224)	122.4(5)	C(266)-C(306)-C(326)	111.1(5)
C(266)-C(216)-N(224)	117.7(5)	C(316)-C(306)-C(326)	108.6(5)
C(236)-C(226)-C(216)	118.9(5)	C(266)-C(306)-H(30J)	108.0
C(236)-C(226)-C(276)	117.3(5)	C(316)-C(306)-H(30J)	108.0
C(216)-C(226)-C(276)	123.8(5)	C(326)-C(306)-H(30J)	108.0
C(246)-C(236)-C(226)	121.4(5)	C(306)-C(316)-H(31Q)	109.5
C(246)-C(236)-H(23F)	119.3	C(306)-C(316)-H(31R)	109.5
C(226)-C(236)-H(23F)	119.3	H(31Q)-C(316)-H(31R)	109.5
C(256)-C(246)-C(236)	119.0(5)	C(306)-C(316)-H(31S)	109.5
C(256)-C(246)-H(24D)	120.5	H(31Q)-C(316)-H(31S)	109.5
C(236)-C(246)-H(24D)	120.5	H(31R)-C(316)-H(31S)	109.5
C(246)-C(256)-C(266)	121.6(5)	C(306)-C(326)-H(32K)	109.5
C(246)-C(256)-H(25D)	119.2	C(306)-C(326)-H(32L)	109.5
C(266)-C(256)-H(25D)	119.2	H(32K)-C(326)-H(32L)	109.5
C(256)-C(266)-C(216)	119.0(5)	C(306)-C(326)-H(32M)	109.5
C(256)-C(266)-C(306)	118.9(5)	H(32K)-C(326)-H(32M)	109.5
C(216)-C(266)-C(306)	122.0(5)	H(32L)-C(326)-H(32M)	109.5
C(226)-C(276)-C(296)	111.5(5)	N(421)-Co(5)-N(411)	96.11(18)
C(226)-C(276)-C(286)	111.9(5)	N(421)-Co(5)-Co(6)	130.68(14)
C(296)-C(276)-C(286)	109.5(5)	N(411)-Co(5)-Co(6)	133.18(13)
C(226)-C(276)-H(27N)	107.9	N(421)-Co(5)-H(5)	118.9(19)
C(296)-C(276)-H(27N)	107.9	N(411)-Co(5)-H(5)	129.1(19)
C(286)-C(276)-H(27N)	107.9	Co(6)-Co(5)-H(5)	34.7(19)
C(276)-C(286)-H(28T)	109.5	N(421)-Co(5)-H(6)	141(2)
C(276)-C(286)-H(28U)	109.5	N(411)-Co(5)-H(6)	110(2)
H(28T)-C(286)-H(28U)	109.5	Co(6)-Co(5)-H(6)	33(2)
C(276)-C(286)-H(28V)	109.5	H(5)-Co(5)-H(6)	65(3)
H(28T)-C(286)-H(28V)	109.5	N(414)-Co(6)-N(424)	95.42(18)
H(28U)-C(286)-H(28V)	109.5	N(414)-Co(6)-Co(5)	131.61(13)
C(276)-C(296)-H(29P)	109.5	N(424)-Co(6)-Co(5)	132.36(13)
C(276)-C(296)-H(29Q)	109.5	N(414)-Co(6)-H(5)	166(2)
H(29P)-C(296)-H(29Q)	109.5	N(424)-Co(6)-H(5)	95(2)

Co(5)-Co(6)-H(5)	38(2)	H(46C)-C(461)-H(46D)	109.5
N(414)-Co(6)-H(6)	106(2)	C(411)-C(471)-H(47A)	109.5
N(424)-Co(6)-H(6)	155(2)	C(411)-C(471)-H(47B)	109.5
Co(5)-Co(6)-H(6)	31(2)	H(47A)-C(471)-H(47B)	109.5
H(5)-Co(6)-H(6)	67(3)	C(411)-C(471)-H(47C)	109.5
C(421)-N(411)-C(412)	122.8(5)	H(47A)-C(471)-H(47C)	109.5
C(421)-N(411)-Co(5)	121.1(4)	H(47B)-C(471)-H(47C)	109.5
C(412)-N(411)-Co(5)	115.9(3)	C(411)-C(481)-H(48A)	109.5
C(441)-N(421)-C(413)	118.7(5)	C(411)-C(481)-H(48B)	109.5
C(441)-N(421)-Co(5)	118.0(4)	H(48A)-C(481)-H(48B)	109.5
C(413)-N(421)-Co(5)	123.0(4)	C(411)-C(481)-H(48C)	109.5
C(444)-N(414)-C(416)	120.7(4)	H(48A)-C(481)-H(48C)	109.5
C(444)-N(414)-Co(6)	119.2(4)	H(48B)-C(481)-H(48C)	109.5
C(416)-N(414)-Co(6)	119.9(3)	C(491)-C(451)-C(511)	106.6(13)
C(481)-C(411)-C(461)	107.0(5)	C(491)-C(451)-C(501)	109.3(14)
C(481)-C(411)-C(471)	109.4(5)	C(511)-C(451)-C(501)	107.2(12)
C(461)-C(411)-C(471)	104.9(5)	C(491)-C(451)-C(441)	108(3)
C(481)-C(411)-C(421)	109.4(5)	C(511)-C(451)-C(441)	118.8(12)
C(461)-C(411)-C(421)	119.5(5)	C(501)-C(451)-C(441)	106.8(11)
C(471)-C(411)-C(421)	106.3(5)	C(49")-C(45")-C(51")	107.1(16)
N(411)-C(421)-C(431)	120.7(5)	C(49")-C(45")-C(50")	106.8(14)
N(411)-C(421)-C(411)	127.0(5)	C(51")-C(45")-C(50")	105.3(11)
C(431)-C(421)-C(411)	112.2(5)	C(49")-C(45")-C(441)	104(3)
C(441)-C(431)-C(421)	131.9(5)	C(51")-C(45")-C(441)	117.1(14)
C(441)-C(431)-H(43B)	114.0	C(50")-C(45")-C(441)	115.5(12)
C(421)-C(431)-H(43B)	114.0	C(462)-C(412)-C(422)	120.5(5)
N(421)-C(441)-C(431)	121.5(5)	C(462)-C(412)-N(411)	119.3(5)
N(421)-C(441)-C(451)	122.2(9)	C(422)-C(412)-N(411)	120.2(5)
C(431)-C(441)-C(451)	116.0(9)	C(432)-C(422)-C(412)	117.6(5)
N(421)-C(441)-C(45")	128.8(9)	C(432)-C(422)-C(472)	121.0(5)
C(431)-C(441)-C(45")	109.6(9)	C(412)-C(422)-C(472)	121.4(5)
C(411)-C(461)-H(46B)	109.5	C(442)-C(432)-C(422)	122.3(6)
C(411)-C(461)-H(46C)	109.5	C(442)-C(432)-H(43C)	118.8
H(46B)-C(461)-H(46C)	109.5	C(422)-C(432)-H(43C)	118.8
C(411)-C(461)-H(46D)	109.5	C(432)-C(442)-C(452)	119.6(6)
H(46B)-C(461)-H(46D)	109.5	C(432)-C(442)-H(44A)	120.2

C(452)-C(442)-H(44A)	120.2	H(51H)-C(512)-H(51I)	109.5
C(442)-C(452)-C(462)	121.4(6)	C(502)-C(522)-H(52B)	109.5
C(442)-C(452)-H(45B)	119.3	C(502)-C(522)-H(52C)	109.5
C(462)-C(452)-H(45B)	119.3	H(52B)-C(522)-H(52C)	109.5
C(452)-C(462)-C(412)	118.4(5)	C(502)-C(522)-H(52D)	109.5
C(452)-C(462)-C(502)	119.3(5)	H(52B)-C(522)-H(52D)	109.5
C(412)-C(462)-C(502)	122.3(5)	H(52C)-C(522)-H(52D)	109.5
C(422)-C(472)-C(482)	113.3(5)	C(423)-C(413)-C(463)	119.6(5)
C(422)-C(472)-C(492)	109.0(5)	C(423)-C(413)-N(421)	120.7(5)
C(482)-C(472)-C(492)	108.8(5)	C(463)-C(413)-N(421)	119.7(5)
C(422)-C(472)-H(47D)	108.5	C(433)-C(423)-C(413)	119.0(6)
C(482)-C(472)-H(47D)	108.5	C(433)-C(423)-C(47')	115.8(15)
C(492)-C(472)-H(47D)	108.5	C(413)-C(423)-C(47')	122.2(15)
C(472)-C(482)-H(48D)	109.5	C(433)-C(423)-C(473)	118.2(6)
C(472)-C(482)-H(48E)	109.5	C(413)-C(423)-C(473)	122.7(6)
H(48D)-C(482)-H(48E)	109.5	C(443)-C(433)-C(423)	121.4(7)
C(472)-C(482)-H(48F)	109.5	C(443)-C(433)-H(43D)	119.3
H(48D)-C(482)-H(48F)	109.5	C(423)-C(433)-H(43D)	119.3
H(48E)-C(482)-H(48F)	109.5	C(433)-C(443)-C(453)	119.3(6)
C(472)-C(492)-H(49G)	109.5	C(433)-C(443)-H(44B)	120.4
C(472)-C(492)-H(49H)	109.5	C(453)-C(443)-H(44B)	120.4
H(49G)-C(492)-H(49H)	109.5	C(463)-C(453)-C(443)	122.1(6)
C(472)-C(492)-H(49I)	109.5	C(463)-C(453)-H(45C)	119.0
H(49G)-C(492)-H(49I)	109.5	C(443)-C(453)-H(45C)	119.0
H(49H)-C(492)-H(49I)	109.5	C(453)-C(463)-C(413)	118.5(6)
C(462)-C(502)-C(522)	109.8(5)	C(453)-C(463)-C(503)	119.6(5)
C(462)-C(502)-C(512)	112.7(5)	C(413)-C(463)-C(503)	121.8(5)
C(522)-C(502)-C(512)	109.4(5)	C(423)-C(473)-C(483)	112.5(6)
C(462)-C(502)-H(50G)	108.3	C(423)-C(473)-C(493)	112.6(6)
C(522)-C(502)-H(50G)	108.3	C(483)-C(473)-C(493)	111.0(7)
C(512)-C(502)-H(50G)	108.3	C(423)-C(473)-H(47E)	106.8
C(502)-C(512)-H(51G)	109.5	C(483)-C(473)-H(47E)	106.8
C(502)-C(512)-H(51H)	109.5	C(493)-C(473)-H(47E)	106.8
H(51G)-C(512)-H(51H)	109.5	C(423)-C(47')-C(48')	99(2)
C(502)-C(512)-H(51I)	109.5	C(423)-C(47')-C(49')	117(2)
H(51G)-C(512)-H(51I)	109.5	C(48')-C(47')-C(49')	112(2)

C(423)-C(47')-H(47F)	109.4	C(414)-C(464)-H(46G)	109.5
C(48')-C(47')-H(47F)	109.4	H(46E)-C(464)-H(46G)	109.5
C(49')-C(47')-H(47F)	109.4	H(46F)-C(464)-H(46G)	109.5
C(463)-C(503)-C(523)	111.6(5)	C(414)-C(474)-H(47G)	109.5
C(463)-C(503)-C(513)	109.4(6)	C(414)-C(474)-H(47H)	109.5
C(523)-C(503)-C(513)	105.2(6)	H(47G)-C(474)-H(47H)	109.5
C(463)-C(503)-H(50H)	110.2	C(414)-C(474)-H(47I)	109.5
C(523)-C(503)-H(50H)	110.2	H(47G)-C(474)-H(47I)	109.5
C(513)-C(503)-H(50H)	110.2	H(47H)-C(474)-H(47I)	109.5
H(51M)-C(51Z)-H(51N)	109.5	C(414)-C(484)-H(48M)	109.5
H(51M)-C(51Z)-H(51O)	109.5	C(414)-C(484)-H(48N)	109.5
H(51N)-C(51Z)-H(51O)	109.5	H(48M)-C(484)-H(48N)	109.5
C(484)-C(414)-C(464)	105.6(5)	C(414)-C(484)-H(48O)	109.5
C(484)-C(414)-C(474)	110.1(5)	H(48M)-C(484)-H(48O)	109.5
C(464)-C(414)-C(474)	106.5(5)	H(48N)-C(484)-H(48O)	109.5
C(484)-C(414)-C(424)	107.8(5)	C(454)-C(494)-H(49P)	109.5
C(464)-C(414)-C(424)	119.1(5)	C(454)-C(494)-H(49Q)	109.5
C(474)-C(414)-C(424)	107.6(5)	H(49P)-C(494)-H(49Q)	109.5
N(424)-C(424)-C(434)	121.4(5)	C(454)-C(494)-H(49R)	109.5
N(424)-C(424)-C(414)	127.0(5)	H(49P)-C(494)-H(49R)	109.5
C(434)-C(424)-C(414)	111.7(5)	H(49Q)-C(494)-H(49R)	109.5
C(444)-C(434)-C(424)	130.3(5)	C(454)-C(504)-H(50I)	109.5
C(444)-C(434)-H(43E)	114.8	C(454)-C(504)-H(50J)	109.5
C(424)-C(434)-H(43E)	114.8	H(50I)-C(504)-H(50J)	109.5
N(414)-C(444)-C(434)	122.3(5)	C(454)-C(504)-H(50K)	109.5
N(414)-C(444)-C(454)	124.2(5)	H(50I)-C(504)-H(50K)	109.5
C(434)-C(444)-C(454)	113.2(5)	H(50J)-C(504)-H(50K)	109.5
C(494)-C(454)-C(514)	108.1(5)	C(454)-C(514)-H(51P)	109.5
C(494)-C(454)-C(504)	107.5(5)	C(454)-C(514)-H(51Q)	109.5
C(514)-C(454)-C(504)	105.3(5)	H(51P)-C(514)-H(51Q)	109.5
C(494)-C(454)-C(444)	105.1(5)	C(454)-C(514)-H(51R)	109.5
C(514)-C(454)-C(444)	118.6(5)	H(51P)-C(514)-H(51R)	109.5
C(504)-C(454)-C(444)	111.9(4)	H(51Q)-C(514)-H(51R)	109.5
C(414)-C(464)-H(46E)	109.5	C(465)-C(415)-C(425)	121.2(5)
C(414)-C(464)-H(46F)	109.5	C(465)-C(415)-N(424)	119.3(5)
H(46E)-C(464)-H(46F)	109.5	C(425)-C(415)-N(424)	119.4(5)

C(435)-C(425)-C(415)	118.2(6)	C(465)-C(505)-H(50L)	107.9
C(435)-C(425)-C(475)	121.3(6)	C(515)-C(505)-H(50L)	107.9
C(415)-C(425)-C(475)	120.5(5)	C(525)-C(505)-H(50L)	107.9
C(445)-C(435)-C(425)	121.1(7)	C(505)-C(515)-H(51S)	109.5
C(445)-C(435)-H(43F)	119.4	C(505)-C(515)-H(51T)	109.5
C(425)-C(435)-H(43F)	119.4	H(51S)-C(515)-H(51T)	109.5
C(435)-C(445)-C(455)	121.0(6)	C(505)-C(515)-H(51U)	109.5
C(435)-C(445)-H(44C)	119.5	H(51S)-C(515)-H(51U)	109.5
C(455)-C(445)-H(44C)	119.5	H(51T)-C(515)-H(51U)	109.5
C(445)-C(455)-C(465)	120.7(6)	C(505)-C(525)-H(52K)	109.5
C(445)-C(455)-H(45D)	119.7	C(505)-C(525)-H(52L)	109.5
C(465)-C(455)-H(45D)	119.7	H(52K)-C(525)-H(52L)	109.5
C(455)-C(465)-C(415)	117.7(6)	C(505)-C(525)-H(52M)	109.5
C(455)-C(465)-C(505)	118.4(6)	H(52K)-C(525)-H(52M)	109.5
C(415)-C(465)-C(505)	123.9(5)	H(52L)-C(525)-H(52M)	109.5
C(425)-C(475)-C(485)	108.9(5)	C(426)-C(416)-C(466)	119.3(5)
C(425)-C(475)-C(495)	113.8(5)	C(426)-C(416)-N(414)	122.3(5)
C(485)-C(475)-C(495)	110.5(5)	C(466)-C(416)-N(414)	118.4(5)
C(425)-C(475)-H(47J)	107.8	C(424)-N(424)-C(415)	122.3(4)
C(485)-C(475)-H(47J)	107.8	C(424)-N(424)-Co(6)	121.5(4)
C(495)-C(475)-H(47J)	107.8	C(415)-N(424)-Co(6)	116.2(3)
C(475)-C(485)-H(48P)	109.5	C(436)-C(426)-C(416)	118.9(5)
C(475)-C(485)-H(48Q)	109.5	C(436)-C(426)-C(476)	117.7(5)
H(48P)-C(485)-H(48Q)	109.5	C(416)-C(426)-C(476)	123.4(5)
C(475)-C(485)-H(48R)	109.5	C(446)-C(436)-C(426)	121.5(6)
H(48P)-C(485)-H(48R)	109.5	C(446)-C(436)-H(43G)	119.3
H(48Q)-C(485)-H(48R)	109.5	C(426)-C(436)-H(43G)	119.3
C(475)-C(495)-H(49S)	109.5	C(456)-C(446)-C(436)	119.5(6)
C(475)-C(495)-H(49T)	109.5	C(456)-C(446)-H(44D)	120.2
H(49S)-C(495)-H(49T)	109.5	C(436)-C(446)-H(44D)	120.2
C(475)-C(495)-H(49U)	109.5	C(446)-C(456)-C(466)	121.5(6)
H(49S)-C(495)-H(49U)	109.5	C(446)-C(456)-H(45E)	119.2
H(49T)-C(495)-H(49U)	109.5	C(466)-C(456)-H(45E)	119.2
C(465)-C(505)-C(515)	109.7(5)	C(456)-C(466)-C(416)	118.9(5)
C(465)-C(505)-C(525)	114.2(5)	C(456)-C(466)-C(506)	118.6(5)
C(515)-C(505)-C(525)	109.1(5)	C(416)-C(466)-C(506)	122.4(5)

C(486)-C(476)-C(426)	110.8(5)	C(27)-C(17)-H(17A)	109.5
C(486)-C(476)-C(496)	108.5(5)	C(27)-C(17)-H(17B)	109.5
C(426)-C(476)-C(496)	112.3(5)	H(17A)-C(17)-H(17B)	109.5
C(486)-C(476)-H(47K)	108.4	C(27)-C(17)-H(17C)	109.5
C(426)-C(476)-H(47K)	108.4	H(17A)-C(17)-H(17C)	109.5
C(496)-C(476)-H(47K)	108.4	H(17B)-C(17)-H(17C)	109.5
C(476)-C(486)-H(48S)	109.5	C(37)-C(27)-C(77)	120.0
C(476)-C(486)-H(48T)	109.5	C(37)-C(27)-C(17)	130.4(12)
H(48S)-C(486)-H(48T)	109.5	C(77)-C(27)-C(17)	109.5(12)
C(476)-C(486)-H(48U)	109.5	C(27)-C(37)-C(47)	120.0
H(48S)-C(486)-H(48U)	109.5	C(27)-C(37)-H(37A)	120.0
H(48T)-C(486)-H(48U)	109.5	C(47)-C(37)-H(37A)	120.0
C(476)-C(496)-H(49V)	109.5	C(57)-C(47)-C(37)	120.0
C(476)-C(496)-H(49W)	109.5	C(57)-C(47)-H(47N)	120.0
H(49V)-C(496)-H(49W)	109.5	C(37)-C(47)-H(47N)	120.0
C(476)-C(496)-H(49X)	109.5	C(47)-C(57)-C(67)	120.0
H(49V)-C(496)-H(49X)	109.5	C(47)-C(57)-H(57A)	120.0
H(49W)-C(496)-H(49X)	109.5	C(67)-C(57)-H(57A)	120.0
C(526)-C(506)-C(466)	112.6(5)	C(77)-C(67)-C(57)	120.0
C(526)-C(506)-C(516)	108.1(5)	C(77)-C(67)-H(67A)	120.0
C(466)-C(506)-C(516)	112.3(5)	C(57)-C(67)-H(67A)	120.0
C(526)-C(506)-H(50M)	107.9	C(67)-C(77)-C(27)	120.0
C(466)-C(506)-H(50M)	107.9	C(67)-C(77)-H(77A)	120.0
C(516)-C(506)-H(50M)	107.9	C(27)-C(77)-H(77A)	120.0
C(506)-C(516)-H(51V)	109.5	C(97)-C(87)-H(87A)	109.5
C(506)-C(516)-H(51W)	109.5	C(97)-C(87)-H(87B)	109.5
H(51V)-C(516)-H(51W)	109.5	H(87A)-C(87)-H(87B)	109.5
C(506)-C(516)-H(51X)	109.5	C(97)-C(87)-H(87C)	109.5
H(51V)-C(516)-H(51X)	109.5	H(87A)-C(87)-H(87C)	109.5
H(51W)-C(516)-H(51X)	109.5	H(87B)-C(87)-H(87C)	109.5
C(506)-C(526)-H(52N)	109.5	C(107)-C(97)-C(147)	120.0
C(506)-C(526)-H(52O)	109.5	C(107)-C(97)-C(87)	119.9(13)
H(52N)-C(526)-H(52O)	109.5	C(147)-C(97)-C(87)	120.1(13)
C(506)-C(526)-H(52P)	109.5	C(117)-C(107)-C(97)	120.0
H(52N)-C(526)-H(52P)	109.5	C(117)-C(107)-H(107)	120.0
H(52O)-C(526)-H(52P)	109.5	C(97)-C(107)-H(107)	120.0

C(107)-C(117)-C(127)	120.0	C(16')-C(15')-H(15D)	109.5
C(107)-C(117)-H(117)	120.0	C(16')-C(15')-H(15E)	109.5
C(127)-C(117)-H(117)	120.0	H(15D)-C(15')-H(15E)	109.5
C(137)-C(127)-C(117)	120.0	C(16')-C(15')-H(15F)	109.5
C(137)-C(127)-H(127)	120.0	H(15D)-C(15')-H(15F)	109.5
C(117)-C(127)-H(127)	120.0	H(15E)-C(15')-H(15F)	109.5
C(147)-C(137)-C(127)	120.0	C(17')-C(16')-C(21')	120.0
C(147)-C(137)-H(137)	120.0	C(17')-C(16')-C(15')	119.7(17)
C(127)-C(137)-H(137)	120.0	C(21')-C(16')-C(15')	120.1(17)
C(137)-C(147)-C(97)	120.0	C(16')-C(17')-C(18')	120.0
C(137)-C(147)-H(147)	120.0	C(16')-C(17')-H(17E)	120.0
C(97)-C(147)-H(147)	120.0	C(18')-C(17')-H(17E)	120.0
C(167)-C(157)-H(15A)	109.5	C(19')-C(18')-C(17')	120.0
C(167)-C(157)-H(15B)	109.5	C(19')-C(18')-H(18B)	120.0
H(15A)-C(157)-H(15B)	109.5	C(17')-C(18')-H(18B)	120.0
C(167)-C(157)-H(15C)	109.5	C(20')-C(19')-C(18')	120.0
H(15A)-C(157)-H(15C)	109.5	C(20')-C(19')-H(19B)	120.0
H(15B)-C(157)-H(15C)	109.5	C(18')-C(19')-H(19B)	120.0
C(177)-C(167)-C(217)	120.0	C(19')-C(20')-C(21')	120.0
C(177)-C(167)-C(157)	121.2(8)	C(19')-C(20')-H(20B)	120.0
C(217)-C(167)-C(157)	118.8(8)	C(21')-C(20')-H(20B)	120.0
C(187)-C(177)-C(167)	120.0	C(20')-C(21')-C(16')	120.0
C(187)-C(177)-H(17D)	120.0	C(20')-C(21')-H(21B)	120.0
C(167)-C(177)-H(17D)	120.0	C(16')-C(21')-H(21B)	120.0
C(177)-C(187)-C(197)	120.0	C(237)-C(227)-H(22A)	109.5
C(177)-C(187)-H(18A)	120.0	C(237)-C(227)-H(22B)	109.5
C(197)-C(187)-H(18A)	120.0	H(22A)-C(227)-H(22B)	109.5
C(207)-C(197)-C(187)	120.0	C(237)-C(227)-H(22C)	109.5
C(207)-C(197)-H(19A)	120.0	H(22A)-C(227)-H(22C)	109.5
C(187)-C(197)-H(19A)	120.0	H(22B)-C(227)-H(22C)	109.5
C(197)-C(207)-C(217)	120.0	C(247)-C(237)-C(287)	120.0
C(197)-C(207)-H(20A)	120.0	C(247)-C(237)-C(227)	119.2(7)
C(217)-C(207)-H(20A)	120.0	C(287)-C(237)-C(227)	120.8(7)
C(207)-C(217)-C(167)	120.0	C(237)-C(247)-C(257)	120.0
C(207)-C(217)-H(21A)	120.0	C(237)-C(247)-H(247)	120.0
C(167)-C(217)-H(21A)	120.0	C(257)-C(247)-H(247)	120.0

C(267)-C(257)-C(247)	120.0	C(24')-C(23')-C(28')	120.0
C(267)-C(257)-H(257)	120.0	C(24')-C(23')-C(22')	120.3(12)
C(247)-C(257)-H(257)	120.0	C(28')-C(23')-C(22')	119.6(12)
C(277)-C(267)-C(257)	120.0	C(25')-C(24')-C(23')	120.0
C(277)-C(267)-H(267)	120.0	C(25')-C(24')-H(24')	120.0
C(257)-C(267)-H(267)	120.0	C(23')-C(24')-H(24')	120.0
C(267)-C(277)-C(287)	120.0	C(24')-C(25')-C(26')	120.0
C(267)-C(277)-H(277)	120.0	C(24')-C(25')-H(25')	120.0
C(287)-C(277)-H(277)	120.0	C(26')-C(25')-H(25')	120.0
C(277)-C(287)-C(237)	120.0	C(27')-C(26')-C(25')	120.0
C(277)-C(287)-H(287)	120.0	C(27')-C(26')-H(26')	120.0
C(237)-C(287)-H(287)	120.0	C(25')-C(26')-H(26')	120.0
C(23')-C(22')-H(22D)	109.5	C(26')-C(27')-C(28')	120.0
C(23')-C(22')-H(22E)	109.5	C(26')-C(27')-H(27')	120.0
H(22D)-C(22')-H(22E)	109.5	C(28')-C(27')-H(27')	120.0
C(23')-C(22')-H(22F)	109.5	C(27')-C(28')-C(23')	120.0
H(22D)-C(22')-H(22F)	109.5	C(27')-C(28')-H(28')	120.0
H(22E)-C(22')-H(22F)	109.5	C(23')-C(28')-H(28')	120.0

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for holkd15. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	15(1)	18(1)	13(1)	-1(1)	0(1)	-2(1)
Co2	15(1)	16(1)	14(1)	-2(1)	-1(1)	-2(1)
N11	14(3)	20(3)	14(2)	-6(2)	3(2)	0(2)
N21	17(3)	18(3)	14(3)	-3(2)	0(2)	-3(2)
N14	12(2)	17(3)	19(3)	-6(2)	-2(2)	-6(2)
N24	22(3)	13(3)	15(3)	-3(2)	-2(2)	2(2)
C11	24(3)	25(3)	12(3)	-2(3)	2(3)	1(3)
C21	20(3)	16(3)	10(3)	-2(2)	3(2)	-4(2)
C31	17(3)	23(3)	16(3)	-5(3)	9(3)	-1(3)
C41	14(3)	19(3)	17(3)	-1(3)	0(3)	2(2)
C51	21(3)	31(4)	20(3)	2(3)	0(3)	-7(3)
C61	38(4)	37(4)	17(3)	10(3)	-1(3)	-6(3)
C71	32(4)	36(4)	19(3)	7(3)	-4(3)	-7(3)
C81	48(4)	42(4)	11(3)	-4(3)	-2(3)	-3(3)
C91	17(3)	53(5)	22(3)	-1(3)	-3(3)	-14(3)
C101	17(3)	62(5)	23(4)	-9(3)	5(3)	-2(3)
C111	33(4)	40(4)	40(4)	-1(3)	-6(3)	-16(3)
C12	26(3)	17(3)	4(3)	0(2)	0(2)	-4(3)
C22	24(3)	20(3)	11(3)	-3(2)	1(3)	-3(3)
C32	25(4)	20(3)	24(3)	-1(3)	-7(3)	0(3)
C42	32(4)	21(3)	23(3)	-1(3)	-6(3)	7(3)
C52	37(4)	19(3)	22(3)	-7(3)	1(3)	-7(3)
C62	24(3)	19(3)	9(3)	1(2)	-2(3)	-4(3)
C72	22(3)	15(3)	20(3)	-3(3)	-7(3)	4(3)
C82	30(4)	21(4)	32(4)	-5(3)	-7(3)	-1(3)
C92	27(4)	30(4)	31(4)	-3(3)	-12(3)	-6(3)
C102	19(3)	18(3)	26(3)	-8(3)	-1(3)	2(3)
C112	34(4)	34(4)	31(4)	-8(3)	-3(3)	-13(3)
C122	57(5)	30(4)	35(4)	-3(3)	-6(4)	-24(3)
C13	11(3)	32(4)	14(3)	9(3)	-2(2)	-10(3)
C23	19(3)	29(4)	16(3)	3(3)	0(3)	-11(3)

C33	26(4)	42(4)	20(3)	1(3)	0(3)	-14(3)
C43	21(4)	51(5)	25(4)	14(3)	-6(3)	-18(3)
C53	13(3)	37(4)	40(4)	8(3)	-4(3)	-2(3)
C63	18(3)	38(4)	22(3)	10(3)	-1(3)	-8(3)
C73	21(3)	37(4)	15(3)	0(3)	0(3)	-14(3)
C83	37(4)	54(5)	34(4)	-13(3)	6(3)	-23(4)
C93	32(4)	37(4)	23(3)	-5(3)	-4(3)	-13(3)
C103	29(4)	19(3)	36(4)	-4(3)	-6(3)	4(3)
C113	32(4)	47(5)	55(5)	-18(4)	2(4)	-5(3)
C123	30(4)	29(4)	66(5)	-2(4)	-16(4)	2(3)
C14	16(3)	27(4)	21(3)	-4(3)	1(3)	-7(3)
C24	11(3)	20(3)	21(3)	-1(3)	-4(3)	5(2)
C34	13(3)	24(3)	26(3)	-5(3)	-5(3)	-5(3)
C44	16(3)	17(3)	19(3)	0(3)	-7(3)	-4(2)
C54	27(4)	25(4)	24(3)	-4(3)	-3(3)	-8(3)
C64	14(3)	31(4)	22(3)	-2(3)	4(3)	-5(3)
C74	16(3)	48(4)	37(4)	-18(3)	3(3)	-2(3)
C84	57(5)	37(4)	31(4)	-6(3)	18(4)	-21(4)
C94	33(4)	28(4)	29(4)	-11(3)	-9(3)	-12(3)
C104	40(4)	24(4)	41(4)	-2(3)	-8(3)	-12(3)
C114	34(4)	33(4)	40(4)	-17(3)	-8(3)	-3(3)
C15	17(3)	24(3)	11(3)	1(3)	4(2)	-9(3)
C25	11(3)	36(4)	13(3)	-2(3)	2(2)	-11(3)
C35	24(4)	38(4)	14(3)	2(3)	-1(3)	-17(3)
C45	40(4)	40(4)	7(3)	-9(3)	5(3)	-23(3)
C55	38(4)	22(4)	28(4)	-12(3)	16(3)	-16(3)
C65	24(3)	24(3)	14(3)	-2(3)	7(3)	-6(3)
C75	20(3)	29(4)	17(3)	4(3)	-7(3)	-2(3)
C85	29(4)	52(5)	56(5)	-1(4)	18(4)	7(4)
C95	33(4)	50(5)	29(4)	5(3)	-5(3)	-3(3)
C105	27(4)	23(3)	23(3)	-5(3)	3(3)	0(3)
C115	31(4)	30(4)	42(4)	-5(3)	10(3)	3(3)
C125	37(4)	21(3)	25(4)	-2(3)	2(3)	-2(3)
C16	25(3)	19(3)	23(3)	-6(3)	-7(3)	-3(3)
C26	23(3)	17(3)	28(4)	-9(3)	-2(3)	2(3)
C36	44(4)	24(4)	27(4)	-7(3)	4(3)	2(3)

C46	50(5)	24(4)	47(5)	-14(3)	-1(4)	8(3)
C56	43(4)	18(4)	41(4)	0(3)	-10(4)	-1(3)
C66	26(4)	21(3)	35(4)	-6(3)	-10(3)	-5(3)
C76	31(4)	21(3)	23(3)	-9(3)	0(3)	8(3)
C86	50(5)	36(4)	23(4)	-9(3)	-6(3)	0(3)
C96	48(5)	26(4)	35(4)	-6(3)	9(3)	0(3)
C106	40(4)	25(4)	26(4)	2(3)	-5(3)	2(3)
C116	51(5)	42(5)	38(4)	3(3)	-14(4)	-6(4)
C126	51(5)	62(5)	28(4)	4(4)	-4(4)	-18(4)
Co3	16(1)	17(1)	14(1)	0(1)	1(1)	-5(1)
Co4	14(1)	14(1)	15(1)	-3(1)	1(1)	-3(1)
N211	22(3)	23(3)	12(3)	-3(2)	-2(2)	-6(2)
N221	20(3)	14(3)	21(3)	-2(2)	-4(2)	0(2)
N214	14(3)	14(3)	14(2)	-5(2)	5(2)	-3(2)
N224	19(3)	12(3)	18(3)	-3(2)	1(2)	-2(2)
C231	33(4)	34(4)	14(3)	1(3)	11(3)	-15(3)
C241	29(4)	26(4)	19(3)	-5(3)	2(3)	-8(3)
C251	39(4)	30(4)	26(4)	4(3)	-2(3)	-9(3)
C221	19(3)	37(4)	20(3)	-9(3)	2(3)	-8(3)
C211	24(4)	60(5)	20(4)	-5(3)	4(3)	-20(3)
C261	21(4)	140(16)	26(4)	-16(6)	11(3)	-16(6)
C271	55(6)	59(6)	39(11)	7(5)	-13(6)	-40(5)
C281	14(3)	58(5)	27(4)	-7(3)	3(3)	-16(3)
C21"	24(4)	60(5)	20(4)	-5(3)	4(3)	-20(3)
C26"	21(4)	140(16)	26(4)	-16(6)	11(3)	-16(6)
C27"	55(6)	59(6)	39(11)	7(5)	-13(6)	-40(5)
C28"	14(3)	58(5)	27(4)	-7(3)	3(3)	-16(3)
C291	54(5)	33(4)	26(4)	2(3)	-13(3)	-8(3)
C301	70(6)	47(5)	34(4)	11(4)	-11(4)	-31(4)
C311	55(5)	32(4)	25(4)	11(3)	-4(3)	3(3)
C212	14(3)	35(4)	22(3)	4(3)	0(3)	-9(3)
C222	17(3)	33(4)	15(3)	-3(3)	2(3)	-10(3)
C232	17(3)	43(4)	20(3)	-2(3)	1(3)	-17(3)
C242	15(3)	31(4)	39(4)	2(3)	-4(3)	-2(3)
C252	15(3)	25(4)	47(4)	-4(3)	-4(3)	2(3)
C262	10(3)	29(4)	35(4)	-6(3)	0(3)	-6(3)

C272	30(4)	34(4)	21(3)	-5(3)	-4(3)	-16(3)
C282	34(4)	28(4)	29(4)	-11(3)	0(3)	-5(3)
C292	46(5)	45(4)	37(4)	-10(3)	-2(4)	-22(4)
C302	22(4)	34(4)	39(4)	-18(3)	-6(3)	4(3)
C312	31(4)	34(4)	60(5)	-14(4)	-16(4)	-2(3)
C322	26(4)	86(6)	58(5)	-45(5)	-2(4)	6(4)
C213	25(3)	12(3)	19(3)	1(2)	-4(3)	0(3)
C223	24(3)	16(3)	20(3)	4(3)	-4(3)	2(3)
C233	36(4)	20(4)	33(4)	0(3)	-7(3)	1(3)
C243	47(5)	17(4)	35(4)	6(3)	4(3)	13(3)
C253	63(5)	13(3)	37(4)	-9(3)	0(4)	-9(3)
C263	37(4)	12(3)	25(4)	-3(3)	7(3)	-3(3)
C273	28(4)	21(3)	19(3)	-4(3)	-12(3)	2(3)
C283	43(5)	45(5)	47(5)	-10(4)	-18(4)	0(4)
C293	26(4)	29(4)	49(4)	-10(3)	7(3)	-8(3)
C303	40(4)	24(4)	58(5)	-17(3)	4(4)	-11(3)
C313	49(5)	54(5)	49(5)	2(4)	-14(4)	-11(4)
C323	102(7)	78(6)	43(5)	-14(4)	-5(5)	-60(6)
C214	20(3)	42(4)	19(3)	-9(3)	1(3)	-11(3)
C224	17(3)	22(3)	22(3)	-4(3)	2(3)	-3(3)
C234	4(3)	36(4)	29(4)	-8(3)	-1(3)	-5(3)
C244	24(3)	11(3)	18(3)	0(2)	1(3)	1(3)
C254	18(3)	26(4)	30(4)	-13(3)	4(3)	-7(3)
C264	27(4)	56(5)	15(3)	-13(3)	12(3)	-15(3)
C274	30(4)	68(5)	31(4)	-14(4)	4(3)	-18(4)
C284	43(4)	43(4)	34(4)	0(3)	16(3)	-23(4)
C294	25(4)	31(4)	46(4)	-19(3)	-4(3)	-9(3)
C304	26(4)	43(4)	27(4)	-8(3)	-13(3)	-10(3)
C314	24(4)	28(4)	34(4)	-8(3)	-6(3)	-12(3)
C215	13(3)	32(4)	14(3)	-8(3)	7(3)	-8(3)
C225	16(3)	30(4)	17(3)	-6(3)	2(3)	-8(3)
C235	16(3)	41(4)	20(3)	-3(3)	-2(3)	-6(3)
C245	23(4)	55(5)	29(4)	-24(4)	4(3)	-12(3)
C255	25(4)	31(4)	33(4)	-16(3)	10(3)	-9(3)
C265	19(3)	28(4)	17(3)	-5(3)	7(3)	-16(3)
C275	28(4)	26(4)	16(3)	3(3)	0(3)	-6(3)

C285	33(4)	32(4)	77(6)	-1(4)	20(4)	0(3)
C295	55(5)	51(5)	29(4)	14(3)	-8(4)	-6(4)
C305	28(4)	18(3)	22(3)	-5(3)	10(3)	-2(3)
C315	46(4)	28(4)	37(4)	-4(3)	10(3)	-2(3)
C325	28(4)	32(4)	33(4)	-9(3)	-2(3)	10(3)
C216	15(3)	16(3)	21(3)	-5(3)	-2(3)	-5(2)
C226	19(3)	22(3)	18(3)	-6(3)	-6(3)	-3(3)
C236	30(4)	28(4)	16(3)	-10(3)	-1(3)	-6(3)
C246	32(4)	23(4)	30(4)	-19(3)	4(3)	1(3)
C256	31(4)	17(3)	22(3)	-5(3)	1(3)	7(3)
C266	26(4)	21(3)	22(3)	5(3)	-5(3)	-8(3)
C276	24(3)	17(3)	21(3)	-2(3)	1(3)	-3(3)
C286	32(4)	40(4)	20(3)	-8(3)	1(3)	-2(3)
C296	40(4)	33(4)	24(4)	-4(3)	5(3)	-5(3)
C306	33(4)	20(3)	17(3)	1(3)	0(3)	5(3)
C316	51(5)	34(4)	41(4)	10(3)	3(4)	-14(4)
C326	49(5)	46(5)	27(4)	-8(3)	-8(3)	3(4)
Co5	15(1)	17(1)	16(1)	-2(1)	-1(1)	-2(1)
Co6	14(1)	21(1)	15(1)	-5(1)	0(1)	-5(1)
N411	19(3)	22(3)	11(2)	-2(2)	-1(2)	-2(2)
N421	21(3)	11(3)	20(3)	-7(2)	-4(2)	0(2)
N414	21(3)	17(3)	13(3)	-1(2)	-4(2)	-4(2)
C411	24(3)	26(4)	22(3)	3(3)	-1(3)	-8(3)
C421	25(3)	22(3)	11(3)	2(3)	2(3)	-7(3)
C431	30(4)	26(4)	10(3)	-2(3)	10(3)	-6(3)
C441	34(4)	13(3)	15(3)	-6(2)	1(3)	0(3)
C461	21(4)	38(4)	25(3)	0(3)	4(3)	-11(3)
C471	40(5)	37(5)	66(5)	8(4)	-16(4)	-18(4)
C481	18(4)	88(6)	25(4)	-7(4)	4(3)	-4(4)
C451	21(5)	25(4)	15(3)	3(3)	-5(3)	0(3)
C491	36(13)	41(5)	10(8)	-2(5)	4(9)	6(7)
C501	42(7)	35(7)	22(3)	7(4)	-4(4)	3(3)
C511	42(7)	35(7)	22(3)	7(4)	-4(4)	3(3)
C45"	21(5)	25(4)	15(3)	3(3)	-5(3)	0(3)
C49"	36(13)	41(5)	10(8)	-2(5)	4(9)	6(7)
C50"	42(7)	35(7)	22(3)	7(4)	-4(4)	3(3)

C51"	42(7)	35(7)	22(3)	7(4)	-4(4)	3(3)
C412	9(3)	20(3)	17(3)	-1(3)	4(2)	-5(2)
C422	12(3)	26(4)	17(3)	0(3)	4(3)	-9(3)
C432	18(3)	32(4)	20(3)	-3(3)	-3(3)	-8(3)
C442	25(4)	26(4)	30(4)	13(3)	-11(3)	-8(3)
C452	20(3)	17(3)	35(4)	8(3)	0(3)	-4(3)
C462	15(3)	19(3)	25(3)	-1(3)	-3(3)	-8(3)
C472	25(4)	28(4)	17(3)	-9(3)	7(3)	-9(3)
C482	49(5)	43(5)	57(5)	-14(4)	-7(4)	-21(4)
C492	45(5)	41(5)	63(5)	-15(4)	16(4)	-14(4)
C502	21(3)	19(3)	35(4)	-3(3)	-5(3)	3(3)
C512	36(4)	43(5)	54(5)	-27(4)	4(4)	-5(3)
C522	17(3)	23(4)	51(4)	-11(3)	-6(3)	-2(3)
C413	34(4)	17(3)	12(3)	-3(2)	-6(3)	-1(3)
C423	25(4)	27(4)	24(3)	-11(3)	-10(3)	5(3)
C433	31(4)	42(5)	45(4)	-13(4)	-18(3)	16(3)
C443	50(5)	28(4)	54(5)	-10(4)	-17(4)	18(4)
C453	55(5)	15(3)	31(4)	-6(3)	-6(4)	5(3)
C463	36(4)	19(3)	15(3)	-3(3)	2(3)	-5(3)
C473	30(4)	23(4)	11(5)	-5(4)	-9(5)	4(4)
C483	16(4)	28(5)	48(7)	-2(5)	-10(5)	-2(4)
C493	61(7)	26(6)	52(8)	-9(5)	-33(6)	-2(5)
C47'	30(4)	23(4)	11(5)	-5(4)	-9(5)	4(4)
C48'	16(4)	28(5)	48(7)	-2(5)	-10(5)	-2(4)
C49'	61(7)	26(6)	52(8)	-9(5)	-33(6)	-2(5)
C503	38(4)	25(4)	42(4)	-14(3)	6(3)	-12(3)
C513	72(10)	55(8)	54(6)	6(6)	-25(7)	-34(7)
C523	42(5)	94(7)	37(5)	0(4)	-7(4)	-28(4)
C50Z	38(4)	25(4)	42(4)	-14(3)	6(3)	-12(3)
C51Z	72(10)	55(8)	54(6)	6(6)	-25(7)	-34(7)
C52Z	42(5)	94(7)	37(5)	0(4)	-7(4)	-28(4)
C414	17(3)	38(4)	23(3)	-6(3)	5(3)	-12(3)
C424	20(3)	19(3)	18(3)	-2(3)	3(3)	-5(3)
C434	16(3)	25(4)	26(3)	-9(3)	-5(3)	-8(3)
C444	12(3)	21(3)	22(3)	1(3)	-3(3)	-6(3)
C454	15(3)	27(4)	24(3)	-8(3)	-1(3)	-3(3)

C464	30(4)	55(5)	18(3)	-9(3)	11(3)	-21(3)
C474	17(4)	69(5)	35(4)	-22(4)	13(3)	-13(3)
C484	38(4)	47(5)	27(4)	-11(3)	16(3)	-22(3)
C494	28(4)	31(4)	22(3)	-3(3)	-11(3)	-10(3)
C504	25(4)	33(4)	31(4)	-9(3)	-3(3)	-14(3)
C514	24(4)	27(4)	34(4)	-17(3)	-7(3)	-10(3)
C415	19(3)	31(4)	18(3)	-13(3)	9(3)	-13(3)
C425	13(3)	40(4)	18(3)	-4(3)	5(3)	-10(3)
C435	22(4)	70(5)	18(4)	-14(4)	5(3)	-16(4)
C445	27(4)	64(5)	28(4)	-21(4)	4(3)	-19(4)
C455	28(4)	43(4)	31(4)	-18(3)	8(3)	-14(3)
C465	14(3)	29(4)	19(3)	-10(3)	6(3)	-5(3)
C475	18(3)	45(4)	16(3)	-2(3)	-5(3)	-7(3)
C485	30(4)	37(4)	55(5)	-2(4)	1(4)	2(3)
C495	62(5)	61(5)	25(4)	11(4)	-8(4)	-26(4)
C505	25(4)	23(4)	37(4)	-14(3)	10(3)	0(3)
C515	42(4)	27(4)	40(4)	-11(3)	13(3)	-4(3)
C525	30(4)	39(4)	50(5)	-19(4)	13(3)	-2(3)
C416	10(3)	22(3)	23(3)	-7(3)	1(3)	-10(2)
N424	16(3)	22(3)	18(3)	-7(2)	-1(2)	-2(2)
C426	16(3)	23(3)	21(3)	-6(3)	2(3)	-1(3)
C436	19(3)	30(4)	23(3)	0(3)	-1(3)	-4(3)
C446	23(4)	23(4)	39(4)	-12(3)	-6(3)	2(3)
C456	33(4)	13(3)	36(4)	-2(3)	-6(3)	0(3)
C466	23(3)	18(3)	24(3)	-2(3)	-6(3)	-6(3)
C476	30(4)	23(3)	13(3)	1(3)	5(3)	-3(3)
C486	44(5)	32(4)	55(5)	3(4)	24(4)	-5(3)
C496	47(5)	48(5)	23(4)	-4(3)	-2(3)	13(4)
C506	39(4)	16(3)	25(4)	1(3)	-10(3)	-4(3)
C516	33(4)	54(5)	27(4)	10(3)	-4(3)	-13(3)
C526	41(4)	50(5)	34(4)	8(3)	-14(3)	-16(4)
C17	74(7)	35(5)	164(12)	-21(6)	-7(7)	-13(5)
C27	74(7)	35(5)	164(12)	-21(6)	-7(7)	-13(5)
C37	65(6)	27(5)	79(7)	-10(4)	-41(5)	-4(4)
C47	89(11)	38(7)	67(9)	2(6)	-9(8)	-14(7)
C57	74(7)	35(5)	164(12)	-21(6)	-7(7)	-13(5)

C67	89(11)	38(7)	67(9)	2(6)	-9(8)	-14(7)
C77	65(6)	27(5)	79(7)	-10(4)	-41(5)	-4(4)
C87	37(9)	45(9)	30(8)	-4(7)	0(7)	-14(7)
C97	17(12)	39(7)	28(6)	-10(5)	-2(11)	7(11)
C107	34(13)	30(7)	45(7)	-13(5)	-11(11)	3(10)
C117	45(12)	34(7)	38(7)	-7(5)	-9(11)	1(11)
C127	17(12)	39(7)	28(6)	-10(5)	-2(11)	7(11)
C137	34(13)	30(7)	45(7)	-13(5)	-11(11)	3(10)
C147	45(12)	34(7)	38(7)	-7(5)	-9(11)	1(11)
C157	78(8)	86(9)	107(14)	-64(10)	26(9)	-23(7)
C167	53(7)	21(5)	59(7)	-9(4)	3(6)	-14(5)
C177	70(8)	49(6)	42(6)	-13(4)	-17(6)	-10(6)
C187	70(10)	57(8)	87(10)	-29(7)	-18(8)	-8(7)
C197	91(11)	50(10)	99(13)	-31(8)	39(10)	-41(8)
C207	132(13)	56(8)	55(8)	-7(6)	-5(9)	-52(9)
C217	63(11)	32(6)	44(6)	7(4)	-22(6)	-12(6)
C15'	91(11)	50(10)	99(13)	-31(8)	39(10)	-41(8)
C16'	53(7)	21(5)	59(7)	-9(4)	3(6)	-14(5)
C17'	63(11)	32(6)	44(6)	7(4)	-22(6)	-12(6)
C18'	70(10)	57(8)	87(10)	-29(7)	-18(8)	-8(7)
C19'	78(8)	86(9)	107(14)	-64(10)	26(9)	-23(7)
C20'	132(13)	56(8)	55(8)	-7(6)	-5(9)	-52(9)
C21'	70(8)	49(6)	42(6)	-13(4)	-17(6)	-10(6)
C227	46(6)	34(6)	45(6)	2(5)	11(5)	5(5)
C237	39(9)	33(3)	45(5)	-18(3)	-21(7)	15(6)
C247	57(9)	24(3)	45(5)	-6(3)	-18(7)	9(6)
C257	58(9)	21(3)	30(4)	1(3)	-13(7)	18(5)
C267	39(9)	33(3)	45(5)	-18(3)	-21(7)	15(6)
C277	57(9)	24(3)	45(5)	-6(3)	-18(7)	9(6)
C287	58(9)	21(3)	30(4)	1(3)	-13(7)	18(5)
C22'	46(6)	34(6)	45(6)	2(5)	11(5)	5(5)
C23'	39(9)	33(3)	45(5)	-18(3)	-21(7)	15(6)
C24'	57(9)	24(3)	45(5)	-6(3)	-18(7)	9(6)
C25'	58(9)	21(3)	30(4)	1(3)	-13(7)	18(5)
C26'	39(9)	33(3)	45(5)	-18(3)	-21(7)	15(6)
C27'	57(9)	24(3)	45(5)	-6(3)	-18(7)	9(6)

C28'	58(9)	21(3)	30(4)	1(3)	-13(7)	18(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for holkd15.

	x	y	z	U(eq)
H1	3970(40)	7910(20)	1986(16)	31
H2	4550(40)	7400(20)	1605(16)	30
H31A	7100	8469	699	24
H61A	6071	9543	-49	48
H61B	6721	9350	345	48
H61C	5605	9703	395	48
H71A	4566	9082	-113	45
H71B	4090	9303	311	45
H71C	4154	8659	271	45
H81A	6133	8579	-203	51
H81B	5942	8088	170	51
H81C	6913	8405	149	51
H91A	9415	8150	1652	45
H91B	8748	7649	1732	45
H91C	8363	8196	1944	45
H10A	9506	8145	957	52
H10B	8555	8350	684	52
H10C	8712	7730	931	52
H11A	8809	9039	1254	55
H11B	7732	9082	1530	55
H11C	7764	9138	1036	55
H32A	1479	9212	856	28
H42A	1650	10129	871	31
H52A	3179	10343	1036	31
H72A	3460	8049	955	23
H82A	2486	8097	1602	42
H82B	2056	7684	1357	42
H82C	1460	8300	1373	42
H92A	2646	8380	325	43
H92B	1557	8412	592	43

H92C	2258	7824	571	43
H10D	5511	9445	1170	26
H11D	4682	9267	1842	48
H11E	4139	9899	1813	48
H11F	5353	9755	1831	48
H12A	5104	10377	779	59
H12B	5824	10343	1144	59
H12C	4630	10578	1209	59
H33A	7159	7850	2951	35
H43A	7873	6924	2964	40
H53A	7876	6487	2392	38
H73A	6218	8758	2061	29
H83A	7715	8865	2370	60
H83B	7069	8806	2814	60
H83C	6755	9323	2466	60
H93A	4810	8462	2488	44
H93B	5006	9042	2601	44
H93C	5360	8473	2895	44
H10E	6785	7104	1441	34
H11G	8621	6904	1401	66
H11H	8121	6452	1224	66
H11I	8525	6312	1676	66
H12D	5822	6507	1921	63
H12E	6848	6086	2012	63
H12F	6435	6183	1563	63
H34A	862	6900	2179	24
H64A	590	7393	3457	34
H64B	1226	7837	3172	34
H64C	1800	7240	3355	34
H74A	-566	7527	2942	50
H74B	-231	7362	2489	50
H74C	60	7921	2603	50
H84A	355	6583	3263	62
H84B	1514	6392	3093	62
H84C	611	6442	2800	62
H94A	804	6574	1109	42

H94B	1744	6911	1097	42
H94C	716	7057	1388	42
H10F	423	5856	1741	51
H10G	179	6404	1960	51
H10H	939	5878	2155	51
H11J	1809	5681	1278	51
H11K	2496	5541	1662	51
H11L	2827	5958	1259	51
H35A	4129	7701	3523	30
H45A	3454	8624	3486	32
H55A	2434	9046	2963	34
H75A	3570	6753	2900	27
H85A	5091	7040	2578	74
H85B	5386	6498	2908	74
H85C	5463	7101	3013	74
H95A	3201	6659	3633	58
H95B	4332	6775	3677	58
H95C	4174	6227	3505	58
H10I	1604	8373	2201	30
H11M	425	8744	2730	54
H11N	371	9142	2293	54
H11O	960	9294	2648	54
H12G	3007	8823	1918	42
H12H	2614	9319	2184	42
H12I	1969	9232	1823	42
H36A	5377	5957	818	39
H46A	5770	5138	1273	49
H56A	5134	5075	1962	41
H76A	3554	7126	1025	31
H86A	3041	6471	647	55
H86B	4121	6457	374	55
H86C	3324	7020	351	55
H96A	5293	7270	935	56
H96B	4767	7479	511	56
H96C	5510	6897	570	56
H10J	3577	6149	2446	38

H11P	5306	5775	2578	66
H11Q	5022	5161	2614	66
H11R	4505	5554	2946	66
H12J	2434	5566	2362	71
H12K	2889	5346	2800	71
H12L	3300	5033	2410	71
H3	9100(40)	2540(20)	1314(16)	31
H4	8500(40)	2970(20)	1711(16)	28
H23A	6331	1622	2553	33
H26A	3856	2011	2421	94
H26B	4632	2423	2477	94
H26C	4894	1770	2634	94
H27A	4445	1279	1937	72
H27B	5487	1105	2158	72
H27C	5526	1290	1665	72
H28A	3775	2215	1712	49
H28B	4767	2259	1388	49
H28C	4421	2717	1690	49
H26D	3851	2270	2434	94
H26E	4734	2651	2405	94
H26F	4867	2037	2663	94
H27D	4297	1354	2196	72
H27E	5482	1197	2275	72
H27F	5145	1273	1814	72
H28D	3745	2272	1740	49
H28E	4722	2156	1416	49
H28F	4518	2720	1613	49
H29A	8049	1310	3374	56
H29B	7311	1766	3098	56
H29C	8526	1745	3016	56
H30A	7274	521	3192	74
H30B	7053	540	2720	74
H30C	6478	1014	2980	74
H31B	9035	532	3099	60
H31C	9569	918	2722	60
H31D	8990	436	2630	60

H23B	5768	2878	406	31
H24A	5132	3779	532	35
H25A	5191	4024	1183	36
H27G	6938	1778	1143	32
H28G	8244	2165	720	44
H28H	7565	2321	334	44
H28I	7970	1683	497	44
H29D	5369	1719	875	60
H29E	6313	1355	651	60
H29F	5835	1948	419	60
H30D	6293	3147	2051	37
H31E	7320	3798	1691	60
H31F	6674	4039	2081	60
H31G	6327	4254	1624	60
H32B	4967	3744	2346	82
H32C	4455	3394	2076	82
H32D	4612	4023	1899	82
H23C	11932	1093	2069	37
H24B	11830	260	1848	44
H25B	10270	99	1660	44
H27H	9845	2154	2276	27
H28J	10479	1564	2870	67
H28K	10934	2140	2790	67
H28L	11626	1589	2663	67
H29G	10970	2362	1682	52
H29H	11925	2054	1928	52
H29I	11276	2611	2064	52
H30E	7881	1009	1741	47
H31H	8767	1045	1070	76
H31I	7853	680	1124	76
H31J	9013	380	1142	76
H32E	7426	120	1812	103
H32F	8041	150	2197	103
H32G	8599	-159	1822	103
H23D	12219	3616	1135	27
H26H	12424	3236	-173	48

H26I	11241	3190	-36	48
H26J	12108	2720	155	48
H27I	13520	3401	237	62
H27J	13272	2993	657	62
H27L	13206	3646	664	62
H28M	12125	4188	15	61
H28N	11664	4295	472	61
H28O	10951	4131	163	61
H29J	11450	4621	2174	48
H29K	10451	4321	2222	48
H29L	10646	4786	1831	48
H30F	12496	3698	2256	45
H30G	12494	3271	1937	45
H30H	11532	3377	2270	45
H31K	12768	4504	1690	41
H31L	12195	4553	1280	41
H31M	12980	4008	1418	41
H23E	8881	3098	-258	31
H24C	9609	2204	-334	40
H25C	10612	1668	154	35
H27M	9383	3864	509	29
H28P	7944	3473	811	75
H28Q	7523	3515	367	75
H28R	7570	4069	555	75
H29M	9640	4082	-239	71
H29N	8714	4487	-41	71
H29O	8482	3993	-262	71
H30I	10720	1935	1143	29
H31N	11517	1044	1085	58
H31O	11621	1185	589	58
H31P	10514	1171	838	58
H32H	12522	1737	1125	49
H32I	12150	2383	974	49
H32J	12612	1980	640	49
H23F	8101	4205	2744	29
H24D	7557	5079	2380	33

H25D	8005	5260	1670	30
H27N	9737	3086	2343	25
H28T	10373	3628	2785	46
H28U	10154	3029	3016	46
H28V	9358	3571	3093	46
H29P	7999	2968	2455	49
H29Q	7877	3249	2868	49
H29R	8590	2663	2847	49
H30J	9401	4302	1037	30
H31Q	10575	4873	1140	65
H31R	9690	5397	1139	65
H31S	10044	5129	723	65
H32K	7628	4678	1012	62
H32L	8319	4962	630	62
H32M	7909	5285	1015	62
H5	2630(40)	2290(20)	4682(16)	32
H6	2010(40)	2750(20)	4961(16)	32
H43B	-244	1603	5962	27
H46B	-2071	2558	4998	42
H46C	-2752	2063	5093	42
H46D	-1740	2015	4777	42
H47A	-2190	1187	5448	71
H47B	-1166	1047	5682	71
H47C	-1097	1103	5187	71
H48A	-1864	2482	5781	67
H48B	-1681	1867	6035	67
H48C	-2699	2074	5802	67
H49A	1177	1314	6816	47
H49B	423	1691	6500	47
H49C	1589	1794	6479	47
H50A	791	448	6608	52
H50B	924	375	6128	52
H50C	11	812	6297	52
H51A	2527	637	6597	52
H51B	2986	1101	6259	52
H51C	2746	545	6121	52

H49D	1422	1382	6786	47
H49E	743	1826	6477	47
H49F	1964	1732	6390	47
H50D	463	618	6706	52
H50E	218	557	6251	52
H50F	-263	1104	6449	52
H51D	2208	504	6612	52
H51E	2856	813	6226	52
H51F	2199	350	6156	52
H43C	-713	2503	3761	27
H44A	-1420	3406	3809	34
H45B	-1304	3782	4404	31
H47D	384	1510	4577	27
H48D	-1152	1427	4289	70
H48E	-195	1008	4130	70
H48F	-592	1567	3834	70
H49G	1723	1862	4136	74
H49H	1098	1908	3740	74
H49I	1509	1310	3984	74
H50G	-175	3065	5320	31
H51G	-2009	3296	5348	64
H51H	-1871	3902	5105	64
H51I	-1497	3712	5560	64
H52B	842	3669	4888	44
H52C	200	3985	5245	44
H52D	-155	4108	4785	44
H43D	5349	883	5580	48
H44B	5178	3	5473	54
H45C	3619	-170	5302	41
H47E	3345	2037	5612	26
H48G	4291	2101	4960	46
H48H	5329	1884	5177	46
H48I	4684	2472	5250	46
H49J	4141	1612	6222	67
H49K	4537	2189	6030	67
H49L	5238	1613	5963	67

H47F	3316	1986	5737	26
H48J	4536	2077	5169	46
H48K	5399	1680	5424	46
H48L	4969	2284	5544	46
H49M	3686	1494	6380	67
H49N	4523	1908	6260	67
H49O	4825	1265	6208	67
H50H	1236	740	5312	40
H51J	1712	-173	5744	86
H51K	2132	-414	5322	86
H51L	939	-191	5408	86
H52E	2064	791	4616	85
H52F	1231	373	4696	85
H52G	2424	134	4701	85
H50N	1423	838	5229	40
H51M	676	310	5712	86
H51N	1301	-252	5576	86
H51O	463	115	5292	86
H52H	1562	791	4628	85
H52I	1545	134	4722	85
H52J	2613	372	4662	85
H43E	5786	3302	4442	25
H46E	5939	2884	3139	50
H46F	4741	3063	3254	50
H46G	5275	2449	3419	50
H47G	7134	2685	3644	59
H47H	6486	2298	3980	59
H47I	6855	2831	4105	59
H48M	6263	3674	3362	55
H48N	6062	3779	3835	55
H48O	5127	3879	3552	55
H49P	6003	3542	5506	39
H49Q	6014	3093	5203	39
H49R	5042	3218	5528	39
H50I	6296	4316	4898	42
H50J	5708	4333	4495	42

H50K	6494	3795	4650	42
H51P	4986	4445	5401	39
H51Q	3956	4175	5432	39
H51R	4234	4620	5038	39
H43F	2221	2774	3094	42
H44C	2808	1851	3063	44
H45D	3904	1340	3528	39
H47J	2989	3574	3793	32
H48P	1491	3286	4121	64
H48Q	1037	3299	3688	64
H48R	1178	3868	3836	64
H49S	3232	3749	3042	74
H49T	2410	4207	3239	74
H49U	2033	3736	3035	74
H50L	4940	1861	4319	35
H51S	3518	1403	4591	55
H51T	4568	993	4657	55
H51U	3894	940	4295	55
H52K	5984	1546	3729	60
H52L	5427	1003	3804	60
H52M	6113	1111	4145	60
H43G	1589	4134	5956	29
H44D	1126	4996	5569	33
H45E	1571	5133	4860	33
H47K	3197	2965	5602	27
H48S	1441	2879	5704	70
H48T	1314	3190	6103	70
H48U	1994	2591	6110	70
H49V	3495	2937	6301	62
H49W	2805	3530	6318	62
H49X	3875	3486	6037	62
H50M	2851	4116	4253	32
H51V	4151	4619	4345	59
H51W	3357	5183	4317	59
H51X	3663	4874	3919	59
H52N	1124	4606	4238	61

H52O	1864	4780	3833	61
H52P	1593	5176	4184	61
H17A	6986	4962	-295	135
H17B	6258	5315	-630	135
H17C	6421	4650	-573	135
H37A	6011	4961	450	65
H47N	4426	4995	846	78
H57A	2930	5020	526	108
H67A	3018	5012	-190	78
H77A	4603	4978	-586	65
H87A	7643	23	229	56
H87B	7764	639	3	56
H87C	7948	464	484	56
H107	9635	888	109	43
H117	11370	600	-75	47
H127	11924	-313	-199	34
H137	10744	-939	-140	43
H147	9009	-651	45	47
H15A	1612	23	3886	129
H15B	1271	-144	3476	129
H15C	1182	497	3527	129
H17D	3380	-90	3909	62
H18A	5032	-70	3576	82
H19A	5263	175	2855	94
H20A	3842	400	2466	92
H21A	2190	380	2800	55
H15D	5117	-182	3537	117
H15E	5171	252	3117	117
H15F	5111	-388	3099	117
H17E	3629	230	2668	55
H18B	1839	344	2713	82
H19B	902	221	3363	103
H20B	1755	-15	3967	92
H21B	3545	-128	3922	62
H22A	5932	5556	3455	67
H22B	6208	5258	3908	67

H22C	6004	4895	3572	67
H247	7809	4433	3845	51
H257	9565	4341	3636	47
H267	10220	5011	3129	46
H277	9119	5774	2830	51
H287	7362	5867	3039	47
H22D	10595	4717	3251	67
H22E	10515	5379	3135	67
H22F	10303	5017	2800	67
H24'	8657	5820	2862	51
H25'	6905	5874	3074	47
H26'	6308	5196	3591	46
H27'	7464	4465	3896	51
H28'	9215	4412	3684	47

Table 6. Torsion angles [°] for holkd15.

N11-Co1-Co2-N24	78.2(2)	C13-N21-C41-C51	-13.9(8)
N21-Co1-Co2-N24	-99.4(2)	Co1-N21-C41-C51	175.7(4)
N11-Co1-Co2-N14	-89.9(2)	C21-C31-C41-N21	20.9(9)
N21-Co1-Co2-N14	92.4(3)	C21-C31-C41-C51	-155.2(6)
N21-Co1-N11-C21	34.8(4)	N21-C41-C51-C101	134.0(6)
Co2-Co1-N11-C21	-143.4(3)	C31-C41-C51-C101	-50.2(7)
N21-Co1-N11-C12	-139.8(4)	N21-C41-C51-C91	10.7(9)
Co2-Co1-N11-C12	41.9(5)	C31-C41-C51-C91	-173.5(5)
N11-Co1-N21-C41	-22.6(4)	N21-C41-C51-C111	-108.9(6)
Co2-Co1-N21-C41	155.5(3)	C31-C41-C51-C111	66.9(6)
N11-Co1-N21-C13	166.5(4)	C21-N11-C12-C22	116.4(6)
Co2-Co1-N21-C13	-15.4(5)	Co1-N11-C12-C22	-69.2(6)
N24-Co2-N14-C24	-16.4(4)	C21-N11-C12-C62	-65.3(6)
Co1-Co2-N14-C24	154.6(3)	Co1-N11-C12-C62	109.2(5)
N24-Co2-N14-C15	162.3(4)	C62-C12-C22-C32	4.4(8)
Co1-Co2-N14-C15	-26.7(5)	N11-C12-C22-C32	-177.3(5)
N14-Co2-N24-C44	28.2(4)	C62-C12-C22-C72	-174.7(5)
Co1-Co2-N24-C44	-143.1(3)	N11-C12-C22-C72	3.6(8)
N14-Co2-N24-C16	-142.3(4)	C12-C22-C32-C42	-0.3(8)
Co1-Co2-N24-C16	46.4(4)	C72-C22-C32-C42	178.9(5)
C12-N11-C21-C31	148.0(5)	C22-C32-C42-C52	-2.5(9)
Co1-N11-C21-C31	-27.0(7)	C32-C42-C52-C62	1.1(9)
C12-N11-C21-C11	-33.1(7)	C42-C52-C62-C12	3.0(8)
Co1-N11-C21-C11	151.9(4)	C42-C52-C62-C102	-172.7(5)
C71-C11-C21-N11	-9.4(8)	C22-C12-C62-C52	-5.6(7)
C81-C11-C21-N11	-128.4(6)	N11-C12-C62-C52	176.0(5)
C61-C11-C21-N11	113.7(6)	C22-C12-C62-C102	169.9(5)
C71-C11-C21-C31	169.6(5)	N11-C12-C62-C102	-8.5(7)
C81-C11-C21-C31	50.6(6)	C32-C22-C72-C82	-74.0(6)
C61-C11-C21-C31	-67.2(6)	C12-C22-C72-C82	105.1(6)
N11-C21-C31-C41	-5.0(10)	C32-C22-C72-C92	49.4(7)
C11-C21-C31-C41	176.0(6)	C12-C22-C72-C92	-131.5(5)
C13-N21-C41-C31	170.6(5)	C52-C62-C102-C112	87.4(6)
Co1-N21-C41-C31	0.2(7)	C12-C62-C102-C112	-88.1(6)

C52-C62-C102-C122	-34.3(7)	C84-C14-C24-C34	53.0(6)
C12-C62-C102-C122	150.2(5)	C74-C14-C24-C34	-65.4(6)
C41-N21-C13-C63	-85.1(6)	N14-C24-C34-C44	25.0(9)
Co1-N21-C13-C63	85.7(5)	C14-C24-C34-C44	-155.0(6)
C41-N21-C13-C23	98.4(6)	C16-N24-C44-C34	150.9(5)
Co1-N21-C13-C23	-90.8(5)	Co2-N24-C44-C34	-19.5(7)
C63-C13-C23-C33	4.0(8)	C16-N24-C44-C54	-34.6(8)
N21-C13-C23-C33	-179.7(5)	Co2-N24-C44-C54	155.0(4)
C63-C13-C23-C73	-177.5(5)	C24-C34-C44-N24	-11.2(10)
N21-C13-C23-C73	-1.2(8)	C24-C34-C44-C54	173.7(6)
C13-C23-C33-C43	-0.5(8)	N24-C44-C54-C104	155.1(5)
C73-C23-C33-C43	-179.1(5)	C34-C44-C54-C104	-30.0(7)
C23-C33-C43-C53	-1.4(9)	N24-C44-C54-C94	-88.1(6)
C33-C43-C53-C63	-0.1(9)	C34-C44-C54-C94	86.8(6)
C43-C53-C63-C13	3.5(9)	N24-C44-C54-C114	31.4(8)
C43-C53-C63-C103	-176.9(5)	C34-C44-C54-C114	-153.7(5)
C23-C13-C63-C53	-5.4(8)	C24-N14-C15-C65	-86.8(6)
N21-C13-C63-C53	178.1(5)	Co2-N14-C15-C65	94.5(5)
C23-C13-C63-C103	174.9(5)	C24-N14-C15-C25	94.9(6)
N21-C13-C63-C103	-1.5(8)	Co2-N14-C15-C25	-83.9(5)
C33-C23-C73-C93	-74.9(7)	C65-C15-C25-C35	1.0(8)
C13-C23-C73-C93	106.6(6)	N14-C15-C25-C35	179.3(5)
C33-C23-C73-C83	48.4(7)	C65-C15-C25-C75	-178.7(5)
C13-C23-C73-C83	-130.1(6)	N14-C15-C25-C75	-0.3(7)
C53-C63-C103-C123	60.0(7)	C15-C25-C35-C45	-0.3(8)
C13-C63-C103-C123	-120.3(6)	C75-C25-C35-C45	179.4(5)
C53-C63-C103-C113	-62.8(7)	C25-C35-C45-C55	-0.8(8)
C13-C63-C103-C113	116.9(6)	C35-C45-C55-C65	1.2(8)
C15-N14-C24-C34	176.7(5)	C25-C15-C65-C55	-0.6(8)
Co2-N14-C24-C34	-4.6(7)	N14-C15-C65-C55	-178.9(5)
C15-N14-C24-C14	-3.3(8)	C25-C15-C65-C105	177.6(5)
Co2-N14-C24-C14	175.4(4)	N14-C15-C65-C105	-0.7(8)
C64-C14-C24-N14	-8.0(9)	C45-C55-C65-C15	-0.5(8)
C84-C14-C24-N14	-127.0(6)	C45-C55-C65-C105	-178.8(5)
C74-C14-C24-N14	114.7(6)	C35-C25-C75-C95	44.2(7)
C64-C14-C24-C34	172.0(5)	C15-C25-C75-C95	-136.2(5)

C35-C25-C75-C85	-79.7(6)	N221-Co3-N211-C221	22.3(5)
C15-C25-C75-C85	99.9(6)	Co4-Co3-N211-C221	-159.0(4)
C15-C65-C105-C125	-106.8(6)	N221-Co3-N211-C212	-163.2(4)
C55-C65-C105-C125	71.4(6)	Co4-Co3-N211-C212	15.6(5)
C15-C65-C105-C115	129.6(6)	N211-Co3-N221-C241	-33.0(4)
C55-C65-C105-C115	-52.2(7)	Co4-Co3-N221-C241	148.1(3)
C44-N24-C16-C66	-72.3(7)	N211-Co3-N221-C213	140.5(4)
Co2-N24-C16-C66	98.2(5)	Co4-Co3-N221-C213	-38.3(5)
C44-N24-C16-C26	108.4(6)	N224-Co4-N214-C224	14.8(5)
Co2-N24-C16-C26	-81.1(6)	Co3-Co4-N214-C224	-157.0(4)
C66-C16-C26-C36	2.0(9)	N224-Co4-N214-C215	-162.1(4)
N24-C16-C26-C36	-178.6(5)	Co3-Co4-N214-C215	26.0(5)
C66-C16-C26-C76	178.9(5)	N214-Co4-N224-C244	-25.2(4)
N24-C16-C26-C76	-1.7(9)	Co3-Co4-N224-C244	146.8(3)
C16-C26-C36-C46	1.5(10)	N214-Co4-N224-C216	143.1(4)
C76-C26-C36-C46	-175.6(6)	Co3-Co4-N224-C216	-44.9(4)
C26-C36-C46-C56	-3.9(11)	C213-N221-C241-C231	-150.3(5)
C36-C46-C56-C66	2.7(10)	Co3-N221-C241-C231	23.2(7)
C46-C56-C66-C16	0.9(9)	C213-N221-C241-C251	36.1(8)
C46-C56-C66-C106	-177.0(6)	Co3-N221-C241-C251	-150.3(4)
C26-C16-C66-C56	-3.2(9)	C221-C231-C241-N221	8.9(10)
N24-C16-C66-C56	177.4(5)	C221-C231-C241-C251	-177.0(6)
C26-C16-C66-C106	174.5(5)	N221-C241-C251-C311	-26.6(9)
N24-C16-C66-C106	-4.8(8)	C231-C241-C251-C311	159.5(6)
C36-C26-C76-C96	-63.1(7)	N221-C241-C251-C291	95.0(6)
C16-C26-C76-C96	119.9(6)	C231-C241-C251-C291	-78.9(6)
C36-C26-C76-C86	59.6(7)	N221-C241-C251-C301	-149.8(6)
C16-C26-C76-C86	-117.4(6)	C231-C241-C251-C301	36.2(7)
C56-C66-C106-C126	-78.8(7)	C212-N211-C221-C231	-174.9(5)
C16-C66-C106-C126	103.4(7)	Co3-N211-C221-C231	-0.7(7)
C56-C66-C106-C116	43.7(8)	C212-N211-C221-C211	9.7(11)
C16-C66-C106-C116	-134.0(6)	Co3-N211-C221-C211	-176.1(8)
N221-Co3-Co4-N224	-85.1(2)	C212-N211-C221-C21"	0(2)
N211-Co3-Co4-N224	96.5(3)	Co3-N211-C221-C21"	174(2)
N221-Co3-Co4-N214	84.0(2)	C241-C231-C221-N211	-22.1(10)
N211-Co3-Co4-N214	-94.4(3)	C241-C231-C221-C211	153.9(8)

C241-C231-C221-C21"	162.3(18)	C212-C262-C302-C322	-121.6(6)
N211-C221-C211-C261	-131.4(13)	C241-N221-C213-C223	-115.1(6)
C231-C221-C211-C261	52.9(11)	Co3-N221-C213-C223	71.6(6)
N211-C221-C211-C281	-7.3(16)	C241-N221-C213-C263	67.4(7)
C231-C221-C211-C281	177.1(9)	Co3-N221-C213-C263	-105.9(5)
N211-C221-C211-C271	111.5(13)	C263-C213-C223-C233	-4.1(8)
C231-C221-C211-C271	-64.1(9)	N221-C213-C223-C233	178.5(5)
N211-C221-C21"-C26"	-113(4)	C263-C213-C223-C273	176.8(5)
C231-C221-C21"-C26"	62(3)	N221-C213-C223-C273	-0.6(8)
N211-C221-C21"-C27"	131(3)	C213-C223-C233-C243	-0.8(9)
C231-C221-C21"-C27"	-54(3)	C273-C223-C233-C243	178.3(5)
C221-N211-C212-C262	86.6(7)	C223-C233-C243-C253	4.1(9)
Co3-N211-C212-C262	-87.9(5)	C233-C243-C253-C263	-2.6(10)
C221-N211-C212-C222	-95.7(7)	C243-C253-C263-C213	-2.2(9)
Co3-N211-C212-C222	89.8(6)	C243-C253-C263-C303	176.0(6)
C262-C212-C222-C232	-2.2(8)	C223-C213-C263-C253	5.5(8)
N211-C212-C222-C232	-179.8(5)	N221-C213-C263-C253	-177.0(5)
C262-C212-C222-C272	178.2(5)	C223-C213-C263-C303	-172.6(6)
N211-C212-C222-C272	0.6(8)	N221-C213-C263-C303	4.9(8)
C212-C222-C232-C242	2.4(8)	C213-C223-C273-C293	-119.6(6)
C272-C222-C232-C242	-178.0(5)	C233-C223-C273-C293	61.4(7)
C222-C232-C242-C252	-2.1(8)	C213-C223-C273-C283	116.9(6)
C232-C242-C252-C262	1.6(9)	C233-C223-C273-C283	-62.2(7)
C242-C252-C262-C212	-1.4(9)	C253-C263-C303-C313	-62.6(8)
C242-C252-C262-C302	179.3(5)	C213-C263-C303-C313	115.4(6)
C222-C212-C262-C252	1.8(8)	C253-C263-C303-C323	60.6(8)
N211-C212-C262-C252	179.4(5)	C213-C263-C303-C323	-121.3(6)
C222-C212-C262-C302	-179.0(5)	C215-N214-C224-C234	-179.2(5)
N211-C212-C262-C302	-1.3(8)	Co4-N214-C224-C234	3.9(8)
C232-C222-C272-C282	71.6(7)	C215-N214-C224-C214	6.3(9)
C212-C222-C272-C282	-108.8(6)	Co4-N214-C224-C214	-170.5(4)
C232-C222-C272-C292	-50.5(7)	C274-C214-C224-N214	-140.3(6)
C212-C222-C272-C292	129.1(6)	C264-C214-C224-N214	-18.3(9)
C252-C262-C302-C312	-64.4(7)	C284-C214-C224-N214	102.9(7)
C212-C262-C302-C312	116.3(6)	C274-C214-C224-C234	44.8(7)
C252-C262-C302-C322	57.6(8)	C264-C214-C224-C234	166.8(5)

C284-C214-C224-C234	-71.9(6)	C215-C225-C275-C295	140.3(6)
N214-C224-C234-C244	-22.5(10)	C255-C265-C305-C315	-13.9(7)
C214-C224-C234-C244	152.8(6)	C215-C265-C305-C315	163.3(5)
C216-N224-C244-C234	-151.0(5)	C255-C265-C305-C325	111.6(6)
Co4-N224-C244-C234	17.4(7)	C215-C265-C305-C325	-71.1(7)
C216-N224-C244-C254	36.4(7)	C244-N224-C216-C226	-109.2(6)
Co4-N224-C244-C254	-155.2(4)	Co4-N224-C216-C226	82.3(6)
C224-C234-C244-N224	10.3(10)	C244-N224-C216-C266	72.5(7)
C224-C234-C244-C254	-176.5(6)	Co4-N224-C216-C266	-96.0(5)
N224-C244-C254-C304	84.5(6)	C266-C216-C226-C236	-6.5(8)
C234-C244-C254-C304	-88.5(6)	N224-C216-C226-C236	175.2(5)
N224-C244-C254-C314	-159.6(5)	C266-C216-C226-C276	176.5(5)
C234-C244-C254-C314	27.3(7)	N224-C216-C226-C276	-1.8(8)
N224-C244-C254-C294	-36.8(8)	C216-C226-C236-C246	2.7(9)
C234-C244-C254-C294	150.1(5)	C276-C226-C236-C246	179.9(5)
C224-N214-C215-C225	-89.7(6)	C226-C236-C246-C256	1.6(9)
Co4-N214-C215-C225	87.4(5)	C236-C246-C256-C266	-2.1(9)
C224-N214-C215-C265	90.6(6)	C246-C256-C266-C216	-1.6(9)
Co4-N214-C215-C265	-92.3(5)	C246-C256-C266-C306	177.6(6)
C265-C215-C225-C235	-6.0(8)	C226-C216-C266-C256	6.0(8)
N214-C215-C225-C235	174.3(5)	N224-C216-C266-C256	-175.6(5)
C265-C215-C225-C275	173.7(5)	C226-C216-C266-C306	-173.2(5)
N214-C215-C225-C275	-6.1(8)	N224-C216-C266-C306	5.2(8)
C215-C225-C235-C245	1.8(8)	C236-C226-C276-C296	64.5(7)
C275-C225-C235-C245	-177.9(5)	C216-C226-C276-C296	-118.4(6)
C225-C235-C245-C255	1.5(9)	C236-C226-C276-C286	-58.5(7)
C235-C245-C255-C265	-0.8(9)	C216-C226-C276-C286	118.5(6)
C245-C255-C265-C215	-3.2(8)	C256-C266-C306-C316	77.6(7)
C245-C255-C265-C305	174.2(5)	C216-C266-C306-C316	-103.2(7)
C225-C215-C265-C255	6.7(8)	C256-C266-C306-C326	-44.8(8)
N214-C215-C265-C255	-173.6(5)	C216-C266-C306-C326	134.3(6)
C225-C215-C265-C305	-170.7(5)	N421-Co5-Co6-N414	-82.6(2)
N214-C215-C265-C305	9.0(7)	N411-Co5-Co6-N414	94.9(3)
C235-C225-C275-C285	82.7(7)	N421-Co5-Co6-N424	86.2(3)
C215-C225-C275-C285	-97.0(7)	N411-Co5-Co6-N424	-96.3(2)
C235-C225-C275-C295	-40.0(7)	N421-Co5-N411-C421	21.8(4)

Co6-Co5-N411-C421	-156.2(3)	N421-C441-C451-C501	-130.3(11)
N421-Co5-N411-C412	-163.9(4)	C431-C441-C451-C501	55.6(15)
Co6-Co5-N411-C412	18.1(4)	N421-C441-C45"-C49"	90.9(17)
N411-Co5-N421-C441	-32.7(4)	C431-C441-C45"-C49"	-84.6(14)
Co6-Co5-N421-C441	145.5(3)	N421-C441-C45"-C51"	-27(2)
N411-Co5-N421-C413	141.0(4)	C431-C441-C45"-C51"	157.2(14)
Co6-Co5-N421-C413	-40.8(5)	N421-C441-C45"-C50"	-152.2(13)
N424-Co6-N414-C444	-30.4(4)	C431-C441-C45"-C50"	32.3(19)
Co5-Co6-N414-C444	141.3(3)	C421-N411-C412-C462	84.9(7)
N424-Co6-N414-C416	144.8(4)	Co5-N411-C412-C462	-89.3(5)
Co5-Co6-N414-C416	-43.5(5)	C421-N411-C412-C422	-96.8(6)
C412-N411-C421-C431	-174.0(5)	Co5-N411-C412-C422	89.0(5)
Co5-N411-C421-C431	-0.1(7)	C462-C412-C422-C432	-3.1(8)
C412-N411-C421-C411	8.9(9)	N411-C412-C422-C432	178.6(5)
Co5-N411-C421-C411	-177.2(4)	C462-C412-C422-C472	178.7(5)
C481-C411-C421-N411	-125.3(6)	N411-C412-C422-C472	0.4(8)
C461-C411-C421-N411	-1.6(9)	C412-C422-C432-C442	0.8(8)
C471-C411-C421-N411	116.6(6)	C472-C422-C432-C442	179.0(5)
C481-C411-C421-C431	57.4(7)	C422-C432-C442-C452	1.2(9)
C461-C411-C421-C431	-178.9(5)	C432-C442-C452-C462	-1.0(9)
C471-C411-C421-C431	-60.6(6)	C442-C452-C462-C412	-1.3(8)
N411-C421-C431-C441	-22.5(10)	C442-C452-C462-C502	179.7(5)
C411-C421-C431-C441	154.9(6)	C422-C412-C462-C452	3.4(8)
C413-N421-C441-C431	-151.0(5)	N411-C412-C462-C452	-178.3(5)
Co5-N421-C441-C431	22.9(7)	C422-C412-C462-C502	-177.7(5)
C413-N421-C441-C451	35.2(12)	N411-C412-C462-C502	0.6(8)
Co5-N421-C441-C451	-150.8(10)	C432-C422-C472-C482	-46.1(7)
C413-N421-C441-C45"	33.9(13)	C412-C422-C472-C482	132.0(6)
Co5-N421-C441-C45"	-152.1(12)	C432-C422-C472-C492	75.2(7)
C421-C431-C441-N421	9.2(10)	C412-C422-C472-C492	-106.6(6)
C421-C431-C441-C451	-176.7(10)	C452-C462-C502-C522	-64.2(7)
C421-C431-C441-C45"	-174.9(11)	C412-C462-C502-C522	116.9(6)
N421-C441-C451-C491	112.3(14)	C452-C462-C502-C512	58.0(7)
C431-C441-C451-C491	-61.7(15)	C412-C462-C502-C512	-120.9(6)
N421-C441-C451-C511	-9(2)	C441-N421-C413-C423	-115.5(6)
C431-C441-C451-C511	176.9(14)	Co5-N421-C413-C423	70.9(6)

C441-N421-C413-C463	64.8(7)	C474-C414-C424-C434	66.7(6)
Co5-N421-C413-C463	-108.8(5)	N424-C424-C434-C444	-24.3(10)
C463-C413-C423-C433	-3.8(9)	C414-C424-C434-C444	155.2(6)
N421-C413-C423-C433	176.5(5)	C416-N414-C444-C434	-155.7(5)
C463-C413-C423-C47'	-163.4(14)	Co6-N414-C444-C434	19.4(7)
N421-C413-C423-C47'	16.9(16)	C416-N414-C444-C454	31.4(8)
C463-C413-C423-C473	172.6(6)	Co6-N414-C444-C454	-153.5(4)
N421-C413-C423-C473	-7.1(9)	C424-C434-C444-N414	12.5(10)
C413-C423-C433-C443	0.3(10)	C424-C434-C444-C454	-173.9(6)
C47'-C423-C433-C443	161.2(14)	N414-C444-C454-C494	89.8(6)
C473-C423-C433-C443	-176.2(7)	C434-C444-C454-C494	-83.6(6)
C423-C433-C443-C453	3.1(11)	N414-C444-C454-C514	-31.0(8)
C433-C443-C453-C463	-3.1(10)	C434-C444-C454-C514	155.5(5)
C443-C453-C463-C413	-0.4(9)	N414-C444-C454-C504	-153.8(5)
C443-C453-C463-C503	176.6(6)	C434-C444-C454-C504	32.7(7)
C423-C413-C463-C453	3.8(8)	C465-C415-C425-C435	-2.3(8)
N421-C413-C463-C453	-176.5(5)	N424-C415-C425-C435	-179.8(5)
C423-C413-C463-C503	-173.1(5)	C465-C415-C425-C475	177.6(5)
N421-C413-C463-C503	6.6(8)	N424-C415-C425-C475	0.0(8)
C433-C423-C473-C483	69.8(8)	C415-C425-C435-C445	1.3(8)
C413-C423-C473-C483	-106.6(8)	C475-C425-C435-C445	-178.6(5)
C433-C423-C473-C493	-56.6(9)	C425-C435-C445-C455	-0.3(9)
C413-C423-C473-C493	127.1(8)	C435-C445-C455-C465	0.3(9)
C433-C423-C47'-C48'	68(2)	C445-C455-C465-C415	-1.3(8)
C413-C423-C47'-C48'	-132.0(18)	C445-C455-C465-C505	-180.0(5)
C433-C423-C47'-C49'	-53(3)	C425-C415-C465-C455	2.3(8)
C413-C423-C47'-C49'	108(3)	N424-C415-C465-C455	179.8(5)
C453-C463-C503-C523	-71.6(8)	C425-C415-C465-C505	-179.1(5)
C413-C463-C503-C523	105.3(7)	N424-C415-C465-C505	-1.6(8)
C453-C463-C503-C513	44.4(9)	C435-C425-C475-C485	79.4(7)
C413-C463-C503-C513	-138.6(7)	C415-C425-C475-C485	-100.5(6)
C484-C414-C424-N424	127.5(6)	C435-C425-C475-C495	-44.3(7)
C464-C414-C424-N424	7.3(9)	C415-C425-C475-C495	135.8(6)
C474-C414-C424-N424	-113.8(6)	C455-C465-C505-C515	-72.5(6)
C484-C414-C424-C434	-52.0(7)	C415-C465-C505-C515	108.9(6)
C464-C414-C424-C434	-172.2(6)	C455-C465-C505-C525	50.3(7)

C415-C465-C505-C525	-128.3(6)	C416-C466-C506-C526	138.3(6)
C444-N414-C416-C426	-106.1(6)	C456-C466-C506-C516	82.9(7)
Co6-N414-C416-C426	78.9(6)	C416-C466-C506-C516	-99.4(6)
C444-N414-C416-C466	74.6(7)	C77-C27-C37-C47	0.0
Co6-N414-C416-C466	-100.5(5)	C17-C27-C37-C47	177(2)
C434-C424-N424-C415	178.9(5)	C27-C37-C47-C57	0.0
C414-C424-N424-C415	-0.5(9)	C37-C47-C57-C67	0.0
C434-C424-N424-Co6	0.8(8)	C47-C57-C67-C77	0.0
C414-C424-N424-Co6	-178.6(4)	C57-C67-C77-C27	0.0
C465-C415-N424-C424	87.6(7)	C37-C27-C77-C67	0.0
C425-C415-N424-C424	-94.8(6)	C17-C27-C77-C67	-177.3(17)
C465-C415-N424-Co6	-94.2(5)	C147-C97-C107-C117	0.0
C425-C415-N424-Co6	83.4(5)	C87-C97-C107-C117	-179.8(15)
N414-Co6-N424-C424	20.6(5)	C97-C107-C117-C127	0.0
Co5-Co6-N424-C424	-151.0(4)	C107-C117-C127-C137	0.0
N414-Co6-N424-C415	-157.6(4)	C117-C127-C137-C147	0.0
Co5-Co6-N424-C415	30.8(5)	C127-C137-C147-C97	0.0
C466-C416-C426-C436	-6.0(8)	C107-C97-C147-C137	0.0
N414-C416-C426-C436	174.7(5)	C87-C97-C147-C137	179.8(15)
C466-C416-C426-C476	176.7(5)	C217-C167-C177-C187	0.0
N414-C416-C426-C476	-2.6(8)	C157-C167-C177-C187	179.3(9)
C416-C426-C436-C446	1.7(9)	C167-C177-C187-C197	0.0
C476-C426-C436-C446	179.1(5)	C177-C187-C197-C207	0.0
C426-C436-C446-C456	2.8(9)	C187-C197-C207-C217	0.0
C436-C446-C456-C466	-3.0(9)	C197-C207-C217-C167	0.0
C446-C456-C466-C416	-1.3(9)	C177-C167-C217-C207	0.0
C446-C456-C466-C506	176.5(5)	C157-C167-C217-C207	-179.3(8)
C426-C416-C466-C456	5.8(8)	C21'-C16'-C17'-C18'	0.0
N414-C416-C466-C456	-174.8(5)	C15'-C16'-C17'-C18'	175(2)
C426-C416-C466-C506	-171.9(5)	C16'-C17'-C18'-C19'	0.0
N414-C416-C466-C506	7.5(8)	C17'-C18'-C19'-C20'	0.0
C436-C426-C476-C486	64.7(7)	C18'-C19'-C20'-C21'	0.0
C416-C426-C476-C486	-117.9(6)	C19'-C20'-C21'-C16'	0.0
C436-C426-C476-C496	-56.8(7)	C17'-C16'-C21'-C20'	0.0
C416-C426-C476-C496	120.6(6)	C15'-C16'-C21'-C20'	-175(2)
C456-C466-C506-C526	-39.4(8)	C287-C237-C247-C257	0.0

C227-C237-C247-C257	-177.7(9)
C237-C247-C257-C267	0.0
C247-C257-C267-C277	0.0
C257-C267-C277-C287	0.0
C267-C277-C287-C237	0.0
C247-C237-C287-C277	0.0
C227-C237-C287-C277	177.6(10)
C28'-C23'-C24'-C25'	0.0
C22'-C23'-C24'-C25'	175.7(15)
C23'-C24'-C25'-C26'	0.0
C24'-C25'-C26'-C27'	0.0
C25'-C26'-C27'-C28'	0.0
C26'-C27'-C28'-C23'	0.0
C24'-C23'-C28'-C27'	0.0
C22'-C23'-C28'-C27'	-175.7(15)

REFERENCE NUMBER: holkd18

CRYSTAL STRUCTURE REPORT

$C_{78}\ H_{123}\ Co_2\ K_2\ N_4$

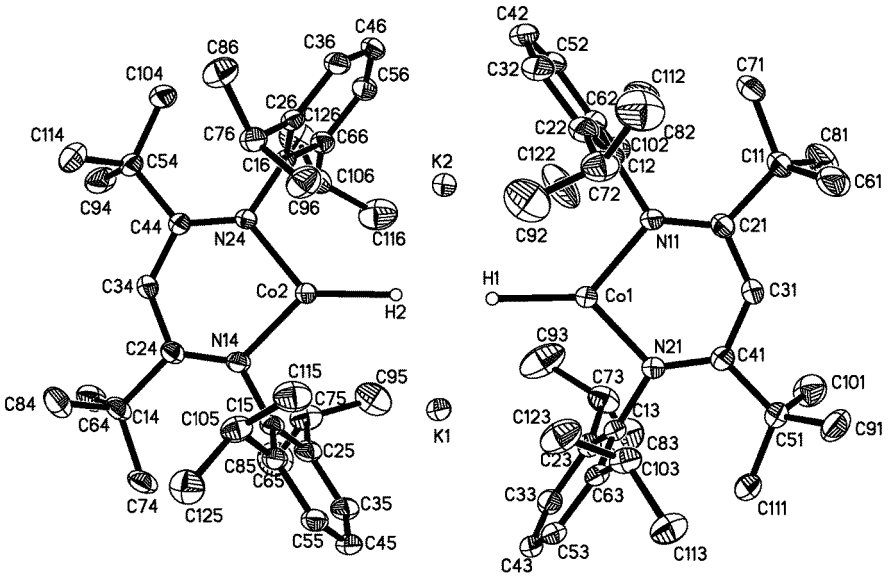
or

$\{[K][LCoH]\}_2 \cdot C_5H_{12} \cdot \frac{1}{2}C_6H_6$

Report prepared for:

K. Ding, Prof. P. Holland

December 21, 2007



William W. Brennessel

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120 Trustee Road

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Data collection

A crystal (0.24 x 0.22 x 0.16 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART APEX II CCD Platform diffractometer for a data collection at 100.0(1) K.[1] A preliminary set of cell constants and an orientation matrix were calculated from 457 reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. The data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 45 seconds and a detector distance of 5.02 cm. A randomly oriented region of reciprocal space was surveyed: four major sections of frames were collected with 0.50º steps in ω at four different ϕ settings and a detector position of -33º in 2θ. The intensity data were corrected for absorption.[2] Final cell constants were calculated from the xyz centroids of 9997 strong reflections from the actual data collection after integration.[3] See Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97[4] and refined using SHELXL-97.[5] The space group *P*-1 was determined based on the lack of systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All carbon-bonded hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The two unique cobalt hydride atoms were found from the difference Fourier map and their positions were refined independently from the cobalt atoms, with relative isotropic displacement parameters (twice the value of those of the bonded cobalt atoms). The final full matrix least squares refinement converged to $R1 = 0.0467$ (F^2, $I > 2\sigma(I)$) and $wR2 = 0.1267$ (F^2, all data).

Structure description

The structure is the one suggested. Per asymmetric unit are two three-coordinate cobalt hydride molecules that form a dinuclear unit via Ph-K-Ph linkages, one co-crystallized pentane solvent molecule, and one half of a co-crystallized benzene solvent molecule. The former two species lie in general positions, while the benzene molecule coincides with a crystallographic inversion center. The angle between N-Co-N planes is 16.69(6)º.

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility, B51 Hutchison Hall, Department of Chemistry, University of Rochester. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel and the X-ray Crystallographic Facility of the Department of Chemistry at the University of Rochester.

[1] *APEX2*, version 2.1-0; Bruker AXS: Madison, WI, 2006.

[2] Sheldrick, G. M. *SADABS*, version 2007/2; University of Göttingen: Göttingen, Germany, 2004.

[3] *SAINT*, version 7.34A; Bruker AXS: Madison, WI, 2006.

[4] Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G. L.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *SIR97: A new program for solving and refining crystal structures*; Istituto di Cristallografia, CNR: Bari, Italy, 1999.

[5] Sheldrick, G. M. *Acta. Cryst.* **2008**, *A64*, 112-122.

Some equations of interest:

$$R_{int} = \Sigma|F_o^2 - \langle F_o^2 \rangle| \,/\, \Sigma|F_o^2|$$

$$R1 = \Sigma||F_o| - |F_c|| \,/\, \Sigma|F_o|$$

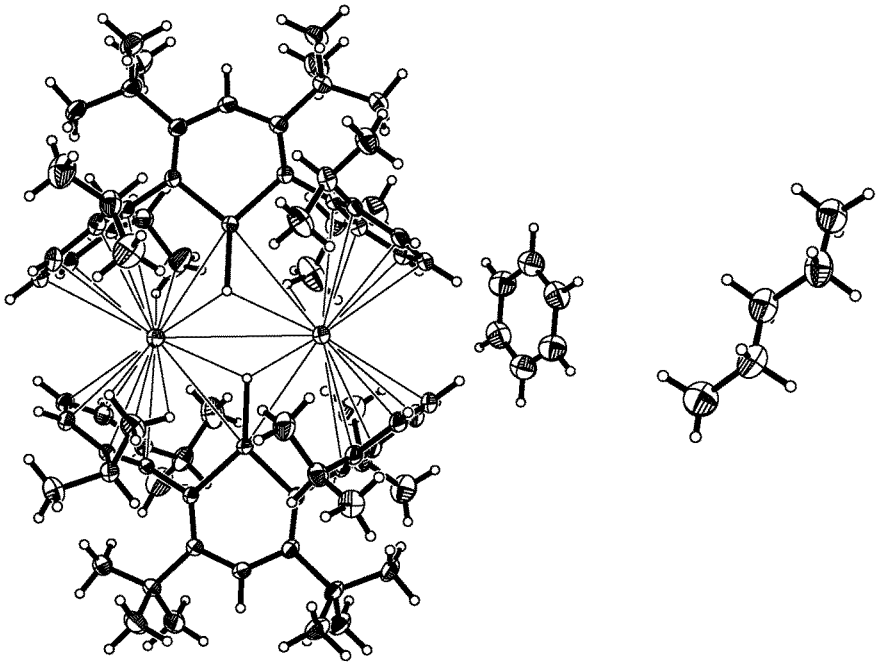
$$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] \,/\, \Sigma[w(F_o^2)^2]]^{1/2}$$

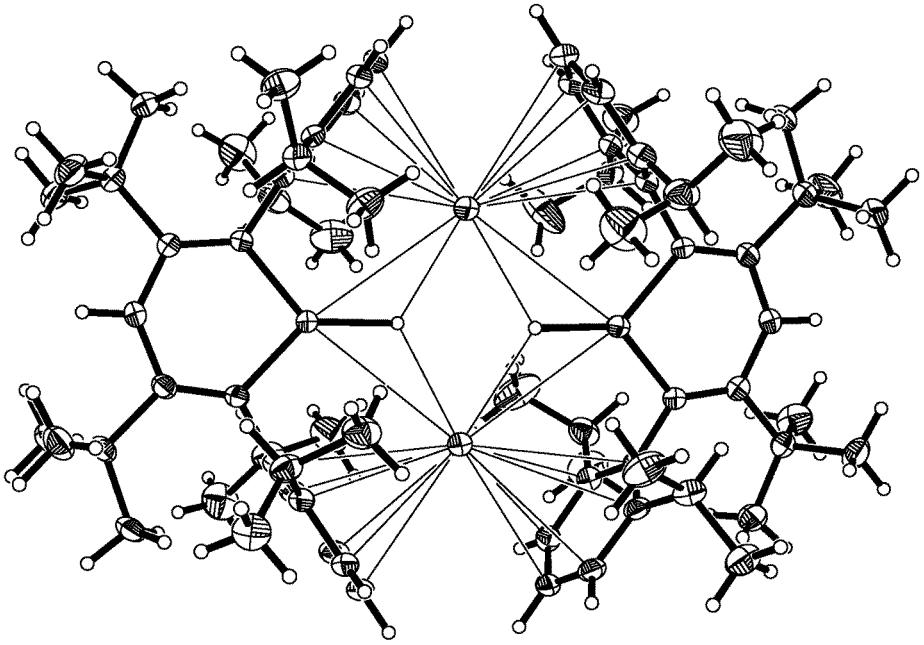
where $w = 1 \,/\, [\sigma^2(F_o^2) + (aP)^2 + bP]$ and

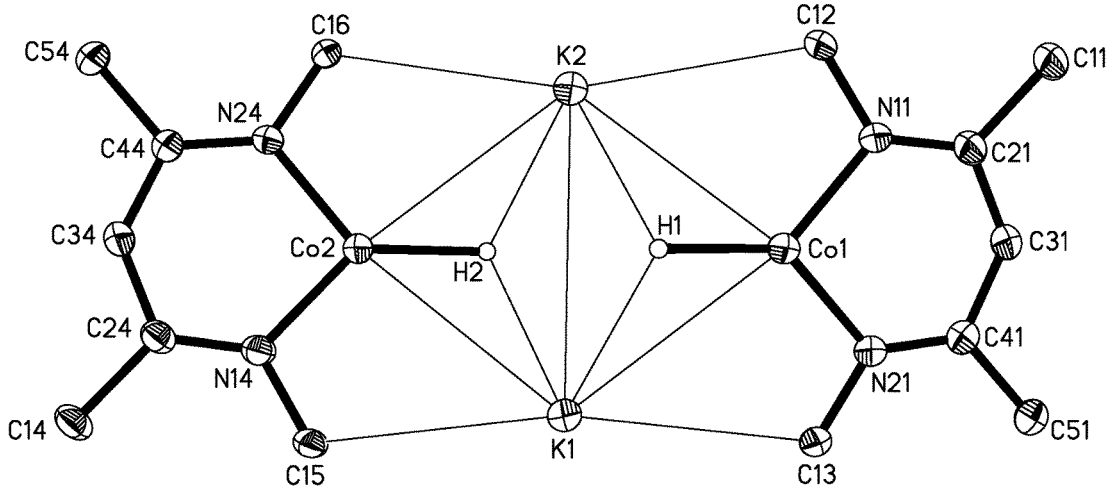
$$P = 1/3 \max(0, F_o^2) + 2/3\, F_c^2$$

$$\text{GOF} = S = [\Sigma[w(F_o^2 - F_c^2)^2] \,/\, (m-n)]^{1/2}$$

where m = number of reflections and n = number of parameters






C16
C12
C54
K2
C11
N24
N11
C44
C21
H1
C34
Co2
Co1
C31
H2
C24
C41
N14
N21
C14
C51
K1
C15
C13

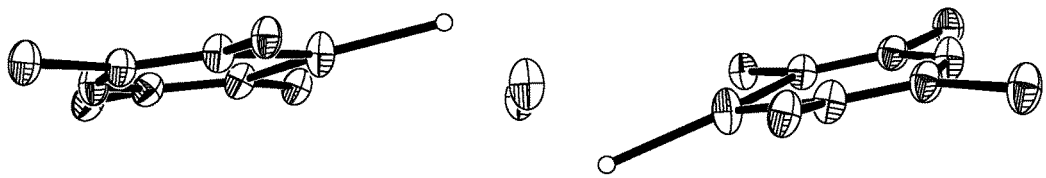


Table 1. Crystal data and structure refinement for holkd18.

Identification code	holkd18	
Empirical formula	C78 H123 Co2 K2 N4	
Formula weight	1312.86	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 14.078(2) Å	α = 75.232(2)°
	b = 15.470(2) Å	β = 69.676(2)°
	c = 19.469(3) Å	γ = 77.776(2)°
Volume	3809.2(9) $Å^3$	
Z	2	
Density (calculated)	1.145 Mg/m^3	
Absorption coefficient	0.587 mm^{-1}	
F(000)	1422	
Crystal color, morphology	deep orange, block	
Crystal size	0.24 x 0.22 x 0.16 mm^3	
Theta range for data collection	1.62 to 32.03°	
Index ranges	$-21 \le h \le 20, -23 \le k \le 23, -29 \le l \le 29$	
Reflections collected	67910	
Independent reflections	26214 [R(int) = 0.0403]	
Observed reflections	16754	
Completeness to theta = 32.03°	98.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9120 and 0.8720	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	26214 / 0 / 811	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	$R1$ = 0.0467, $wR2$ = 0.1106	
R indices (all data)	$R1$ = 0.0865, $wR2$ = 0.1267	
Largest diff. peak and hole	1.328 and -0.424 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for holkd18. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	-778(1)	3388(1)	7752(1)	26(1)
Co2	2276(1)	329(1)	7159(1)	25(1)
K1	1946(1)	2630(1)	7392(1)	29(1)
K2	-435(1)	1084(1)	7642(1)	29(1)
N11	-2195(1)	3538(1)	7827(1)	23(1)
N21	-590(1)	4631(1)	7367(1)	22(1)
N14	3638(1)	80(1)	7216(1)	22(1)
N24	2107(1)	-893(1)	7249(1)	20(1)
C11	-3958(1)	4484(1)	7876(1)	31(1)
C21	-2771(1)	4335(1)	7706(1)	25(1)
C31	-2330(1)	5137(1)	7441(1)	27(1)
C41	-1320(1)	5312(1)	7265(1)	23(1)
C51	-1187(1)	6331(1)	6976(1)	26(1)
C61	-4437(2)	5032(2)	8499(1)	48(1)
C71	-4487(1)	3640(1)	8130(1)	40(1)
C81	-4225(2)	5018(2)	7167(2)	52(1)
C91	-1870(2)	6859(1)	7583(1)	39(1)
C101	-1516(2)	6681(1)	6268(1)	43(1)
C111	-113(2)	6571(1)	6779(1)	38(1)
C12	-2488(1)	2663(1)	7985(1)	24(1)
C22	-2701(1)	2147(1)	8722(1)	30(1)
C32	-2897(1)	1261(1)	8846(1)	35(1)
C42	-2911(1)	890(1)	8276(1)	35(1)
C52	-2697(1)	1396(1)	7558(1)	31(1)
C62	-2471(1)	2278(1)	7395(1)	26(1)
C72	-2725(2)	2514(1)	9378(1)	37(1)
C82	-3764(2)	2508(2)	9987(1)	56(1)
C92	-1887(2)	2004(2)	9715(1)	57(1)
C102	-2162(1)	2777(1)	6585(1)	30(1)
C112	-2834(2)	2688(2)	6149(1)	44(1)
C122	-1054(2)	2434(2)	6186(1)	71(1)

C13	458(1)	4679(1)	7237(1)	22(1)
C23	1183(1)	4618(1)	6528(1)	25(1)
C33	2212(1)	4604(1)	6436(1)	29(1)
C43	2543(1)	4631(1)	7020(1)	29(1)
C53	1826(1)	4666(1)	7720(1)	27(1)
C63	789(1)	4699(1)	7841(1)	23(1)
C73	857(2)	4541(1)	5880(1)	34(1)
C83	1320(2)	5171(2)	5152(1)	53(1)
C93	1157(2)	3570(2)	5758(1)	60(1)
C103	29(1)	4759(1)	8611(1)	29(1)
C113	118(2)	5565(1)	8892(1)	37(1)
C123	149(2)	3884(1)	9172(1)	43(1)
C14	5349(1)	-930(1)	7245(1)	26(1)
C24	4205(1)	-730(1)	7264(1)	22(1)
C34	3781(1)	-1501(1)	7320(1)	24(1)
C44	2819(1)	-1611(1)	7310(1)	21(1)
C54	2709(1)	-2607(1)	7350(1)	25(1)
C64	5979(1)	-1387(1)	6577(1)	36(1)
C74	5878(1)	-118(1)	7151(1)	33(1)
C84	5429(2)	-1576(1)	7978(1)	36(1)
C94	3561(2)	-2962(1)	6699(1)	39(1)
C104	1709(1)	-2768(1)	7299(1)	35(1)
C114	2828(2)	-3190(1)	8095(1)	39(1)
C15	3933(1)	918(1)	7180(1)	23(1)
C25	4230(1)	1517(1)	6479(1)	26(1)
C35	4431(1)	2365(1)	6461(1)	30(1)
C45	4348(1)	2634(1)	7108(1)	28(1)
C55	4046(1)	2054(1)	7791(1)	27(1)
C65	3828(1)	1193(1)	7843(1)	23(1)
C75	4327(2)	1251(1)	5753(1)	35(1)
C85	5428(2)	1206(2)	5224(1)	48(1)
C95	3604(2)	1907(2)	5363(1)	48(1)
C105	3463(1)	592(1)	8609(1)	29(1)
C115	2369(2)	957(2)	9032(1)	38(1)
C125	4173(2)	485(2)	9077(1)	38(1)
C16	1087(1)	-887(1)	7265(1)	21(1)

C26	301(1)	-1030(1)	7960(1)	22(1)
C36	-703(1)	-949(1)	7959(1)	26(1)
C46	-952(1)	-719(1)	7300(1)	29(1)
C56	-186(1)	-567(1)	6625(1)	28(1)
C66	836(1)	-648(1)	6589(1)	24(1)
C76	535(1)	-1238(1)	8696(1)	26(1)
C86	-53(2)	-1975(1)	9279(1)	37(1)
C96	301(2)	-382(1)	9017(1)	37(1)
C106	1647(1)	-483(1)	5831(1)	35(1)
C116	1518(2)	513(2)	5444(1)	53(1)
C126	1637(2)	-1087(2)	5325(1)	51(1)
C17	7133(2)	4610(2)	10022(2)	59(1)
C27	7260(2)	5428(2)	10264(1)	49(1)
C37	6917(2)	6295(2)	9805(1)	46(1)
C47	7120(2)	7126(2)	9971(1)	51(1)
C57	6842(2)	8003(2)	9459(1)	52(1)
C18	5720(2)	4694(2)	5367(1)	48(1)
C28	5640(2)	4195(2)	4895(1)	46(1)
C38	4918(2)	4498(2)	4529(1)	47(1)

Table 3. Bond lengths [Å] and angles [°] for holkd18.

Co(1)-N(11)	1.9162(14)	K(2)-C(22)	3.4913(18)
Co(1)-N(21)	1.9164(14)	K(2)-C(56)	3.5039(18)
Co(1)-K(2)	3.5453(7)	K(2)-H(1)	2.67(2)
Co(1)-K(1)	3.6363(7)	K(2)-H(2)	2.60(2)
Co(1)-H(1)	1.84(2)	N(11)-C(21)	1.339(2)
Co(2)-N(14)	1.9106(13)	N(11)-C(12)	1.426(2)
Co(2)-N(24)	1.9121(13)	N(21)-C(41)	1.335(2)
Co(2)-K(2)	3.6047(7)	N(21)-C(13)	1.422(2)
Co(2)-K(1)	3.6144(7)	N(14)-C(24)	1.335(2)
Co(2)-H(2)	1.78(2)	N(14)-C(15)	1.422(2)
K(1)-C(33)	3.1676(18)	N(24)-C(44)	1.340(2)
K(1)-C(55)	3.2033(18)	N(24)-C(16)	1.4238(19)
K(1)-C(43)	3.2173(17)	C(11)-C(71)	1.526(3)
K(1)-C(45)	3.2322(18)	C(11)-C(61)	1.536(3)
K(1)-C(23)	3.2644(18)	C(11)-C(81)	1.541(3)
K(1)-C(65)	3.2957(17)	C(11)-C(21)	1.564(2)
K(1)-C(35)	3.3257(18)	C(21)-C(31)	1.404(2)
K(1)-C(53)	3.3291(17)	C(31)-C(41)	1.411(2)
K(1)-C(15)	3.4090(17)	C(31)-H(31A)	0.9500
K(1)-C(13)	3.4162(16)	C(41)-C(51)	1.560(2)
K(1)-C(25)	3.4218(17)	C(51)-C(111)	1.527(3)
K(1)-C(63)	3.4497(17)	C(51)-C(91)	1.537(3)
K(1)-K(2)	4.3426(7)	C(51)-C(101)	1.538(3)
K(1)-H(1)	2.67(2)	C(61)-H(61A)	0.9800
K(1)-H(2)	2.64(2)	C(61)-H(61B)	0.9800
K(2)-C(36)	3.1256(18)	C(61)-H(61C)	0.9800
K(2)-C(52)	3.1729(18)	C(71)-H(71A)	0.9800
K(2)-C(62)	3.1805(17)	C(71)-H(71B)	0.9800
K(2)-C(26)	3.1826(16)	C(71)-H(71C)	0.9800
K(2)-C(46)	3.3004(17)	C(81)-H(81A)	0.9800
K(2)-C(42)	3.3209(19)	C(81)-H(81B)	0.9800
K(2)-C(12)	3.3573(17)	C(81)-H(81C)	0.9800
K(2)-C(16)	3.4221(16)	C(91)-H(91A)	0.9800
K(2)-C(32)	3.4450(19)	C(91)-H(91B)	0.9800

C(91)-H(91C)	0.9800	C(13)-C(23)	1.415(2)
C(101)-H(10A)	0.9800	C(13)-C(63)	1.418(2)
C(101)-H(10B)	0.9800	C(23)-C(33)	1.392(2)
C(101)-H(10C)	0.9800	C(23)-C(73)	1.522(3)
C(111)-H(11A)	0.9800	C(33)-C(43)	1.384(3)
C(111)-H(11B)	0.9800	C(33)-H(33A)	0.9500
C(111)-H(11C)	0.9800	C(43)-C(53)	1.391(3)
C(12)-C(62)	1.414(2)	C(43)-H(43A)	0.9500
C(12)-C(22)	1.416(3)	C(53)-C(63)	1.388(2)
C(22)-C(32)	1.400(3)	C(53)-H(53A)	0.9500
C(22)-C(72)	1.511(3)	C(63)-C(103)	1.521(3)
C(32)-C(42)	1.381(3)	C(73)-C(83)	1.519(3)
C(32)-H(32A)	0.9500	C(73)-C(93)	1.529(3)
C(42)-C(52)	1.381(3)	C(73)-H(73A)	1.0000
C(42)-H(42A)	0.9500	C(83)-H(83A)	0.9800
C(52)-C(62)	1.398(2)	C(83)-H(83B)	0.9800
C(52)-H(52A)	0.9500	C(83)-H(83C)	0.9800
C(62)-C(102)	1.523(3)	C(93)-H(93A)	0.9800
C(72)-C(92)	1.525(3)	C(93)-H(93B)	0.9800
C(72)-C(82)	1.531(3)	C(93)-H(93C)	0.9800
C(72)-H(72A)	1.0000	C(103)-C(113)	1.526(3)
C(82)-H(82A)	0.9800	C(103)-C(123)	1.528(3)
C(82)-H(82B)	0.9800	C(103)-H(10E)	1.0000
C(82)-H(82C)	0.9800	C(113)-H(11G)	0.9800
C(92)-H(92A)	0.9800	C(113)-H(11H)	0.9800
C(92)-H(92B)	0.9800	C(113)-H(11I)	0.9800
C(92)-H(92C)	0.9800	C(123)-H(12D)	0.9800
C(102)-C(112)	1.520(3)	C(123)-H(12E)	0.9800
C(102)-C(122)	1.528(3)	C(123)-H(12F)	0.9800
C(102)-H(10D)	1.0000	C(14)-C(74)	1.532(2)
C(112)-H(11D)	0.9800	C(14)-C(64)	1.542(2)
C(112)-H(11E)	0.9800	C(14)-C(84)	1.544(3)
C(112)-H(11F)	0.9800	C(14)-C(24)	1.565(2)
C(122)-H(12A)	0.9800	C(24)-C(34)	1.407(2)
C(122)-H(12B)	0.9800	C(34)-C(44)	1.407(2)
C(122)-H(12C)	0.9800	C(34)-H(34A)	0.9500

C(44)-C(54)	1.560(2)	C(85)-H(85A)	0.9800
C(54)-C(104)	1.522(2)	C(85)-H(85B)	0.9800
C(54)-C(94)	1.538(3)	C(85)-H(85C)	0.9800
C(54)-C(114)	1.544(3)	C(95)-H(95A)	0.9800
C(64)-H(64A)	0.9800	C(95)-H(95B)	0.9800
C(64)-H(64B)	0.9800	C(95)-H(95C)	0.9800
C(64)-H(64C)	0.9800	C(105)-C(125)	1.532(3)
C(74)-H(74A)	0.9800	C(105)-C(115)	1.535(3)
C(74)-H(74B)	0.9800	C(105)-H(10I)	1.0000
C(74)-H(74C)	0.9800	C(115)-H(11M)	0.9800
C(84)-H(84A)	0.9800	C(115)-H(11N)	0.9800
C(84)-H(84B)	0.9800	C(115)-H(11O)	0.9800
C(84)-H(84C)	0.9800	C(125)-H(12G)	0.9800
C(94)-H(94A)	0.9800	C(125)-H(12H)	0.9800
C(94)-H(94B)	0.9800	C(125)-H(12I)	0.9800
C(94)-H(94C)	0.9800	C(16)-C(66)	1.418(2)
C(104)-H(10F)	0.9800	C(16)-C(26)	1.420(2)
C(104)-H(10G)	0.9800	C(26)-C(36)	1.394(2)
C(104)-H(10H)	0.9800	C(26)-C(76)	1.520(2)
C(114)-H(11J)	0.9800	C(36)-C(46)	1.386(3)
C(114)-H(11K)	0.9800	C(36)-H(36A)	0.9500
C(114)-H(11L)	0.9800	C(46)-C(56)	1.383(3)
C(15)-C(65)	1.410(2)	C(46)-H(46A)	0.9500
C(15)-C(25)	1.421(2)	C(56)-C(66)	1.396(2)
C(25)-C(35)	1.389(2)	C(56)-H(56A)	0.9500
C(25)-C(75)	1.524(3)	C(66)-C(106)	1.520(3)
C(35)-C(45)	1.386(3)	C(76)-C(96)	1.533(3)
C(35)-H(35A)	0.9500	C(76)-C(86)	1.536(2)
C(45)-C(55)	1.382(3)	C(76)-H(76A)	1.0000
C(45)-H(45A)	0.9500	C(86)-H(86A)	0.9800
C(55)-C(65)	1.400(2)	C(86)-H(86B)	0.9800
C(55)-H(55A)	0.9500	C(86)-H(86C)	0.9800
C(65)-C(105)	1.521(2)	C(96)-H(96A)	0.9800
C(75)-C(85)	1.533(3)	C(96)-H(96B)	0.9800
C(75)-C(95)	1.533(3)	C(96)-H(96C)	0.9800
C(75)-H(75A)	1.0000	C(106)-C(126)	1.525(3)

C(106)-C(116)	1.536(3)	K(2)-Co(1)-K(1)	74.399(10)
C(106)-H(10J)	1.0000	N(11)-Co(1)-H(1)	128.2(7)
C(116)-H(11P)	0.9800	N(21)-Co(1)-H(1)	134.1(7)
C(116)-H(11Q)	0.9800	K(2)-Co(1)-H(1)	47.3(7)
C(116)-H(11R)	0.9800	K(1)-Co(1)-H(1)	45.0(7)
C(126)-H(12J)	0.9800	N(14)-Co(2)-N(24)	96.59(6)
C(126)-H(12K)	0.9800	N(14)-Co(2)-K(2)	159.66(4)
C(126)-H(12L)	0.9800	N(24)-Co(2)-K(2)	93.13(4)
C(17)-C(27)	1.522(3)	N(14)-Co(2)-K(1)	93.23(4)
C(17)-H(17A)	0.9800	N(24)-Co(2)-K(1)	164.45(4)
C(17)-H(17B)	0.9800	K(2)-Co(2)-K(1)	73.960(10)
C(17)-H(17C)	0.9800	N(14)-Co(2)-H(2)	133.5(7)
C(27)-C(37)	1.498(3)	N(24)-Co(2)-H(2)	129.4(7)
C(27)-H(27A)	0.9900	K(2)-Co(2)-H(2)	43.0(7)
C(27)-H(27B)	0.9900	K(1)-Co(2)-H(2)	44.0(7)
C(37)-C(47)	1.506(3)	C(33)-K(1)-C(55)	101.39(5)
C(37)-H(37A)	0.9900	C(33)-K(1)-C(43)	25.02(5)
C(37)-H(37B)	0.9900	C(55)-K(1)-C(43)	83.29(4)
C(47)-C(57)	1.531(3)	C(33)-K(1)-C(45)	79.84(5)
C(47)-H(47A)	0.9900	C(55)-K(1)-C(45)	24.80(5)
C(47)-H(47B)	0.9900	C(43)-K(1)-C(45)	67.20(4)
C(57)-H(57A)	0.9800	C(33)-K(1)-C(23)	24.93(4)
C(57)-H(57B)	0.9800	C(55)-K(1)-C(23)	125.81(4)
C(57)-H(57C)	0.9800	C(43)-K(1)-C(23)	43.94(4)
C(18)-C(28)	1.387(3)	C(45)-K(1)-C(23)	104.76(4)
C(18)-C(38)#1	1.392(3)	C(33)-K(1)-C(65)	123.47(4)
C(18)-H(18A)	0.9500	C(55)-K(1)-C(65)	24.82(4)
C(28)-C(38)	1.375(3)	C(43)-K(1)-C(65)	107.88(4)
C(28)-H(28A)	0.9500	C(45)-K(1)-C(65)	43.63(4)
C(38)-C(18)#1	1.392(3)	C(23)-K(1)-C(65)	148.38(4)
C(38)-H(38A)	0.9500	C(33)-K(1)-C(35)	79.36(5)
N(11)-Co(1)-N(21)	96.73(6)	C(55)-K(1)-C(35)	42.96(5)
N(11)-Co(1)-K(2)	92.25(4)	C(43)-K(1)-C(35)	76.82(5)
N(21)-Co(1)-K(2)	154.63(4)	C(45)-K(1)-C(35)	24.34(5)
N(11)-Co(1)-K(1)	165.48(4)	C(23)-K(1)-C(35)	101.75(5)
N(21)-Co(1)-K(1)	93.30(4)	C(65)-K(1)-C(35)	49.99(4)

C(33)-K(1)-C(53)	43.08(5)	C(43)-K(1)-C(63)	42.55(4)
C(55)-K(1)-C(53)	88.48(4)	C(45)-K(1)-C(63)	104.50(4)
C(43)-K(1)-C(53)	24.47(5)	C(23)-K(1)-C(63)	42.72(4)
C(45)-K(1)-C(53)	80.95(4)	C(65)-K(1)-C(63)	131.76(4)
C(23)-K(1)-C(53)	50.06(4)	C(35)-K(1)-C(63)	119.03(4)
C(65)-K(1)-C(53)	112.28(4)	C(53)-K(1)-C(63)	23.54(4)
C(35)-K(1)-C(53)	96.90(5)	C(15)-K(1)-C(63)	152.47(4)
C(33)-K(1)-C(15)	121.25(4)	C(13)-K(1)-C(63)	23.83(4)
C(55)-K(1)-C(15)	42.72(4)	C(25)-K(1)-C(63)	142.66(4)
C(43)-K(1)-C(15)	116.22(4)	C(33)-K(1)-Co(2)	140.68(4)
C(45)-K(1)-C(15)	49.70(4)	C(55)-K(1)-Co(2)	85.37(3)
C(23)-K(1)-C(15)	141.41(4)	C(43)-K(1)-Co(2)	155.47(4)
C(65)-K(1)-C(15)	24.21(4)	C(45)-K(1)-Co(2)	94.27(3)
C(35)-K(1)-C(15)	42.06(4)	C(23)-K(1)-Co(2)	136.10(3)
C(53)-K(1)-C(15)	129.58(4)	C(65)-K(1)-Co(2)	61.35(3)
C(33)-K(1)-C(13)	42.85(4)	C(35)-K(1)-Co(2)	80.05(3)
C(55)-K(1)-C(13)	130.13(4)	C(53)-K(1)-Co(2)	173.47(3)
C(43)-K(1)-C(13)	49.91(4)	C(15)-K(1)-Co(2)	44.99(3)
C(45)-K(1)-C(13)	117.11(4)	C(13)-K(1)-Co(2)	144.40(3)
C(23)-K(1)-C(13)	24.32(4)	C(25)-K(1)-Co(2)	56.35(3)
C(65)-K(1)-C(13)	154.19(4)	C(63)-K(1)-Co(2)	160.76(3)
C(35)-K(1)-C(13)	122.08(4)	C(33)-K(1)-Co(1)	84.94(3)
C(53)-K(1)-C(13)	41.93(4)	C(55)-K(1)-Co(1)	155.77(4)
C(15)-K(1)-C(13)	164.10(4)	C(43)-K(1)-Co(1)	94.41(3)
C(33)-K(1)-C(25)	98.93(5)	C(45)-K(1)-Co(1)	161.07(3)
C(55)-K(1)-C(25)	49.77(4)	C(23)-K(1)-Co(1)	60.71(3)
C(43)-K(1)-C(25)	100.22(4)	C(65)-K(1)-Co(1)	149.73(3)
C(45)-K(1)-C(25)	42.54(4)	C(35)-K(1)-Co(1)	159.35(4)
C(23)-K(1)-C(25)	117.42(4)	C(53)-K(1)-Co(1)	80.25(3)
C(65)-K(1)-C(25)	42.82(4)	C(15)-K(1)-Co(1)	149.15(3)
C(35)-K(1)-C(25)	23.71(4)	C(13)-K(1)-Co(1)	44.79(3)
C(53)-K(1)-C(25)	120.52(4)	C(25)-K(1)-Co(1)	153.02(3)
C(15)-K(1)-C(25)	24.02(4)	C(63)-K(1)-Co(1)	56.72(3)
C(13)-K(1)-C(25)	141.00(4)	Co(2)-K(1)-Co(1)	104.643(11)
C(33)-K(1)-C(63)	49.69(4)	C(33)-K(1)-K(2)	125.95(4)
C(55)-K(1)-C(63)	110.03(4)	C(55)-K(1)-K(2)	131.69(3)

C(43)-K(1)-K(2)	144.57(3)	C(13)-K(1)-H(2)	116.5(5)
C(45)-K(1)-K(2)	147.07(3)	C(25)-K(1)-H(2)	74.8(5)
C(23)-K(1)-K(2)	102.34(3)	C(63)-K(1)-H(2)	136.7(5)
C(65)-K(1)-K(2)	107.44(3)	Co(2)-K(1)-H(2)	28.0(5)
C(35)-K(1)-K(2)	130.37(3)	Co(1)-K(1)-H(2)	81.0(5)
C(53)-K(1)-K(2)	131.48(3)	K(2)-K(1)-H(2)	33.8(5)
C(15)-K(1)-K(2)	97.40(3)	H(1)-K(1)-H(2)	69.3(7)
C(13)-K(1)-K(2)	95.10(3)	C(36)-K(2)-C(52)	82.99(5)
C(25)-K(1)-K(2)	107.42(3)	C(36)-K(2)-C(62)	108.39(4)
C(63)-K(1)-K(2)	108.07(3)	C(52)-K(2)-C(62)	25.42(4)
Co(2)-K(1)-K(2)	52.918(9)	C(36)-K(2)-C(26)	25.51(4)
Co(1)-K(1)-K(2)	51.844(11)	C(52)-K(2)-C(26)	108.48(4)
C(33)-K(1)-H(1)	113.7(5)	C(62)-K(2)-C(26)	133.86(4)
C(55)-K(1)-H(1)	135.2(5)	C(36)-K(2)-C(46)	24.71(5)
C(43)-K(1)-H(1)	118.5(5)	C(52)-K(2)-C(46)	69.34(4)
C(45)-K(1)-H(1)	159.5(5)	C(62)-K(2)-C(46)	92.87(4)
C(23)-K(1)-H(1)	89.8(5)	C(26)-K(2)-C(46)	43.94(4)
C(65)-K(1)-H(1)	120.8(5)	C(36)-K(2)-C(42)	70.74(4)
C(35)-K(1)-H(1)	164.6(5)	C(52)-K(2)-C(42)	24.41(5)
C(53)-K(1)-H(1)	98.3(5)	C(62)-K(2)-C(42)	43.73(5)
C(15)-K(1)-H(1)	123.8(5)	C(26)-K(2)-C(42)	94.88(4)
C(13)-K(1)-H(1)	71.8(5)	C(46)-K(2)-C(42)	66.75(4)
C(25)-K(1)-H(1)	140.9(5)	C(36)-K(2)-C(12)	120.39(4)
C(63)-K(1)-H(1)	76.3(5)	C(52)-K(2)-C(12)	43.41(4)
Co(2)-K(1)-H(1)	84.6(5)	C(62)-K(2)-C(12)	24.78(4)
Co(1)-K(1)-H(1)	29.1(5)	C(26)-K(2)-C(12)	143.47(4)
K(2)-K(1)-H(1)	35.5(5)	C(46)-K(2)-C(12)	112.35(4)
C(33)-K(1)-H(2)	124.4(5)	C(42)-K(2)-C(12)	49.67(4)
C(55)-K(1)-H(2)	112.8(5)	C(36)-K(2)-C(16)	43.09(4)
C(43)-K(1)-H(2)	149.1(5)	C(52)-K(2)-C(16)	118.45(4)
C(45)-K(1)-H(2)	117.0(5)	C(62)-K(2)-C(16)	139.93(4)
C(23)-K(1)-H(2)	110.6(5)	C(26)-K(2)-C(16)	24.48(4)
C(65)-K(1)-H(2)	89.3(5)	C(46)-K(2)-C(16)	49.28(4)
C(35)-K(1)-H(2)	96.9(5)	C(42)-K(2)-C(16)	112.99(4)
C(53)-K(1)-H(2)	158.4(5)	C(12)-K(2)-C(16)	161.60(4)
C(15)-K(1)-H(2)	70.8(5)	C(36)-K(2)-C(32)	83.09(5)

C(52)-K(2)-C(32)	41.94(5)	C(56)-K(2)-Co(1)	149.91(3)
C(62)-K(2)-C(32)	49.55(5)	C(36)-K(2)-Co(2)	86.37(3)
C(26)-K(2)-C(32)	102.58(4)	C(52)-K(2)-Co(2)	158.33(4)
C(46)-K(2)-C(32)	86.46(5)	C(62)-K(2)-Co(2)	155.61(4)
C(42)-K(2)-C(32)	23.46(5)	C(26)-K(2)-Co(2)	62.07(3)
C(12)-K(2)-C(32)	41.64(4)	C(46)-K(2)-Co(2)	93.60(3)
C(16)-K(2)-C(32)	125.62(4)	C(42)-K(2)-Co(2)	156.94(3)
C(36)-K(2)-C(22)	106.30(4)	C(12)-K(2)-Co(2)	152.96(3)
C(52)-K(2)-C(22)	49.32(5)	C(16)-K(2)-Co(2)	45.08(3)
C(62)-K(2)-C(22)	42.76(5)	C(32)-K(2)-Co(2)	154.41(4)
C(26)-K(2)-C(22)	124.13(4)	C(22)-K(2)-Co(2)	152.35(3)
C(46)-K(2)-C(22)	108.21(4)	C(56)-K(2)-Co(2)	78.61(3)
C(42)-K(2)-C(22)	41.72(4)	Co(1)-K(2)-Co(2)	106.756(11)
C(12)-K(2)-C(22)	23.77(4)	C(36)-K(2)-K(1)	137.22(3)
C(16)-K(2)-C(22)	148.19(4)	C(52)-K(2)-K(1)	139.76(3)
C(32)-K(2)-C(22)	23.27(4)	C(62)-K(2)-K(1)	114.35(3)
C(36)-K(2)-C(56)	41.76(5)	C(26)-K(2)-K(1)	111.72(3)
C(52)-K(2)-C(56)	80.89(4)	C(46)-K(2)-K(1)	145.73(3)
C(62)-K(2)-C(56)	99.25(4)	C(42)-K(2)-K(1)	147.51(3)
C(26)-K(2)-C(56)	49.15(4)	C(12)-K(2)-K(1)	100.00(3)
C(46)-K(2)-C(56)	23.20(4)	C(16)-K(2)-K(1)	98.20(3)
C(42)-K(2)-C(56)	85.77(5)	C(32)-K(2)-K(1)	126.78(4)
C(12)-K(2)-C(56)	123.14(4)	C(22)-K(2)-K(1)	105.95(3)
C(16)-K(2)-C(56)	40.91(4)	C(56)-K(2)-K(1)	125.59(3)
C(32)-K(2)-C(56)	107.62(5)	Co(1)-K(2)-K(1)	53.757(10)
C(22)-K(2)-C(56)	127.13(4)	Co(2)-K(2)-K(1)	53.123(11)
C(36)-K(2)-Co(1)	163.08(4)	C(36)-K(2)-H(1)	146.5(5)
C(52)-K(2)-Co(1)	87.75(3)	C(52)-K(2)-H(1)	114.0(5)
C(62)-K(2)-Co(1)	63.43(3)	C(62)-K(2)-H(1)	92.0(5)
C(26)-K(2)-Co(1)	159.21(3)	C(26)-K(2)-H(1)	128.9(5)
C(46)-K(2)-Co(1)	156.05(3)	C(46)-K(2)-H(1)	171.2(5)
C(42)-K(2)-Co(1)	95.28(3)	C(42)-K(2)-H(1)	112.6(5)
C(12)-K(2)-Co(1)	46.26(3)	C(12)-K(2)-H(1)	70.6(5)
C(16)-K(2)-Co(1)	151.71(3)	C(16)-K(2)-H(1)	127.3(5)
C(32)-K(2)-Co(1)	80.57(3)	C(32)-K(2)-H(1)	91.2(5)
C(22)-K(2)-Co(1)	57.29(3)	C(22)-K(2)-H(1)	70.9(5)

C(56)-K(2)-H(1)	161.2(5)	C(81)-C(11)-C(21)	109.30(16)
Co(1)-K(2)-H(1)	30.5(5)	N(11)-C(21)-C(31)	120.52(15)
Co(2)-K(2)-H(1)	84.9(5)	N(11)-C(21)-C(11)	125.61(15)
K(1)-K(2)-H(1)	35.6(5)	C(31)-C(21)-C(11)	113.77(14)
C(36)-K(2)-H(2)	111.9(5)	C(21)-C(31)-C(41)	132.30(16)
C(52)-K(2)-H(2)	147.2(5)	C(21)-C(31)-H(31A)	113.9
C(62)-K(2)-H(2)	129.4(5)	C(41)-C(31)-H(31A)	113.9
C(26)-K(2)-H(2)	89.2(5)	N(21)-C(41)-C(31)	119.60(15)
C(46)-K(2)-H(2)	112.0(5)	N(21)-C(41)-C(51)	126.41(14)
C(42)-K(2)-H(2)	171.5(5)	C(31)-C(41)-C(51)	113.98(14)
C(12)-K(2)-H(2)	127.2(5)	C(111)-C(51)-C(91)	105.73(16)
C(16)-K(2)-H(2)	68.9(5)	C(111)-C(51)-C(101)	106.80(16)
C(32)-K(2)-H(2)	161.1(5)	C(91)-C(51)-C(101)	109.40(16)
C(22)-K(2)-H(2)	139.5(5)	C(111)-C(51)-C(41)	116.84(14)
C(56)-K(2)-H(2)	91.3(5)	C(91)-C(51)-C(41)	108.94(14)
Co(1)-K(2)-H(2)	83.3(5)	C(101)-C(51)-C(41)	108.93(15)
Co(2)-K(2)-H(2)	27.9(5)	C(11)-C(61)-H(61A)	109.5
K(1)-K(2)-H(2)	34.3(5)	C(11)-C(61)-H(61B)	109.5
H(1)-K(2)-H(2)	70.0(7)	H(61A)-C(61)-H(61B)	109.5
C(21)-N(11)-C(12)	127.25(14)	C(11)-C(61)-H(61C)	109.5
C(21)-N(11)-Co(1)	124.76(11)	H(61A)-C(61)-H(61C)	109.5
C(12)-N(11)-Co(1)	107.88(10)	H(61B)-C(61)-H(61C)	109.5
C(41)-N(21)-C(13)	127.53(14)	C(11)-C(71)-H(71A)	109.5
C(41)-N(21)-Co(1)	125.76(11)	C(11)-C(71)-H(71B)	109.5
C(13)-N(21)-Co(1)	106.69(10)	H(71A)-C(71)-H(71B)	109.5
C(24)-N(14)-C(15)	127.07(14)	C(11)-C(71)-H(71C)	109.5
C(24)-N(14)-Co(2)	125.93(11)	H(71A)-C(71)-H(71C)	109.5
C(15)-N(14)-Co(2)	106.98(10)	H(71B)-C(71)-H(71C)	109.5
C(44)-N(24)-C(16)	127.60(13)	C(11)-C(81)-H(81A)	109.5
C(44)-N(24)-Co(2)	125.28(11)	C(11)-C(81)-H(81B)	109.5
C(16)-N(24)-Co(2)	107.09(9)	H(81A)-C(81)-H(81B)	109.5
C(71)-C(11)-C(61)	106.79(17)	C(11)-C(81)-H(81C)	109.5
C(71)-C(11)-C(81)	106.10(17)	H(81A)-C(81)-H(81C)	109.5
C(61)-C(11)-C(81)	109.35(18)	H(81B)-C(81)-H(81C)	109.5
C(71)-C(11)-C(21)	116.84(15)	C(51)-C(91)-H(91A)	109.5
C(61)-C(11)-C(21)	108.28(15)	C(51)-C(91)-H(91B)	109.5

H(91A)-C(91)-H(91B)	109.5	C(32)-C(42)-K(2)	83.32(11)
C(51)-C(91)-H(91C)	109.5	C(52)-C(42)-H(42A)	120.4
H(91A)-C(91)-H(91C)	109.5	C(32)-C(42)-H(42A)	120.4
H(91B)-C(91)-H(91C)	109.5	K(2)-C(42)-H(42A)	115.1
C(51)-C(101)-H(10A)	109.5	C(42)-C(52)-C(62)	121.57(18)
C(51)-C(101)-H(10B)	109.5	C(42)-C(52)-K(2)	83.81(11)
H(10A)-C(101)-H(10B)	109.5	C(62)-C(52)-K(2)	77.59(10)
C(51)-C(101)-H(10C)	109.5	C(42)-C(52)-H(52A)	119.2
H(10A)-C(101)-H(10C)	109.5	C(62)-C(52)-H(52A)	119.2
H(10B)-C(101)-H(10C)	109.5	K(2)-C(52)-H(52A)	109.3
C(51)-C(111)-H(11A)	109.5	C(52)-C(62)-C(12)	118.92(17)
C(51)-C(111)-H(11B)	109.5	C(52)-C(62)-C(102)	119.14(16)
H(11A)-C(111)-H(11B)	109.5	C(12)-C(62)-C(102)	121.87(15)
C(51)-C(111)-H(11C)	109.5	C(52)-C(62)-K(2)	76.99(10)
H(11A)-C(111)-H(11C)	109.5	C(12)-C(62)-K(2)	84.63(10)
H(11B)-C(111)-H(11C)	109.5	C(102)-C(62)-K(2)	105.56(10)
C(62)-C(12)-C(22)	119.89(15)	C(22)-C(72)-C(92)	111.72(18)
C(62)-C(12)-N(11)	119.93(16)	C(22)-C(72)-C(82)	112.54(17)
C(22)-C(12)-N(11)	119.90(15)	C(92)-C(72)-C(82)	109.7(2)
C(62)-C(12)-K(2)	70.59(9)	C(22)-C(72)-H(72A)	107.6
C(22)-C(12)-K(2)	83.43(10)	C(92)-C(72)-H(72A)	107.6
N(11)-C(12)-K(2)	111.26(9)	C(82)-C(72)-H(72A)	107.6
C(32)-C(22)-C(12)	118.41(17)	C(72)-C(82)-H(82A)	109.5
C(32)-C(22)-C(72)	118.88(18)	C(72)-C(82)-H(82B)	109.5
C(12)-C(22)-C(72)	122.71(16)	H(82A)-C(82)-H(82B)	109.5
C(32)-C(22)-K(2)	76.51(10)	C(72)-C(82)-H(82C)	109.5
C(12)-C(22)-K(2)	72.80(9)	H(82A)-C(82)-H(82C)	109.5
C(72)-C(22)-K(2)	121.15(12)	H(82B)-C(82)-H(82C)	109.5
C(42)-C(32)-C(22)	121.92(19)	C(72)-C(92)-H(92A)	109.5
C(42)-C(32)-K(2)	73.22(11)	C(72)-C(92)-H(92B)	109.5
C(22)-C(32)-K(2)	80.22(10)	H(92A)-C(92)-H(92B)	109.5
C(42)-C(32)-H(32A)	119.0	C(72)-C(92)-H(92C)	109.5
C(22)-C(32)-H(32A)	119.0	H(92A)-C(92)-H(92C)	109.5
K(2)-C(32)-H(32A)	118.2	H(92B)-C(92)-H(92C)	109.5
C(52)-C(42)-C(32)	119.25(17)	C(112)-C(102)-C(62)	113.75(16)
C(52)-C(42)-K(2)	71.78(10)	C(112)-C(102)-C(122)	108.69(19)

C(62)-C(102)-C(122)	109.82(16)	C(53)-C(43)-K(1)	82.27(10)
C(112)-C(102)-H(10D)	108.1	C(33)-C(43)-H(43A)	120.6
C(62)-C(102)-H(10D)	108.1	C(53)-C(43)-H(43A)	120.6
C(122)-C(102)-H(10D)	108.1	K(1)-C(43)-H(43A)	112.3
C(102)-C(112)-H(11D)	109.5	C(63)-C(53)-C(43)	121.81(17)
C(102)-C(112)-H(11E)	109.5	C(63)-C(53)-K(1)	83.11(9)
H(11D)-C(112)-H(11E)	109.5	C(43)-C(53)-K(1)	73.26(10)
C(102)-C(112)-H(11F)	109.5	C(63)-C(53)-H(53A)	119.1
H(11D)-C(112)-H(11F)	109.5	C(43)-C(53)-H(53A)	119.1
H(11E)-C(112)-H(11F)	109.5	K(1)-C(53)-H(53A)	114.8
C(102)-C(122)-H(12A)	109.5	C(53)-C(63)-C(13)	118.77(16)
C(102)-C(122)-H(12B)	109.5	C(53)-C(63)-C(103)	120.09(16)
H(12A)-C(122)-H(12B)	109.5	C(13)-C(63)-C(103)	121.13(15)
C(102)-C(122)-H(12C)	109.5	C(53)-C(63)-K(1)	73.35(9)
H(12A)-C(122)-H(12C)	109.5	C(13)-C(63)-K(1)	76.76(9)
H(12B)-C(122)-H(12C)	109.5	C(103)-C(63)-K(1)	120.52(10)
C(23)-C(13)-C(63)	119.84(15)	C(83)-C(73)-C(23)	113.77(17)
C(23)-C(13)-N(21)	120.45(15)	C(83)-C(73)-C(93)	108.83(18)
C(63)-C(13)-N(21)	119.41(15)	C(23)-C(73)-C(93)	109.16(17)
C(23)-C(13)-K(1)	71.82(9)	C(83)-C(73)-H(73A)	108.3
C(63)-C(13)-K(1)	79.41(9)	C(23)-C(73)-H(73A)	108.3
N(21)-C(13)-K(1)	114.34(9)	C(93)-C(73)-H(73A)	108.3
C(33)-C(23)-C(13)	118.83(16)	C(73)-C(83)-H(83A)	109.5
C(33)-C(23)-C(73)	120.13(16)	C(73)-C(83)-H(83B)	109.5
C(13)-C(23)-C(73)	121.02(15)	H(83A)-C(83)-H(83B)	109.5
C(33)-C(23)-K(1)	73.64(10)	C(73)-C(83)-H(83C)	109.5
C(13)-C(23)-K(1)	83.86(10)	H(83A)-C(83)-H(83C)	109.5
C(73)-C(23)-K(1)	110.97(11)	H(83B)-C(83)-H(83C)	109.5
C(43)-C(33)-C(23)	121.82(17)	C(73)-C(93)-H(93A)	109.5
C(43)-C(33)-K(1)	79.50(10)	C(73)-C(93)-H(93B)	109.5
C(23)-C(33)-K(1)	81.43(10)	H(93A)-C(93)-H(93B)	109.5
C(43)-C(33)-H(33A)	119.1	C(73)-C(93)-H(93C)	109.5
C(23)-C(33)-H(33A)	119.1	H(93A)-C(93)-H(93C)	109.5
K(1)-C(33)-H(33A)	109.9	H(93B)-C(93)-H(93C)	109.5
C(33)-C(43)-C(53)	118.88(16)	C(63)-C(103)-C(113)	112.03(15)
C(33)-C(43)-K(1)	75.48(10)	C(63)-C(103)-C(123)	110.96(16)

C(113)-C(103)-C(123)	110.65(16)	C(114)-C(54)-C(44)	109.18(14)
C(63)-C(103)-H(10E)	107.7	C(14)-C(64)-H(64A)	109.5
C(113)-C(103)-H(10E)	107.7	C(14)-C(64)-H(64B)	109.5
C(123)-C(103)-H(10E)	107.7	H(64A)-C(64)-H(64B)	109.5
C(103)-C(113)-H(11G)	109.5	C(14)-C(64)-H(64C)	109.5
C(103)-C(113)-H(11H)	109.5	H(64A)-C(64)-H(64C)	109.5
H(11G)-C(113)-H(11H)	109.5	H(64B)-C(64)-H(64C)	109.5
C(103)-C(113)-H(11I)	109.5	C(14)-C(74)-H(74A)	109.5
H(11G)-C(113)-H(11I)	109.5	C(14)-C(74)-H(74B)	109.5
H(11H)-C(113)-H(11I)	109.5	H(74A)-C(74)-H(74B)	109.5
C(103)-C(123)-H(12D)	109.5	C(14)-C(74)-H(74C)	109.5
C(103)-C(123)-H(12E)	109.5	H(74A)-C(74)-H(74C)	109.5
H(12D)-C(123)-H(12E)	109.5	H(74B)-C(74)-H(74C)	109.5
C(103)-C(123)-H(12F)	109.5	C(14)-C(84)-H(84A)	109.5
H(12D)-C(123)-H(12F)	109.5	C(14)-C(84)-H(84B)	109.5
H(12E)-C(123)-H(12F)	109.5	H(84A)-C(84)-H(84B)	109.5
C(74)-C(14)-C(64)	105.71(15)	C(14)-C(84)-H(84C)	109.5
C(74)-C(14)-C(84)	107.07(15)	H(84A)-C(84)-H(84C)	109.5
C(64)-C(14)-C(84)	109.42(15)	H(84B)-C(84)-H(84C)	109.5
C(74)-C(14)-C(24)	116.97(14)	C(54)-C(94)-H(94A)	109.5
C(64)-C(14)-C(24)	108.53(14)	C(54)-C(94)-H(94B)	109.5
C(84)-C(14)-C(24)	108.96(14)	H(94A)-C(94)-H(94B)	109.5
N(14)-C(24)-C(34)	119.79(14)	C(54)-C(94)-H(94C)	109.5
N(14)-C(24)-C(14)	126.29(14)	H(94A)-C(94)-H(94C)	109.5
C(34)-C(24)-C(14)	113.90(14)	H(94B)-C(94)-H(94C)	109.5
C(24)-C(34)-C(44)	132.02(15)	C(54)-C(104)-H(10F)	109.5
C(24)-C(34)-H(34A)	114.0	C(54)-C(104)-H(10G)	109.5
C(44)-C(34)-H(34A)	114.0	H(10F)-C(104)-H(10G)	109.5
N(24)-C(44)-C(34)	120.30(14)	C(54)-C(104)-H(10H)	109.5
N(24)-C(44)-C(54)	125.88(14)	H(10F)-C(104)-H(10H)	109.5
C(34)-C(44)-C(54)	113.79(14)	H(10G)-C(104)-H(10H)	109.5
C(104)-C(54)-C(94)	106.12(15)	C(54)-C(114)-H(11J)	109.5
C(104)-C(54)-C(114)	106.82(15)	C(54)-C(114)-H(11K)	109.5
C(94)-C(54)-C(114)	108.98(15)	H(11J)-C(114)-H(11K)	109.5
C(104)-C(54)-C(44)	116.59(14)	C(54)-C(114)-H(11L)	109.5
C(94)-C(54)-C(44)	108.92(14)	H(11J)-C(114)-H(11L)	109.5

H(11K)-C(114)-H(11L)	109.5	C(105)-C(65)-K(1)	112.21(10)
C(65)-C(15)-C(25)	120.19(15)	C(25)-C(75)-C(85)	112.18(17)
C(65)-C(15)-N(14)	120.11(15)	C(25)-C(75)-C(95)	110.36(17)
C(25)-C(15)-N(14)	119.37(15)	C(85)-C(75)-C(95)	110.30(18)
C(65)-C(15)-K(1)	73.39(9)	C(25)-C(75)-H(75A)	108.0
C(25)-C(15)-K(1)	78.50(9)	C(85)-C(75)-H(75A)	108.0
N(14)-C(15)-K(1)	113.42(9)	C(95)-C(75)-H(75A)	108.0
C(35)-C(25)-C(15)	118.70(16)	C(75)-C(85)-H(85A)	109.5
C(35)-C(25)-C(75)	119.67(17)	C(75)-C(85)-H(85B)	109.5
C(15)-C(25)-C(75)	121.64(15)	H(85A)-C(85)-H(85B)	109.5
C(35)-C(25)-K(1)	74.26(10)	C(75)-C(85)-H(85C)	109.5
C(15)-C(25)-K(1)	77.48(9)	H(85A)-C(85)-H(85C)	109.5
C(75)-C(25)-K(1)	118.31(11)	H(85B)-C(85)-H(85C)	109.5
C(45)-C(35)-C(25)	121.44(17)	C(75)-C(95)-H(95A)	109.5
C(45)-C(35)-K(1)	74.05(10)	C(75)-C(95)-H(95B)	109.5
C(25)-C(35)-K(1)	82.03(10)	H(95A)-C(95)-H(95B)	109.5
C(45)-C(35)-H(35A)	119.3	C(75)-C(95)-H(95C)	109.5
C(25)-C(35)-H(35A)	119.3	H(95A)-C(95)-H(95C)	109.5
K(1)-C(35)-H(35A)	115.0	H(95B)-C(95)-H(95C)	109.5
C(55)-C(45)-C(35)	119.67(16)	C(65)-C(105)-C(125)	112.58(15)
C(55)-C(45)-K(1)	76.43(10)	C(65)-C(105)-C(115)	110.36(15)
C(35)-C(45)-K(1)	81.61(10)	C(125)-C(105)-C(115)	110.26(16)
C(55)-C(45)-H(45A)	120.2	C(65)-C(105)-H(10I)	107.8
C(35)-C(45)-H(45A)	120.2	C(125)-C(105)-H(10I)	107.8
K(1)-C(45)-H(45A)	112.3	C(115)-C(105)-H(10I)	107.8
C(45)-C(55)-C(65)	121.41(16)	C(105)-C(115)-H(11M)	109.5
C(45)-C(55)-K(1)	78.77(10)	C(105)-C(115)-H(11N)	109.5
C(65)-C(55)-K(1)	81.29(10)	H(11M)-C(115)-H(11N)	109.5
C(45)-C(55)-H(55A)	119.3	C(105)-C(115)-H(11O)	109.5
C(65)-C(55)-H(55A)	119.3	H(11M)-C(115)-H(11O)	109.5
K(1)-C(55)-H(55A)	110.7	H(11N)-C(115)-H(11O)	109.5
C(55)-C(65)-C(15)	118.57(16)	C(105)-C(125)-H(12G)	109.5
C(55)-C(65)-C(105)	119.47(15)	C(105)-C(125)-H(12H)	109.5
C(15)-C(65)-C(105)	121.94(15)	H(12G)-C(125)-H(12H)	109.5
C(55)-C(65)-K(1)	73.89(10)	C(105)-C(125)-H(12I)	109.5
C(15)-C(65)-K(1)	82.40(10)	H(12G)-C(125)-H(12I)	109.5

H(12H)-C(125)-H(12I)	109.5	C(96)-C(76)-C(86)	109.55(16)
C(66)-C(16)-C(26)	119.83(14)	C(26)-C(76)-H(76A)	107.9
C(66)-C(16)-N(24)	119.98(14)	C(96)-C(76)-H(76A)	107.9
C(26)-C(16)-N(24)	119.87(15)	C(86)-C(76)-H(76A)	107.9
C(66)-C(16)-K(2)	84.58(9)	C(76)-C(86)-H(86A)	109.5
C(26)-C(16)-K(2)	68.27(8)	C(76)-C(86)-H(86B)	109.5
N(24)-C(16)-K(2)	112.09(9)	H(86A)-C(86)-H(86B)	109.5
C(36)-C(26)-C(16)	118.68(16)	C(76)-C(86)-H(86C)	109.5
C(36)-C(26)-C(76)	120.05(15)	H(86A)-C(86)-H(86C)	109.5
C(16)-C(26)-C(76)	121.24(14)	H(86B)-C(86)-H(86C)	109.5
C(36)-C(26)-K(2)	74.96(9)	C(76)-C(96)-H(96A)	109.5
C(16)-C(26)-K(2)	87.25(9)	C(76)-C(96)-H(96B)	109.5
C(76)-C(26)-K(2)	105.93(10)	H(96A)-C(96)-H(96B)	109.5
C(46)-C(36)-C(26)	121.72(17)	C(76)-C(96)-H(96C)	109.5
C(46)-C(36)-K(2)	84.72(10)	H(96A)-C(96)-H(96C)	109.5
C(26)-C(36)-K(2)	79.53(9)	H(96B)-C(96)-H(96C)	109.5
C(46)-C(36)-H(36A)	119.1	C(66)-C(106)-C(126)	112.19(17)
C(26)-C(36)-H(36A)	119.1	C(66)-C(106)-C(116)	110.72(17)
K(2)-C(36)-H(36A)	106.3	C(126)-C(106)-C(116)	110.11(18)
C(56)-C(46)-C(36)	119.33(16)	C(66)-C(106)-H(10J)	107.9
C(56)-C(46)-K(2)	86.69(10)	C(126)-C(106)-H(10J)	107.9
C(36)-C(46)-K(2)	70.57(10)	C(116)-C(106)-H(10J)	107.9
C(56)-C(46)-H(46A)	120.3	C(106)-C(116)-H(11P)	109.5
C(36)-C(46)-H(46A)	120.3	C(106)-C(116)-H(11Q)	109.5
K(2)-C(46)-H(46A)	112.7	H(11P)-C(116)-H(11Q)	109.5
C(46)-C(56)-C(66)	121.67(17)	C(106)-C(116)-H(11R)	109.5
C(46)-C(56)-K(2)	70.11(10)	H(11P)-C(116)-H(11R)	109.5
C(66)-C(56)-K(2)	81.64(10)	H(11Q)-C(116)-H(11R)	109.5
C(46)-C(56)-H(56A)	119.2	C(106)-C(126)-H(12J)	109.5
C(66)-C(56)-H(56A)	119.2	C(106)-C(126)-H(12K)	109.5
K(2)-C(56)-H(56A)	119.9	H(12J)-C(126)-H(12K)	109.5
C(56)-C(66)-C(16)	118.75(16)	C(106)-C(126)-H(12L)	109.5
C(56)-C(66)-C(106)	119.35(16)	H(12J)-C(126)-H(12L)	109.5
C(16)-C(66)-C(106)	121.90(15)	H(12K)-C(126)-H(12L)	109.5
C(26)-C(76)-C(96)	110.47(14)	C(27)-C(17)-H(17A)	109.5
C(26)-C(76)-C(86)	112.88(14)	C(27)-C(17)-H(17B)	109.5

H(17A)-C(17)-H(17B)	109.5	C(37)-C(47)-H(47B)	108.8
C(27)-C(17)-H(17C)	109.5	C(57)-C(47)-H(47B)	108.8
H(17A)-C(17)-H(17C)	109.5	H(47A)-C(47)-H(47B)	107.7
H(17B)-C(17)-H(17C)	109.5	C(47)-C(57)-H(57A)	109.5
C(37)-C(27)-C(17)	111.9(2)	C(47)-C(57)-H(57B)	109.5
C(37)-C(27)-H(27A)	109.2	H(57A)-C(57)-H(57B)	109.5
C(17)-C(27)-H(27A)	109.2	C(47)-C(57)-H(57C)	109.5
C(37)-C(27)-H(27B)	109.2	H(57A)-C(57)-H(57C)	109.5
C(17)-C(27)-H(27B)	109.2	H(57B)-C(57)-H(57C)	109.5
H(27A)-C(27)-H(27B)	107.9	C(28)-C(18)-C(38)#1	120.8(2)
C(27)-C(37)-C(47)	114.1(2)	C(28)-C(18)-H(18A)	119.6
C(27)-C(37)-H(37A)	108.7	C(38)#1-C(18)-H(18A)	119.6
C(47)-C(37)-H(37A)	108.7	C(38)-C(28)-C(18)	119.7(2)
C(27)-C(37)-H(37B)	108.7	C(38)-C(28)-H(28A)	120.2
C(47)-C(37)-H(37B)	108.7	C(18)-C(28)-H(28A)	120.2
H(37A)-C(37)-H(37B)	107.6	C(28)-C(38)-C(18)#1	119.5(2)
C(37)-C(47)-C(57)	113.7(2)	C(28)-C(38)-H(38A)	120.2
C(37)-C(47)-H(47A)	108.8	C(18)#1-C(38)-H(38A)	120.2
C(57)-C(47)-H(47A)	108.8		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for holkd18. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	18(1)	18(1)	43(1)	-6(1)	-11(1)	-2(1)
Co2	17(1)	18(1)	41(1)	-9(1)	-10(1)	-1(1)
K1	21(1)	21(1)	47(1)	-10(1)	-10(1)	-3(1)
K2	22(1)	22(1)	46(1)	-8(1)	-12(1)	-3(1)
N11	19(1)	20(1)	34(1)	-9(1)	-8(1)	-4(1)
N21	19(1)	20(1)	27(1)	-6(1)	-8(1)	-3(1)
N14	17(1)	23(1)	28(1)	-10(1)	-5(1)	-4(1)
N24	16(1)	19(1)	27(1)	-6(1)	-7(1)	-3(1)
C11	20(1)	31(1)	47(1)	-16(1)	-12(1)	0(1)
C21	19(1)	26(1)	33(1)	-11(1)	-9(1)	-1(1)
C31	20(1)	23(1)	40(1)	-10(1)	-11(1)	2(1)
C41	23(1)	21(1)	26(1)	-8(1)	-7(1)	-2(1)
C51	26(1)	20(1)	33(1)	-5(1)	-9(1)	-2(1)
C61	24(1)	50(1)	73(2)	-38(1)	-3(1)	-4(1)
C71	18(1)	38(1)	68(2)	-23(1)	-11(1)	-1(1)
C81	32(1)	57(1)	70(2)	-7(1)	-30(1)	1(1)
C91	42(1)	25(1)	48(1)	-15(1)	-5(1)	-5(1)
C101	53(1)	36(1)	44(1)	1(1)	-23(1)	-9(1)
C111	33(1)	20(1)	57(1)	-1(1)	-14(1)	-7(1)
C12	15(1)	23(1)	38(1)	-11(1)	-7(1)	-3(1)
C22	21(1)	31(1)	35(1)	-8(1)	-3(1)	-7(1)
C32	24(1)	33(1)	41(1)	-3(1)	-2(1)	-11(1)
C42	24(1)	25(1)	55(1)	-11(1)	-7(1)	-9(1)
C52	19(1)	28(1)	49(1)	-16(1)	-10(1)	-5(1)
C62	17(1)	24(1)	42(1)	-12(1)	-11(1)	-2(1)
C72	35(1)	41(1)	33(1)	-10(1)	-3(1)	-14(1)
C82	49(1)	73(2)	43(1)	-23(1)	3(1)	-18(1)
C92	54(2)	76(2)	47(1)	-17(1)	-22(1)	-9(1)
C102	29(1)	27(1)	40(1)	-11(1)	-16(1)	-2(1)
C112	40(1)	60(1)	44(1)	-18(1)	-18(1)	-11(1)
C122	28(1)	102(2)	49(2)	27(2)	-6(1)	-3(1)

C13	20(1)	17(1)	31(1)	-4(1)	-9(1)	-4(1)
C23	23(1)	23(1)	30(1)	-6(1)	-7(1)	-4(1)
C33	23(1)	24(1)	38(1)	-7(1)	-4(1)	-4(1)
C43	21(1)	18(1)	50(1)	-6(1)	-13(1)	-4(1)
C53	30(1)	19(1)	41(1)	-5(1)	-19(1)	-5(1)
C63	26(1)	16(1)	31(1)	-3(1)	-11(1)	-6(1)
C73	27(1)	47(1)	29(1)	-13(1)	-5(1)	-7(1)
C83	72(2)	49(1)	41(1)	4(1)	-28(1)	-16(1)
C93	102(2)	51(1)	34(1)	-8(1)	-19(1)	-34(2)
C103	33(1)	27(1)	28(1)	-3(1)	-11(1)	-11(1)
C113	44(1)	34(1)	34(1)	-11(1)	-8(1)	-13(1)
C123	65(2)	34(1)	34(1)	1(1)	-19(1)	-19(1)
C14	15(1)	32(1)	35(1)	-14(1)	-8(1)	0(1)
C24	17(1)	26(1)	25(1)	-9(1)	-6(1)	-2(1)
C34	19(1)	21(1)	34(1)	-7(1)	-10(1)	1(1)
C44	20(1)	18(1)	27(1)	-6(1)	-7(1)	-2(1)
C54	24(1)	18(1)	35(1)	-8(1)	-9(1)	-3(1)
C64	21(1)	43(1)	46(1)	-24(1)	-6(1)	1(1)
C74	16(1)	40(1)	47(1)	-19(1)	-10(1)	-3(1)
C84	27(1)	43(1)	43(1)	-11(1)	-18(1)	2(1)
C94	34(1)	28(1)	55(1)	-20(1)	-4(1)	-5(1)
C104	30(1)	24(1)	58(1)	-13(1)	-16(1)	-5(1)
C114	47(1)	23(1)	49(1)	-1(1)	-21(1)	-8(1)
C15	15(1)	23(1)	31(1)	-10(1)	-4(1)	-4(1)
C25	18(1)	31(1)	29(1)	-8(1)	-2(1)	-8(1)
C35	24(1)	31(1)	34(1)	-2(1)	-6(1)	-11(1)
C45	22(1)	24(1)	42(1)	-8(1)	-11(1)	-7(1)
C55	22(1)	27(1)	36(1)	-13(1)	-10(1)	-4(1)
C65	19(1)	23(1)	30(1)	-10(1)	-7(1)	-4(1)
C75	34(1)	41(1)	28(1)	-11(1)	0(1)	-14(1)
C85	41(1)	62(2)	32(1)	-12(1)	4(1)	-10(1)
C95	46(1)	70(2)	35(1)	-16(1)	-14(1)	-9(1)
C105	32(1)	29(1)	28(1)	-10(1)	-6(1)	-9(1)
C115	34(1)	45(1)	34(1)	-10(1)	-1(1)	-14(1)
C125	42(1)	43(1)	31(1)	-6(1)	-13(1)	-7(1)
C16	18(1)	15(1)	31(1)	-7(1)	-9(1)	-2(1)

C26	20(1)	17(1)	30(1)	-7(1)	-6(1)	-4(1)
C36	19(1)	25(1)	36(1)	-10(1)	-5(1)	-5(1)
C46	19(1)	25(1)	47(1)	-14(1)	-14(1)	-1(1)
C56	28(1)	26(1)	36(1)	-8(1)	-17(1)	-4(1)
C66	23(1)	24(1)	29(1)	-9(1)	-10(1)	-3(1)
C76	24(1)	24(1)	29(1)	-6(1)	-7(1)	-5(1)
C86	44(1)	33(1)	32(1)	-1(1)	-9(1)	-15(1)
C96	50(1)	32(1)	35(1)	-10(1)	-17(1)	-9(1)
C106	27(1)	50(1)	29(1)	-10(1)	-9(1)	-7(1)
C116	60(2)	59(2)	36(1)	2(1)	-10(1)	-26(1)
C126	47(1)	70(2)	38(1)	-26(1)	-8(1)	-7(1)
C17	59(2)	65(2)	55(2)	-19(1)	-14(1)	-7(1)
C27	37(1)	64(2)	45(1)	-12(1)	-11(1)	-8(1)
C37	44(1)	62(2)	38(1)	-18(1)	-10(1)	-12(1)
C47	49(1)	65(2)	43(1)	-15(1)	-11(1)	-19(1)
C57	52(1)	61(2)	47(1)	-19(1)	-13(1)	-11(1)
C18	49(1)	51(1)	41(1)	-14(1)	-8(1)	-3(1)
C28	49(1)	42(1)	38(1)	-5(1)	-6(1)	-6(1)
C38	54(1)	47(1)	41(1)	-13(1)	-7(1)	-13(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for holkd18.

	x	y	z	U(eq)
H1	-2(18)	2380(16)	8117(13)	52
H2	1460(17)	1346(15)	6956(13)	50
H31A	-2802	5663	7367	32
H61A	-4261	4697	8948	71
H61B	-5182	5135	8612	71
H61C	-4174	5613	8335	71
H71A	-4353	3280	8589	60
H71B	-4222	3281	7738	60
H71C	-5225	3817	8227	60
H81A	-4962	5066	7259	78
H81B	-3854	4703	6752	78
H81C	-4027	5623	7040	78
H91A	-1790	7500	7407	59
H91B	-1669	6629	8038	59
H91C	-2586	6786	7693	59
H10A	-1415	7316	6074	65
H10B	-2240	6626	6390	65
H10C	-1103	6325	5889	65
H11A	-131	7227	6631	56
H11B	349	6288	6364	56
H11C	131	6351	7215	56
H32A	-3025	905	9336	42
H42A	-3066	293	8376	42
H52A	-2703	1140	7166	37
H72A	-2593	3156	9187	44
H82A	-4297	2860	9773	84
H82B	-3751	2776	10388	84
H82C	-3911	1886	10189	84
H92A	-1222	2016	9325	85
H92B	-2013	1377	9928	85

H92C	-1888	2291	10110	85
H10D	-2207	3432	6581	36
H11D	-3548	2902	6401	67
H11E	-2771	2054	6121	67
H11F	-2617	3050	5643	67
H12A	-866	2744	5661	106
H12B	-983	1783	6214	106
H12C	-603	2555	6426	106
H33A	2700	4575	5958	35
H43A	3248	4626	6945	35
H53A	2053	4666	8126	33
H73A	96	4686	6018	41
H83A	1168	5792	5233	79
H83B	1028	5130	4774	79
H83C	2062	4997	4980	79
H93A	890	3155	6231	89
H93B	1904	3434	5577	89
H93C	869	3497	5387	89
H10E	-674	4844	8568	34
H11G	18	6121	8532	55
H11H	798	5495	8946	55
H11I	-404	5596	9376	55
H12D	58	3378	8994	64
H12E	-366	3929	9658	64
H12F	834	3783	9226	64
H34A	4228	-2050	7374	29
H64A	6700	-1513	6556	53
H64B	5914	-984	6113	53
H64C	5725	-1953	6638	53
H74A	5539	175	7581	49
H74B	5835	312	6692	49
H74C	6597	-323	7118	49
H84A	5004	-1297	8404	54
H84B	6143	-1695	7975	54
H84C	5192	-2144	8020	54
H94A	3483	-3581	6710	59

H94B	4229	-2956	6748	59
H94C	3511	-2577	6224	59
H10F	1143	-2598	7727	53
H10G	1740	-3407	7301	53
H10H	1599	-2401	6835	53
H11J	2283	-2972	8513	59
H11K	3494	-3149	8130	59
H11L	2781	-3820	8116	59
H35A	4630	2769	5994	36
H45A	4497	3214	7084	34
H55A	3985	2244	8233	32
H75A	4117	637	5881	42
H85A	5872	748	5465	73
H85B	5662	1795	5108	73
H85C	5453	1047	4762	73
H95A	2903	1926	5706	73
H95B	3637	1703	4917	73
H95C	3810	2511	5216	73
H10I	3450	-20	8531	35
H11M	1916	995	8737	58
H11N	2360	1558	9114	58
H11O	2133	549	9515	58
H12G	4857	212	8817	57
H12H	3904	95	9564	57
H12I	4213	1078	9150	57
H36A	-1231	-1055	8422	32
H46A	-1642	-666	7313	34
H56A	-359	-403	6175	33
H76A	1282	-1458	8593	31
H86A	78	-2515	9067	55
H86B	-787	-1755	9420	55
H86C	175	-2124	9722	55
H96A	712	74	8658	55
H96B	469	-525	9485	55
H96C	-427	-147	9113	55
H10J	2331	-625	5913	41

H11P	1512	896	5776	79
H11Q	871	660	5327	79
H11R	2087	619	4980	79
H12J	1769	-1721	5562	76
H12K	2169	-958	4843	76
H12L	968	-971	5246	76
H17A	7396	4058	10317	89
H17B	7514	4637	9491	89
H17C	6407	4607	10101	89
H27A	6856	5408	10797	58
H27B	7988	5406	10216	58
H37A	6174	6338	9893	56
H37B	7269	6282	9270	56
H47A	7855	7063	9921	61
H47B	6724	7166	10495	61
H57A	7002	8513	9592	77
H57B	6111	8084	9519	77
H57C	7237	7973	8938	77
H18A	6216	4482	5621	58
H28A	6081	3646	4825	55
H38A	4855	4159	4207	57

Table 6. Torsion angles [°] for holkd18.

N14-Co2-K1-C33	92.26(7)	N24-Co2-K1-C63	-25.04(19)
N24-Co2-K1-C33	-138.57(16)	K2-Co2-K1-C63	9.73(10)
K2-Co2-K1-C33	-103.80(5)	N14-Co2-K1-Co1	-167.66(4)
N14-Co2-K1-C55	-10.08(5)	N24-Co2-K1-Co1	-38.49(16)
N24-Co2-K1-C55	119.09(16)	K2-Co2-K1-Co1	-3.724(11)
K2-Co2-K1-C55	153.86(4)	N14-Co2-K1-K2	-163.94(4)
N14-Co2-K1-C43	52.55(10)	N24-Co2-K1-K2	-34.77(16)
N24-Co2-K1-C43	-178.28(17)	N11-Co1-K1-C33	121.22(19)
K2-Co2-K1-C43	-143.52(9)	N21-Co1-K1-C33	-12.46(6)
N14-Co2-K1-C45	13.10(6)	K2-Co1-K1-C33	145.00(4)
N24-Co2-K1-C45	142.27(16)	N11-Co1-K1-C55	-132.2(2)
K2-Co2-K1-C45	177.03(4)	N21-Co1-K1-C55	94.17(9)
N14-Co2-K1-C23	129.58(6)	K2-Co1-K1-C55	-108.38(8)
N24-Co2-K1-C23	-101.25(16)	N11-Co1-K1-C43	144.41(18)
K2-Co2-K1-C23	-66.48(5)	N21-Co1-K1-C43	10.73(6)
N14-Co2-K1-C65	-16.68(5)	K2-Co1-K1-C43	168.18(4)
N24-Co2-K1-C65	112.49(16)	N11-Co1-K1-C45	157.7(2)
K2-Co2-K1-C65	147.26(4)	N21-Co1-K1-C45	23.99(12)
N14-Co2-K1-C35	32.93(6)	K2-Co1-K1-C45	-178.55(11)
N24-Co2-K1-C35	162.10(16)	N11-Co1-K1-C23	115.01(19)
K2-Co2-K1-C35	-163.13(4)	N21-Co1-K1-C23	-18.66(5)
N14-Co2-K1-C53	-29.7(3)	K2-Co1-K1-C23	138.79(4)
N24-Co2-K1-C53	99.5(3)	N11-Co1-K1-C65	-77.62(19)
K2-Co2-K1-C53	134.2(3)	N21-Co1-K1-C65	148.70(7)
N14-Co2-K1-C15	5.88(6)	K2-Co1-K1-C65	-53.84(6)
N24-Co2-K1-C15	135.05(16)	N11-Co1-K1-C35	80.8(2)
K2-Co2-K1-C15	169.82(4)	N21-Co1-K1-C35	-52.91(10)
N14-Co2-K1-C13	165.87(7)	K2-Co1-K1-C35	104.55(10)
N24-Co2-K1-C13	-64.96(17)	N11-Co1-K1-C53	164.43(19)
K2-Co2-K1-C13	-30.20(5)	N21-Co1-K1-C53	30.76(5)
N14-Co2-K1-C25	33.49(6)	K2-Co1-K1-C53	-171.79(4)
N24-Co2-K1-C25	162.66(16)	N11-Co1-K1-C15	-28.9(2)
K2-Co2-K1-C25	-162.57(4)	N21-Co1-K1-C15	-162.60(7)
N14-Co2-K1-C63	-154.21(10)	K2-Co1-K1-C15	-5.14(6)

N11-Co1-K1-C13	138.38(19)	N21-Co1-K2-C16	54.74(12)
N21-Co1-K1-C13	4.71(6)	K1-Co1-K2-C16	-8.56(7)
K2-Co1-K1-C13	162.16(4)	N11-Co1-K2-C32	-34.84(6)
N11-Co1-K1-C25	21.5(2)	N21-Co1-K2-C32	-145.74(10)
N21-Co1-K1-C25	-112.21(8)	K1-Co1-K2-C32	150.97(4)
K2-Co1-K1-C25	45.25(7)	N11-Co1-K2-C22	-34.67(6)
N11-Co1-K1-C63	165.26(19)	N21-Co1-K2-C22	-145.57(10)
N21-Co1-K1-C63	31.59(5)	K1-Co1-K2-C22	151.13(4)
K2-Co1-K1-C63	-170.96(4)	N11-Co1-K2-C56	74.15(8)
N11-Co1-K1-Co2	-20.00(18)	N21-Co1-K2-C56	-36.75(12)
N21-Co1-K1-Co2	-153.68(4)	K1-Co1-K2-C56	-100.04(6)
K2-Co1-K1-Co2	3.778(12)	N11-Co1-K2-Co2	170.36(5)
N11-Co1-K1-K2	-23.78(18)	N21-Co1-K2-Co2	59.46(10)
N21-Co1-K1-K2	-157.46(4)	K1-Co1-K2-Co2	-3.828(12)
N11-Co1-K2-C36	-49.97(13)	N11-Co1-K2-K1	174.19(5)
N21-Co1-K2-C36	-160.87(15)	N21-Co1-K2-K1	63.29(10)
K1-Co1-K2-C36	135.84(12)	N14-Co2-K2-C36	-112.61(13)
N11-Co1-K2-C52	6.74(6)	N24-Co2-K2-C36	5.94(6)
N21-Co1-K2-C52	-104.16(10)	K1-Co2-K2-C36	-165.26(4)
K1-Co1-K2-C52	-167.45(4)	N14-Co2-K2-C52	-173.22(15)
N11-Co1-K2-C62	14.45(6)	N24-Co2-K2-C52	-54.67(11)
N21-Co1-K2-C62	-96.45(10)	K1-Co2-K2-C52	134.14(10)
K1-Co1-K2-C62	-159.74(4)	N14-Co2-K2-C62	118.65(15)
N11-Co1-K2-C26	-135.46(10)	N24-Co2-K2-C62	-122.80(9)
N21-Co1-K2-C26	113.64(13)	K1-Co2-K2-C62	66.01(8)
K1-Co1-K2-C26	50.35(9)	N14-Co2-K2-C26	-104.48(13)
N11-Co1-K2-C46	23.27(10)	N24-Co2-K2-C26	14.07(5)
N21-Co1-K2-C46	-87.63(13)	K1-Co2-K2-C26	-157.12(4)
K1-Co1-K2-C46	-150.92(9)	N14-Co2-K2-C46	-136.26(13)
N11-Co1-K2-C42	-16.51(6)	N24-Co2-K2-C46	-17.71(6)
N21-Co1-K2-C42	-127.41(10)	K1-Co2-K2-C46	171.10(4)
K1-Co1-K2-C42	169.30(4)	N14-Co2-K2-C42	-105.79(16)
N11-Co1-K2-C12	-7.66(6)	N24-Co2-K2-C42	12.76(11)
N21-Co1-K2-C12	-118.56(11)	K1-Co2-K2-C42	-158.43(10)
K1-Co1-K2-C12	178.15(5)	N14-Co2-K2-C12	59.65(15)
N11-Co1-K2-C16	165.64(8)	N24-Co2-K2-C12	178.20(9)

K1-Co2-K2-C12	7.00(8)	C23-K1-K2-C52	-16.39(7)
N14-Co2-K2-C16	-126.66(13)	C65-K1-K2-C52	174.38(7)
N24-Co2-K2-C16	-8.11(6)	C35-K1-K2-C52	-133.75(7)
K1-Co2-K2-C16	-179.30(4)	C53-K1-K2-C52	30.47(8)
N14-Co2-K2-C32	-46.93(15)	C15-K1-K2-C52	-163.02(7)
N24-Co2-K2-C32	71.62(9)	C13-K1-K2-C52	7.12(7)
K1-Co2-K2-C32	-99.58(8)	C25-K1-K2-C52	-140.63(7)
N14-Co2-K2-C22	6.39(15)	C63-K1-K2-C52	27.58(7)
N24-Co2-K2-C22	124.94(8)	Co2-K1-K2-C52	-155.78(6)
K1-Co2-K2-C22	-46.26(7)	Co1-K1-K2-C52	19.64(6)
N14-Co2-K2-C56	-154.05(13)	C33-K1-K2-C62	-25.02(6)
N24-Co2-K2-C56	-35.50(5)	C55-K1-K2-C62	168.44(6)
K1-Co2-K2-C56	153.30(3)	C43-K1-K2-C62	-0.75(8)
N14-Co2-K2-Co1	56.50(12)	C45-K1-K2-C62	-160.99(8)
N24-Co2-K2-Co1	175.05(4)	C23-K1-K2-C62	-16.15(5)
K1-Co2-K2-Co1	3.860(12)	C65-K1-K2-C62	174.62(5)
N14-Co2-K2-K1	52.65(12)	C35-K1-K2-C62	-133.51(6)
N24-Co2-K2-K1	171.19(4)	C53-K1-K2-C62	30.70(6)
C33-K1-K2-C36	152.48(7)	C15-K1-K2-C62	-162.78(5)
C55-K1-K2-C36	-14.06(7)	C13-K1-K2-C62	7.36(5)
C43-K1-K2-C36	176.75(8)	C25-K1-K2-C62	-140.39(5)
C45-K1-K2-C36	16.51(9)	C63-K1-K2-C62	27.82(5)
C23-K1-K2-C36	161.35(6)	Co2-K1-K2-C62	-155.54(4)
C65-K1-K2-C36	-7.88(6)	Co1-K1-K2-C62	19.87(4)
C35-K1-K2-C36	43.99(7)	C33-K1-K2-C26	152.22(5)
C53-K1-K2-C36	-151.80(7)	C55-K1-K2-C26	-14.32(6)
C15-K1-K2-C36	14.72(6)	C43-K1-K2-C26	176.49(7)
C13-K1-K2-C36	-175.14(6)	C45-K1-K2-C26	16.25(8)
C25-K1-K2-C36	37.11(7)	C23-K1-K2-C26	161.09(5)
C63-K1-K2-C36	-154.68(6)	C65-K1-K2-C26	-8.14(5)
Co2-K1-K2-C36	21.96(5)	C35-K1-K2-C26	43.73(6)
Co1-K1-K2-C36	-162.62(6)	C53-K1-K2-C26	-152.06(6)
C33-K1-K2-C52	-25.26(8)	C15-K1-K2-C26	14.45(5)
C55-K1-K2-C52	168.20(7)	C13-K1-K2-C26	-175.40(5)
C43-K1-K2-C52	-0.99(9)	C25-K1-K2-C26	36.85(5)
C45-K1-K2-C52	-161.23(9)	C63-K1-K2-C26	-154.95(5)

Co2-K1-K2-C26	21.70(3)	C35-K1-K2-C12	-154.74(6)
Co1-K1-K2-C26	-162.89(4)	C53-K1-K2-C12	9.47(6)
C33-K1-K2-C46	114.59(8)	C15-K1-K2-C12	175.98(4)
C55-K1-K2-C46	-51.94(8)	C13-K1-K2-C12	-13.87(5)
C43-K1-K2-C46	138.87(9)	C25-K1-K2-C12	-161.62(5)
C45-K1-K2-C46	-21.37(10)	C63-K1-K2-C12	6.58(5)
C23-K1-K2-C46	123.47(7)	Co2-K1-K2-C12	-176.77(3)
C65-K1-K2-C46	-45.76(7)	Co1-K1-K2-C12	-1.36(3)
C35-K1-K2-C46	6.11(8)	C33-K1-K2-C16	131.02(5)
C53-K1-K2-C46	170.32(7)	C55-K1-K2-C16	-35.52(6)
C15-K1-K2-C46	-23.17(7)	C43-K1-K2-C16	155.29(7)
C13-K1-K2-C46	146.98(7)	C45-K1-K2-C16	-4.95(7)
C25-K1-K2-C46	-0.78(7)	C23-K1-K2-C16	139.89(4)
C63-K1-K2-C46	167.43(7)	C65-K1-K2-C16	-29.34(4)
Co2-K1-K2-C46	-15.92(6)	C35-K1-K2-C16	22.53(6)
Co1-K1-K2-C46	159.49(7)	C53-K1-K2-C16	-173.26(5)
C33-K1-K2-C42	-65.03(9)	C15-K1-K2-C16	-6.74(4)
C55-K1-K2-C42	128.43(9)	C13-K1-K2-C16	163.40(4)
C43-K1-K2-C42	-40.75(10)	C25-K1-K2-C16	15.65(5)
C45-K1-K2-C42	159.00(10)	C63-K1-K2-C16	-176.14(4)
C23-K1-K2-C42	-56.15(8)	Co2-K1-K2-C16	0.50(3)
C65-K1-K2-C42	134.62(8)	Co1-K1-K2-C16	175.92(3)
C35-K1-K2-C42	-173.52(8)	C33-K1-K2-C32	-81.60(6)
C53-K1-K2-C42	-9.30(9)	C55-K1-K2-C32	111.86(6)
C15-K1-K2-C42	157.21(8)	C43-K1-K2-C32	-57.33(8)
C13-K1-K2-C42	-32.64(8)	C45-K1-K2-C32	142.43(8)
C25-K1-K2-C42	179.60(8)	C23-K1-K2-C32	-72.73(6)
C63-K1-K2-C42	-12.19(8)	C65-K1-K2-C32	118.04(6)
Co2-K1-K2-C42	164.45(8)	C35-K1-K2-C32	169.91(6)
Co1-K1-K2-C42	-20.13(7)	C53-K1-K2-C32	-25.88(7)
C33-K1-K2-C12	-46.25(6)	C15-K1-K2-C32	140.64(5)
C55-K1-K2-C12	147.21(6)	C13-K1-K2-C32	-49.22(6)
C43-K1-K2-C12	-21.98(8)	C25-K1-K2-C32	163.03(6)
C45-K1-K2-C12	177.78(7)	C63-K1-K2-C32	-28.76(6)
C23-K1-K2-C12	-37.38(5)	Co2-K1-K2-C32	147.88(5)
C65-K1-K2-C12	153.39(5)	Co1-K1-K2-C32	-36.71(5)

C33-K1-K2-C22	-69.89(6)	C15-K1-K2-Co1	177.34(3)
C55-K1-K2-C22	123.57(6)	C13-K1-K2-Co1	-12.51(3)
C43-K1-K2-C22	-45.62(8)	C25-K1-K2-Co1	-160.27(4)
C45-K1-K2-C22	154.14(7)	C63-K1-K2-Co1	7.94(3)
C23-K1-K2-C22	-61.02(5)	Co2-K1-K2-Co1	-175.416(14)
C65-K1-K2-C22	129.75(5)	C33-K1-K2-Co2	130.52(5)
C35-K1-K2-C22	-178.38(6)	C55-K1-K2-Co2	-36.02(5)
C53-K1-K2-C22	-14.16(6)	C43-K1-K2-Co2	154.79(7)
C15-K1-K2-C22	152.35(5)	C45-K1-K2-Co2	-5.45(7)
C13-K1-K2-C22	-37.51(5)	C23-K1-K2-Co2	139.39(3)
C25-K1-K2-C22	174.74(5)	C65-K1-K2-Co2	-29.84(3)
C63-K1-K2-C22	-17.05(5)	C35-K1-K2-Co2	22.03(5)
Co2-K1-K2-C22	159.59(4)	C53-K1-K2-Co2	-173.76(5)
Co1-K1-K2-C22	-24.99(3)	C15-K1-K2-Co2	-7.24(3)
C33-K1-K2-C56	97.72(6)	C13-K1-K2-Co2	162.90(3)
C55-K1-K2-C56	-68.81(6)	C25-K1-K2-Co2	15.15(3)
C43-K1-K2-C56	122.00(8)	C63-K1-K2-Co2	-176.64(3)
C45-K1-K2-C56	-38.24(8)	Co1-K1-K2-Co2	175.416(14)
C23-K1-K2-C56	106.60(5)	N21-Co1-N11-C21	-6.49(15)
C65-K1-K2-C56	-62.63(5)	K2-Co1-N11-C21	-162.72(14)
C35-K1-K2-C56	-10.76(6)	K1-Co1-N11-C21	-139.85(15)
C53-K1-K2-C56	153.45(6)	N21-Co1-N11-C12	170.01(11)
C15-K1-K2-C56	-40.04(5)	K2-Co1-N11-C12	13.78(11)
C13-K1-K2-C56	130.11(5)	K1-Co1-N11-C12	36.7(3)
C25-K1-K2-C56	-17.65(5)	N11-Co1-N21-C41	3.74(15)
C63-K1-K2-C56	150.56(5)	K2-Co1-N21-C41	113.70(14)
Co2-K1-K2-C56	-32.80(4)	K1-Co1-N21-C41	173.22(13)
Co1-K1-K2-C56	142.62(4)	N11-Co1-N21-C13	-177.81(11)
C33-K1-K2-Co1	-44.90(4)	K2-Co1-N21-C13	-67.86(15)
C55-K1-K2-Co1	148.57(5)	K1-Co1-N21-C13	-8.34(10)
C43-K1-K2-Co1	-20.62(7)	N24-Co2-N14-C24	2.98(15)
C45-K1-K2-Co1	179.14(7)	K2-Co2-N14-C24	120.99(14)
C23-K1-K2-Co1	-36.02(3)	K1-Co2-N14-C24	170.91(14)
C65-K1-K2-Co1	154.75(3)	N24-Co2-N14-C15	-178.39(11)
C35-K1-K2-Co1	-153.38(5)	K2-Co2-N14-C15	-60.39(18)
C53-K1-K2-Co1	10.83(5)	K1-Co2-N14-C15	-10.47(10)

N14-Co2-N24-C44	-1.40(15)	C36-K2-C12-C62	-66.56(11)
K2-Co2-N24-C44	-163.50(13)	C52-K2-C12-C62	-32.23(10)
K1-Co2-N24-C44	-130.22(14)	C26-K2-C12-C62	-81.55(13)
N14-Co2-N24-C16	176.65(11)	C46-K2-C12-C62	-40.39(11)
K2-Co2-N24-C16	14.55(10)	C42-K2-C12-C62	-65.02(11)
K1-Co2-N24-C16	47.8(2)	C16-K2-C12-C62	-43.33(19)
C12-N11-C21-C31	-169.90(17)	C32-K2-C12-C62	-96.13(11)
Co1-N11-C21-C31	5.9(2)	C22-K2-C12-C62	-124.92(15)
C12-N11-C21-C11	13.7(3)	C56-K2-C12-C62	-17.09(12)
Co1-N11-C21-C11	-170.43(13)	Co1-K2-C12-C62	126.57(11)
C71-C11-C21-N11	-6.3(3)	Co2-K2-C12-C62	122.40(10)
C61-C11-C21-N11	114.2(2)	K1-K2-C12-C62	128.09(10)
C81-C11-C21-N11	-126.7(2)	C36-K2-C12-C22	58.36(11)
C71-C11-C21-C31	177.14(18)	C52-K2-C12-C22	92.69(11)
C61-C11-C21-C31	-62.3(2)	C62-K2-C12-C22	124.92(15)
C81-C11-C21-C31	56.7(2)	C26-K2-C12-C22	43.38(13)
N11-C21-C31-C41	-0.9(3)	C46-K2-C12-C22	84.53(11)
C11-C21-C31-C41	175.82(19)	C42-K2-C12-C22	59.90(10)
C13-N21-C41-C31	-178.60(16)	C16-K2-C12-C22	81.59(18)
Co1-N21-C41-C31	-0.5(2)	C32-K2-C12-C22	28.79(10)
C13-N21-C41-C51	-0.2(3)	C56-K2-C12-C22	107.84(10)
Co1-N21-C41-C51	177.95(12)	Co1-K2-C12-C22	-108.51(11)
C21-C31-C41-N21	-2.0(3)	Co2-K2-C12-C22	-112.67(10)
C21-C31-C41-C51	179.37(19)	K1-K2-C12-C22	-106.99(10)
N21-C41-C51-C111	1.1(3)	C36-K2-C12-N11	177.94(11)
C31-C41-C51-C111	179.61(17)	C52-K2-C12-N11	-147.73(15)
N21-C41-C51-C91	-118.56(19)	C62-K2-C12-N11	-115.50(17)
C31-C41-C51-C91	59.9(2)	C26-K2-C12-N11	162.95(10)
N21-C41-C51-C101	122.17(19)	C46-K2-C12-N11	-155.89(11)
C31-C41-C51-C101	-59.3(2)	C42-K2-C12-N11	179.48(14)
C21-N11-C12-C62	81.5(2)	C16-K2-C12-N11	-158.83(12)
Co1-N11-C12-C62	-94.85(15)	C32-K2-C12-N11	148.37(15)
C21-N11-C12-C22	-104.6(2)	C22-K2-C12-N11	119.58(17)
Co1-N11-C12-C22	79.06(16)	C56-K2-C12-N11	-132.58(11)
C21-N11-C12-K2	160.74(14)	Co1-K2-C12-N11	11.07(9)
Co1-N11-C12-K2	-15.65(12)	Co2-K2-C12-N11	6.91(17)

K1-K2-C12-N11	12.59(12)	C26-K2-C22-C72	91.30(14)
C62-C12-C22-C32	-0.5(2)	C46-K2-C22-C72	137.45(14)
N11-C12-C22-C32	-174.35(15)	C42-K2-C22-C72	144.03(17)
K2-C12-C22-C32	-63.57(15)	C12-K2-C22-C72	-118.29(18)
C62-C12-C22-C72	179.53(16)	C16-K2-C22-C72	98.03(15)
N11-C12-C22-C72	5.6(2)	C32-K2-C22-C72	115.8(2)
K2-C12-C22-C72	116.41(16)	C56-K2-C22-C72	152.75(13)
C62-C12-C22-K2	63.12(13)	Co1-K2-C22-C72	-63.78(13)
N11-C12-C22-K2	-110.78(14)	Co2-K2-C22-C72	-2.95(19)
C36-K2-C22-C32	-4.18(13)	K1-K2-C22-C72	-39.89(14)
C52-K2-C22-C32	61.05(12)	C12-C22-C32-C42	-1.5(3)
C62-K2-C22-C32	95.49(13)	C72-C22-C32-C42	178.53(17)
C26-K2-C22-C32	-24.51(14)	K2-C22-C32-C42	-63.10(17)
C46-K2-C22-C32	21.64(13)	C12-C22-C32-K2	61.61(14)
C42-K2-C22-C32	28.22(11)	C72-C22-C32-K2	-118.37(16)
C12-K2-C22-C32	125.90(17)	C36-K2-C32-C42	-56.28(12)
C16-K2-C22-C32	-17.78(16)	C52-K2-C32-C42	30.91(11)
C56-K2-C22-C32	36.94(14)	C62-K2-C32-C42	65.12(12)
Co1-K2-C22-C32	-179.59(13)	C26-K2-C32-C42	-72.84(12)
Co2-K2-C22-C32	-118.76(12)	C46-K2-C32-C42	-31.69(12)
K1-K2-C22-C32	-155.70(11)	C12-K2-C32-C42	98.33(14)
C36-K2-C22-C12	-130.08(10)	C16-K2-C32-C42	-63.66(13)
C52-K2-C22-C12	-64.85(10)	C22-K2-C32-C42	127.76(19)
C62-K2-C22-C12	-30.41(9)	C56-K2-C32-C42	-22.06(13)
C26-K2-C22-C12	-150.41(9)	Co1-K2-C32-C42	128.11(12)
C46-K2-C22-C12	-104.26(10)	Co2-K2-C32-C42	-122.64(12)
C42-K2-C22-C12	-97.68(12)	K1-K2-C32-C42	157.36(10)
C16-K2-C22-C12	-143.68(10)	C36-K2-C32-C22	175.96(12)
C32-K2-C22-C12	-125.90(17)	C52-K2-C32-C22	-96.85(13)
C56-K2-C22-C12	-88.96(11)	C62-K2-C32-C22	-62.64(12)
Co1-K2-C22-C12	54.51(9)	C26-K2-C32-C22	159.40(12)
Co2-K2-C22-C12	115.34(10)	C46-K2-C32-C22	-159.45(12)
K1-K2-C22-C12	78.40(10)	C42-K2-C32-C22	-127.76(19)
C36-K2-C22-C72	111.63(14)	C12-K2-C32-C22	-29.43(10)
C52-K2-C22-C72	176.86(16)	C16-K2-C32-C22	168.58(11)
C62-K2-C22-C72	-148.70(16)	C56-K2-C32-C22	-149.82(11)

Co1-K2-C32-C22	0.35(11)	C46-K2-C52-C42	79.06(11)
Co2-K2-C32-C22	109.60(12)	C12-K2-C52-C42	-92.87(13)
K1-K2-C32-C22	29.60(14)	C16-K2-C52-C42	83.17(12)
C22-C32-C42-C52	1.9(3)	C32-K2-C52-C42	-29.66(10)
K2-C32-C42-C52	-64.77(15)	C22-K2-C52-C42	-60.81(11)
C22-C32-C42-K2	66.62(17)	C56-K2-C52-C42	99.93(11)
C36-K2-C42-C52	-117.19(12)	Co1-K2-C52-C42	-108.03(11)
C62-K2-C42-C52	30.87(10)	Co2-K2-C52-C42	118.95(13)
C26-K2-C42-C52	-125.57(11)	K1-K2-C52-C42	-123.76(10)
C46-K2-C42-C52	-90.98(11)	C36-K2-C52-C62	-177.95(12)
C12-K2-C42-C52	64.22(11)	C26-K2-C52-C62	-177.02(11)
C16-K2-C42-C52	-108.51(11)	C46-K2-C52-C62	-156.67(13)
C32-K2-C42-C52	123.81(17)	C42-K2-C52-C62	124.27(17)
C22-K2-C42-C52	95.82(12)	C12-K2-C52-C62	31.39(10)
C56-K2-C42-C52	-77.22(11)	C16-K2-C52-C62	-152.57(11)
Co1-K2-C42-C52	72.60(11)	C32-K2-C52-C62	94.61(13)
Co2-K2-C42-C52	-124.41(11)	C22-K2-C52-C62	63.46(11)
K1-K2-C42-C52	88.78(13)	C56-K2-C52-C62	-135.80(12)
C36-K2-C42-C32	119.00(13)	Co1-K2-C52-C62	16.24(11)
C52-K2-C42-C32	-123.81(17)	Co2-K2-C52-C62	-116.78(12)
C62-K2-C42-C32	-92.94(13)	K1-K2-C52-C62	0.50(15)
C26-K2-C42-C32	110.62(12)	C42-C52-C62-C12	-1.6(3)
C46-K2-C42-C32	145.20(13)	K2-C52-C62-C12	-76.27(14)
C12-K2-C42-C32	-59.59(11)	C42-C52-C62-C102	175.38(16)
C16-K2-C42-C32	127.68(11)	K2-C52-C62-C102	100.74(14)
C22-K2-C42-C32	-27.99(11)	C42-C52-C62-K2	74.64(16)
C56-K2-C42-C32	158.96(12)	C22-C12-C62-C52	2.0(2)
Co1-K2-C42-C32	-51.21(12)	N11-C12-C62-C52	175.86(14)
Co2-K2-C42-C32	111.78(13)	K2-C12-C62-C52	71.92(14)
K1-K2-C42-C32	-35.03(16)	C22-C12-C62-C102	-174.96(15)
C32-C42-C52-C62	-0.3(3)	N11-C12-C62-C102	-1.1(2)
K2-C42-C52-C62	-71.32(15)	K2-C12-C62-C102	-104.99(15)
C32-C42-C52-K2	71.06(16)	C22-C12-C62-K2	-69.97(14)
C36-K2-C52-C42	57.78(11)	N11-C12-C62-K2	103.93(13)
C62-K2-C52-C42	-124.27(17)	C36-K2-C62-C52	2.14(13)
C26-K2-C52-C42	58.71(12)	C26-K2-C62-C52	3.92(14)

C46-K2-C62-C52	21.78(12)	C12-C22-C72-C92	-115.8(2)
C42-K2-C62-C52	-29.61(11)	K2-C22-C72-C92	-27.1(2)
C12-K2-C62-C52	-121.35(17)	C32-C22-C72-C82	-59.8(3)
C16-K2-C62-C52	38.99(15)	C12-C22-C72-C82	120.3(2)
C32-K2-C62-C52	-61.10(12)	K2-C22-C72-C82	-151.02(15)
C22-K2-C62-C52	-92.22(13)	C52-C62-C102-C112	45.4(2)
C56-K2-C62-C52	44.22(12)	C12-C62-C102-C112	-137.72(17)
Co1-K2-C62-C52	-161.79(12)	K2-C62-C102-C112	128.92(14)
Co2-K2-C62-C52	127.02(11)	C52-C62-C102-C122	-76.7(2)
K1-K2-C62-C52	-179.64(10)	C12-C62-C102-C122	100.2(2)
C36-K2-C62-C12	123.49(10)	K2-C62-C102-C122	6.9(2)
C52-K2-C62-C12	121.35(17)	C41-N21-C13-C23	-89.4(2)
C26-K2-C62-C12	125.26(10)	Co1-N21-C13-C23	92.19(15)
C46-K2-C62-C12	143.12(10)	C41-N21-C13-C63	96.8(2)
C42-K2-C62-C12	91.74(12)	Co1-N21-C13-C63	-81.61(15)
C16-K2-C62-C12	160.34(9)	C41-N21-C13-K1	-171.86(13)
C32-K2-C62-C12	60.24(10)	Co1-N21-C13-K1	9.74(12)
C22-K2-C62-C12	29.12(9)	C33-K1-C13-C23	31.52(10)
C56-K2-C62-C12	165.57(10)	C55-K1-C13-C23	89.59(11)
Co1-K2-C62-C12	-40.45(9)	C43-K1-C13-C23	64.99(10)
Co2-K2-C62-C12	-111.63(11)	C45-K1-C13-C23	64.04(11)
K1-K2-C62-C12	-58.30(11)	C65-K1-C13-C23	100.02(13)
C36-K2-C62-C102	-114.89(11)	C35-K1-C13-C23	36.56(11)
C52-K2-C62-C102	-117.03(17)	C53-K1-C13-C23	97.50(11)
C26-K2-C62-C102	-113.12(11)	C15-K1-C13-C23	32.8(2)
C46-K2-C62-C102	-95.25(11)	C25-K1-C13-C23	17.13(13)
C42-K2-C62-C102	-146.64(13)	C63-K1-C13-C23	126.46(14)
C12-K2-C62-C102	121.62(16)	Co2-K1-C13-C23	-85.12(10)
C16-K2-C62-C102	-78.04(12)	Co1-K1-C13-C23	-122.87(11)
C32-K2-C62-C102	-178.14(13)	K2-K1-C13-C23	-108.87(9)
C22-K2-C62-C102	150.75(13)	C33-K1-C13-C63	-94.94(11)
C56-K2-C62-C102	-72.81(11)	C55-K1-C13-C63	-36.87(12)
Co1-K2-C62-C102	81.17(10)	C43-K1-C13-C63	-61.47(10)
Co2-K2-C62-C102	9.99(16)	C45-K1-C13-C63	-62.42(11)
K1-K2-C62-C102	63.32(11)	C23-K1-C13-C63	-126.46(14)
C32-C22-C72-C92	64.1(2)	C65-K1-C13-C63	-26.44(15)

C35-K1-C13-C63	-89.90(10)	C13-K1-C23-C33	122.49(16)
C53-K1-C13-C63	-28.96(9)	C25-K1-C23-C33	-45.46(12)
C15-K1-C13-C63	-93.62(18)	C63-K1-C23-C33	93.87(12)
C25-K1-C13-C63	-109.33(11)	Co2-K1-C23-C33	-114.28(10)
Co2-K1-C13-C63	148.42(8)	Co1-K1-C23-C33	165.21(12)
Co1-K1-C13-C63	110.67(10)	K2-K1-C23-C33	-162.77(10)
K2-K1-C13-C63	124.67(9)	C33-K1-C23-C13	-122.49(16)
C33-K1-C13-N21	147.43(14)	C55-K1-C23-C13	-109.48(10)
C55-K1-C13-N21	-154.50(10)	C43-K1-C23-C13	-92.44(11)
C43-K1-C13-N21	-179.10(14)	C45-K1-C23-C13	-124.14(10)
C45-K1-C13-N21	179.95(11)	C65-K1-C23-C13	-125.13(10)
C23-K1-C13-N21	115.91(16)	C35-K1-C23-C13	-148.97(9)
C65-K1-C13-N21	-144.07(11)	C53-K1-C23-C13	-59.78(10)
C35-K1-C13-N21	152.47(10)	C15-K1-C23-C13	-166.22(9)
C53-K1-C13-N21	-146.59(14)	C25-K1-C23-C13	-167.95(9)
C15-K1-C13-N21	148.75(14)	C63-K1-C23-C13	-28.62(9)
C25-K1-C13-N21	133.04(11)	Co2-K1-C23-C13	123.23(9)
C63-K1-C13-N21	-117.63(16)	Co1-K1-C23-C13	42.72(8)
Co2-K1-C13-N21	30.79(14)	K2-K1-C23-C13	74.75(9)
Co1-K1-C13-N21	-6.96(9)	C33-K1-C23-C73	116.60(17)
K2-K1-C13-N21	7.03(11)	C55-K1-C23-C73	129.60(11)
C63-C13-C23-C33	-1.8(2)	C43-K1-C23-C73	146.64(14)
N21-C13-C23-C33	-175.57(15)	C45-K1-C23-C73	114.94(11)
K1-C13-C23-C33	-67.50(14)	C65-K1-C23-C73	113.95(12)
C63-C13-C23-C73	176.52(16)	C35-K1-C23-C73	90.11(12)
N21-C13-C23-C73	2.7(2)	C53-K1-C23-C73	179.30(14)
K1-C13-C23-C73	110.82(16)	C15-K1-C23-C73	72.86(13)
C63-C13-C23-K1	65.71(14)	C13-K1-C23-C73	-120.92(16)
N21-C13-C23-K1	-108.07(13)	C25-K1-C23-C73	71.13(12)
C55-K1-C23-C33	13.01(13)	C63-K1-C23-C73	-149.53(14)
C43-K1-C23-C33	30.05(10)	Co2-K1-C23-C73	2.31(14)
C45-K1-C23-C33	-1.65(12)	Co1-K1-C23-C73	-78.20(11)
C65-K1-C23-C33	-2.65(16)	K2-K1-C23-C73	-46.17(11)
C35-K1-C23-C33	-26.48(12)	C13-C23-C33-C43	1.3(3)
C53-K1-C23-C33	62.71(11)	C73-C23-C33-C43	-177.04(16)
C15-K1-C23-C33	-43.74(14)	K1-C23-C33-C43	-71.92(16)

C13-C23-C33-K1	73.21(14)	C53-K1-C43-C33	-122.59(16)
C73-C23-C33-K1	-105.13(15)	C15-K1-C43-C33	108.18(10)
C55-K1-C33-C43	-44.50(11)	C13-K1-C43-C33	-62.47(10)
C45-K1-C33-C43	-56.86(10)	C25-K1-C43-C33	89.22(11)
C23-K1-C33-C43	124.77(17)	C63-K1-C43-C33	-94.13(11)
C65-K1-C33-C43	-56.90(12)	Co2-K1-C43-C33	73.20(13)
C35-K1-C33-C43	-81.61(11)	Co1-K1-C43-C33	-68.02(10)
C53-K1-C33-C43	30.72(10)	K2-K1-C43-C33	-51.89(13)
C15-K1-C33-C43	-85.53(11)	C33-K1-C43-C53	122.59(16)
C13-K1-C33-C43	94.05(12)	C55-K1-C43-C53	-101.19(11)
C25-K1-C33-C43	-95.06(11)	C45-K1-C43-C53	-120.79(11)
C63-K1-C33-C43	62.19(10)	C23-K1-C43-C53	92.66(11)
Co2-K1-C33-C43	-141.15(9)	C65-K1-C43-C53	-104.65(10)
Co1-K1-C33-C43	111.85(10)	C35-K1-C43-C53	-144.36(11)
K2-K1-C33-C43	145.71(9)	C15-K1-C43-C53	-129.23(10)
C55-K1-C33-C23	-169.27(11)	C13-K1-C43-C53	60.12(10)
C43-K1-C33-C23	-124.77(17)	C25-K1-C43-C53	-148.18(10)
C45-K1-C33-C23	178.38(11)	C63-K1-C43-C53	28.46(9)
C65-K1-C33-C23	178.34(10)	Co2-K1-C43-C53	-164.21(8)
C35-K1-C33-C23	153.62(11)	Co1-K1-C43-C53	54.58(10)
C53-K1-C33-C23	-94.04(12)	K2-K1-C43-C53	70.71(13)
C15-K1-C33-C23	149.71(10)	C33-C43-C53-C63	-1.8(2)
C13-K1-C33-C23	-30.72(10)	K1-C43-C53-C63	-70.49(15)
C25-K1-C33-C23	140.17(11)	C33-C43-C53-K1	68.66(14)
C63-K1-C33-C23	-62.57(10)	C33-K1-C53-C63	94.76(12)
Co2-K1-C33-C23	94.08(11)	C55-K1-C53-C63	-156.72(11)
Co1-K1-C33-C23	-12.92(10)	C43-K1-C53-C63	126.21(16)
K2-K1-C33-C23	20.95(12)	C45-K1-C53-C63	179.52(11)
C23-C33-C43-C53	0.5(3)	C23-K1-C53-C63	61.50(10)
K1-C33-C43-C53	-72.45(14)	C65-K1-C53-C63	-149.50(10)
C23-C33-C43-K1	72.94(16)	C35-K1-C53-C63	161.07(11)
C55-K1-C43-C33	136.22(11)	C15-K1-C53-C63	-169.42(10)
C45-K1-C43-C33	116.62(11)	C13-K1-C53-C63	29.32(9)
C23-K1-C43-C33	-29.93(10)	C25-K1-C53-C63	163.25(10)
C65-K1-C43-C33	132.75(10)	Co2-K1-C53-C63	-137.2(3)
C35-K1-C43-C33	93.05(11)	Co1-K1-C53-C63	1.74(10)

K2-K1-C53-C63	-6.88(13)	C25-K1-C63-C53	-24.17(14)
C33-K1-C53-C43	-31.45(10)	Co2-K1-C63-C53	166.43(10)
C55-K1-C53-C43	77.07(11)	Co1-K1-C63-C53	-177.95(12)
C45-K1-C53-C43	53.31(11)	K2-K1-C63-C53	174.58(10)
C23-K1-C53-C43	-64.71(11)	C33-K1-C63-C13	62.70(10)
C65-K1-C53-C43	84.30(11)	C55-K1-C63-C13	150.77(9)
C35-K1-C53-C43	34.86(11)	C43-K1-C63-C13	96.29(11)
C15-K1-C53-C43	64.37(12)	C45-K1-C63-C13	125.42(10)
C13-K1-C53-C43	-96.89(12)	C23-K1-C63-C13	29.23(9)
C25-K1-C53-C43	37.04(12)	C65-K1-C63-C13	164.94(9)
C63-K1-C53-C43	-126.21(16)	C35-K1-C63-C13	104.29(10)
Co2-K1-C53-C43	96.6(3)	C53-K1-C63-C13	125.91(16)
Co1-K1-C53-C43	-124.47(10)	C15-K1-C63-C13	143.73(10)
K2-K1-C53-C43	-133.09(9)	C25-K1-C63-C13	101.74(11)
C43-C53-C63-C13	1.3(2)	Co2-K1-C63-C13	-67.66(15)
K1-C53-C63-C13	-64.09(14)	Co1-K1-C63-C13	-52.04(9)
C43-C53-C63-C103	-178.54(15)	K2-K1-C63-C13	-59.51(10)
K1-C53-C63-C103	116.06(14)	C33-K1-C63-C103	-178.75(14)
C43-C53-C63-K1	65.40(15)	C55-K1-C63-C103	-90.68(12)
C23-C13-C63-C53	0.5(2)	C43-K1-C63-C103	-145.16(15)
N21-C13-C63-C53	174.37(14)	C45-K1-C63-C103	-116.03(12)
K1-C13-C63-C53	62.29(14)	C23-K1-C63-C103	147.78(14)
C23-C13-C63-C103	-179.62(15)	C65-K1-C63-C103	-76.51(13)
N21-C13-C63-C103	-5.8(2)	C35-K1-C63-C103	-137.16(12)
K1-C13-C63-C103	-117.86(14)	C53-K1-C63-C103	-115.54(17)
C23-C13-C63-K1	-61.76(13)	C15-K1-C63-C103	-97.72(14)
N21-C13-C63-K1	112.08(13)	C13-K1-C63-C103	118.55(16)
C33-K1-C63-C53	-63.21(11)	C25-K1-C63-C103	-139.71(12)
C55-K1-C63-C53	24.86(12)	Co2-K1-C63-C103	50.89(18)
C43-K1-C63-C53	-29.62(10)	Co1-K1-C63-C103	66.51(11)
C45-K1-C63-C53	-0.49(12)	K2-K1-C63-C103	59.04(12)
C23-K1-C63-C53	-96.68(12)	C33-C23-C73-C83	-48.4(2)
C65-K1-C63-C53	39.03(13)	C13-C23-C73-C83	133.31(19)
C35-K1-C63-C53	-21.62(12)	K1-C23-C73-C83	-131.14(16)
C15-K1-C63-C53	17.83(16)	C33-C23-C73-C93	73.4(2)
C13-K1-C63-C53	-125.91(16)	C13-C23-C73-C93	-104.9(2)

K1-C23-C73-C93	-9.37(19)	Co2-N14-C15-K1	12.10(12)
C53-C63-C103-C113	55.7(2)	C33-K1-C15-C65	102.90(10)
C13-C63-C103-C113	-124.14(17)	C55-K1-C15-C65	31.37(9)
K1-C63-C103-C113	143.25(13)	C43-K1-C15-C65	74.86(10)
C53-C63-C103-C123	-68.5(2)	C45-K1-C15-C65	64.64(10)
C13-C63-C103-C123	111.65(18)	C23-K1-C15-C65	122.83(10)
K1-C63-C103-C123	19.04(19)	C35-K1-C15-C65	97.15(11)
C15-N14-C24-C34	177.86(16)	C53-K1-C15-C65	50.27(11)
Co2-N14-C24-C34	-3.8(2)	C13-K1-C15-C65	101.85(17)
C15-N14-C24-C14	-3.7(3)	C25-K1-C15-C65	126.60(14)
Co2-N14-C24-C14	174.63(12)	C63-K1-C15-C65	41.14(14)
C74-C14-C24-N14	-1.0(3)	Co2-K1-C15-C65	-124.81(11)
C64-C14-C24-N14	-120.44(19)	Co1-K1-C15-C65	-112.56(9)
C84-C14-C24-N14	120.49(18)	K2-K1-C15-C65	-116.63(9)
C74-C14-C24-C34	177.46(16)	C33-K1-C15-C25	-23.69(11)
C64-C14-C24-C34	58.1(2)	C55-K1-C15-C25	-95.23(11)
C84-C14-C24-C34	-61.01(19)	C43-K1-C15-C25	-51.73(11)
N14-C24-C34-C44	2.7(3)	C45-K1-C15-C25	-61.95(10)
C14-C24-C34-C44	-175.86(18)	C23-K1-C15-C25	-3.76(13)
C16-N24-C44-C34	-176.91(16)	C65-K1-C15-C25	-126.60(14)
Co2-N24-C44-C34	0.7(2)	C35-K1-C15-C25	-29.45(9)
C16-N24-C44-C54	5.1(3)	C53-K1-C15-C25	-76.33(11)
Co2-N24-C44-C54	-177.23(12)	C13-K1-C15-C25	-24.7(2)
C24-C34-C44-N24	-1.1(3)	C63-K1-C15-C25	-85.46(13)
C24-C34-C44-C54	177.07(18)	Co2-K1-C15-C25	108.59(10)
N24-C44-C54-C104	1.4(3)	Co1-K1-C15-C25	120.85(9)
C34-C44-C54-C104	-176.71(16)	K2-K1-C15-C25	116.77(9)
N24-C44-C54-C94	121.34(19)	C33-K1-C15-N14	-140.91(11)
C34-C44-C54-C94	-56.7(2)	C55-K1-C15-N14	147.56(14)
N24-C44-C54-C114	-119.75(18)	C43-K1-C15-N14	-168.94(11)
C34-C44-C54-C114	62.2(2)	C45-K1-C15-N14	-179.16(14)
C24-N14-C15-C65	-85.6(2)	C23-K1-C15-N14	-120.98(11)
Co2-N14-C15-C65	95.84(15)	C65-K1-C15-N14	116.19(16)
C24-N14-C15-C25	101.0(2)	C35-K1-C15-N14	-146.66(14)
Co2-N14-C15-C25	-77.58(16)	C53-K1-C15-N14	166.46(10)
C24-N14-C15-K1	-169.30(13)	C13-K1-C15-N14	-141.96(14)

C25-K1-C15-N14	-117.21(16)	Co2-K1-C25-C15	-53.61(9)
C63-K1-C15-N14	157.33(10)	Co1-K1-C25-C15	-103.94(11)
Co2-K1-C15-N14	-8.62(9)	K2-K1-C25-C15	-68.12(10)
Co1-K1-C15-N14	3.63(16)	C33-K1-C25-C75	-80.96(13)
K2-K1-C15-N14	-0.44(11)	C55-K1-C25-C75	-178.37(15)
C65-C15-C25-C35	1.1(2)	C43-K1-C25-C75	-106.31(13)
N14-C15-C25-C35	174.54(15)	C45-K1-C25-C75	-145.16(15)
K1-C15-C25-C35	64.00(14)	C23-K1-C25-C75	-63.26(13)
C65-C15-C25-C75	-178.58(16)	C65-K1-C25-C75	148.36(15)
N14-C15-C25-C75	-5.2(2)	C35-K1-C25-C75	-115.61(18)
K1-C15-C25-C75	-115.70(16)	C53-K1-C25-C75	-121.00(12)
C65-C15-C25-K1	-62.88(14)	C15-K1-C25-C75	119.39(17)
N14-C15-C25-K1	110.54(13)	C13-K1-C25-C75	-71.11(14)
C33-K1-C25-C35	34.65(12)	C63-K1-C25-C75	-110.05(13)
C55-K1-C25-C35	-62.76(11)	Co2-K1-C25-C75	65.77(12)
C43-K1-C25-C35	9.30(12)	Co1-K1-C25-C75	15.45(17)
C45-K1-C25-C35	-29.55(11)	K2-K1-C25-C75	51.27(13)
C23-K1-C25-C35	52.35(12)	C15-C25-C35-C45	0.0(3)
C65-K1-C25-C35	-96.03(12)	C75-C25-C35-C45	179.72(17)
C53-K1-C25-C35	-5.39(13)	K1-C25-C35-C45	65.74(16)
C15-K1-C25-C35	-125.00(16)	C15-C25-C35-K1	-65.73(14)
C13-K1-C25-C35	44.50(14)	C75-C25-C35-K1	113.98(15)
C63-K1-C25-C35	5.56(15)	C33-K1-C35-C45	88.85(11)
Co2-K1-C25-C35	-178.62(12)	C55-K1-C35-C45	-30.93(10)
Co1-K1-C25-C35	131.06(10)	C43-K1-C35-C45	63.40(11)
K2-K1-C25-C35	166.88(10)	C23-K1-C35-C45	99.88(11)
C33-K1-C25-C15	159.65(10)	C65-K1-C35-C45	-64.06(11)
C55-K1-C25-C15	62.24(10)	C53-K1-C35-C45	49.33(11)
C43-K1-C25-C15	134.30(10)	C15-K1-C35-C45	-96.15(12)
C45-K1-C25-C15	95.45(11)	C13-K1-C35-C45	85.37(11)
C23-K1-C25-C15	177.36(9)	C25-K1-C35-C45	-126.00(17)
C65-K1-C25-C15	28.97(9)	C63-K1-C35-C45	57.85(12)
C35-K1-C25-C15	125.00(16)	Co2-K1-C35-C45	-124.83(11)
C53-K1-C25-C15	119.62(10)	Co1-K1-C35-C45	129.96(11)
C13-K1-C25-C15	169.50(9)	K2-K1-C35-C45	-142.52(9)
C63-K1-C25-C15	130.56(10)	C33-K1-C35-C25	-145.15(12)

C55-K1-C35-C25	95.07(12)	C25-K1-C45-C35	28.76(10)
C43-K1-C35-C25	-170.60(12)	C63-K1-C45-C35	-130.12(11)
C45-K1-C35-C25	126.00(17)	Co2-K1-C45-C35	54.17(11)
C23-K1-C35-C25	-134.12(11)	Co1-K1-C45-C35	-123.57(12)
C65-K1-C35-C25	61.94(11)	K2-K1-C45-C35	58.52(14)
C53-K1-C35-C25	175.33(11)	C35-C45-C55-C65	0.5(3)
C15-K1-C35-C25	29.85(10)	K1-C45-C55-C65	72.41(15)
C13-K1-C35-C25	-148.63(10)	C35-C45-C55-K1	-71.92(15)
C63-K1-C35-C25	-176.15(10)	C33-K1-C55-C45	-30.14(11)
Co2-K1-C35-C25	1.17(10)	C43-K1-C55-C45	-47.51(10)
Co1-K1-C35-C25	-104.04(13)	C23-K1-C55-C45	-35.69(12)
K2-K1-C35-C25	-16.52(13)	C65-K1-C55-C45	124.61(16)
C25-C35-C45-C55	-0.8(3)	C35-K1-C55-C45	30.34(10)
K1-C35-C45-C55	69.08(15)	C53-K1-C55-C45	-71.49(11)
C25-C35-C45-K1	-69.89(16)	C15-K1-C55-C45	94.05(12)
C33-K1-C45-C55	150.00(11)	C13-K1-C55-C45	-66.21(12)
C43-K1-C45-C55	127.40(11)	C25-K1-C55-C45	61.98(10)
C23-K1-C45-C55	150.71(10)	C63-K1-C55-C45	-81.16(11)
C65-K1-C45-C55	-30.05(9)	Co2-K1-C55-C45	110.70(10)
C35-K1-C45-C55	-123.39(16)	Co1-K1-C55-C45	-133.33(10)
C53-K1-C45-C55	106.29(11)	K2-K1-C55-C45	138.78(9)
C15-K1-C45-C55	-62.54(10)	C33-K1-C55-C65	-154.75(10)
C13-K1-C45-C55	128.19(10)	C43-K1-C55-C65	-172.12(11)
C25-K1-C45-C55	-94.63(12)	C45-K1-C55-C65	-124.61(16)
C63-K1-C45-C55	106.48(10)	C23-K1-C55-C65	-160.30(10)
Co2-K1-C45-C55	-69.22(10)	C35-K1-C55-C65	-94.28(12)
Co1-K1-C45-C55	113.03(13)	C53-K1-C55-C65	163.90(11)
K2-K1-C45-C55	-64.87(13)	C15-K1-C55-C65	-30.56(9)
C33-K1-C45-C35	-86.61(11)	C13-K1-C55-C65	169.18(9)
C55-K1-C45-C35	123.39(16)	C25-K1-C55-C65	-62.63(10)
C43-K1-C45-C35	-109.20(12)	C63-K1-C55-C65	154.23(10)
C23-K1-C45-C35	-85.90(11)	Co2-K1-C55-C65	-13.91(10)
C65-K1-C45-C35	93.34(12)	Co1-K1-C55-C65	102.06(11)
C53-K1-C45-C35	-130.32(11)	K2-K1-C55-C65	14.17(12)
C15-K1-C45-C35	60.85(11)	C45-C55-C65-C15	0.6(2)
C13-K1-C45-C35	-108.42(11)	K1-C55-C65-C15	71.70(14)

C45-C55-C65-C105	-177.84(16)	K2-K1-C65-C15	68.31(10)
K1-C55-C65-C105	-106.78(14)	C33-K1-C65-C105	145.88(10)
C45-C55-C65-K1	-71.06(15)	C55-K1-C65-C105	115.79(16)
C25-C15-C65-C55	-1.4(2)	C43-K1-C65-C105	124.02(11)
N14-C15-C65-C55	-174.80(14)	C45-K1-C65-C105	145.82(13)
K1-C15-C65-C55	-66.96(14)	C23-K1-C65-C105	147.22(11)
C25-C15-C65-C105	177.01(15)	C35-K1-C65-C105	178.32(13)
N14-C15-C65-C105	3.6(2)	C53-K1-C65-C105	98.36(11)
K1-C15-C65-C105	111.48(15)	C15-K1-C65-C105	-121.47(15)
C25-C15-C65-K1	65.53(14)	C13-K1-C65-C105	96.54(14)
N14-C15-C65-K1	-107.84(13)	C25-K1-C65-C105	-150.21(13)
C33-K1-C65-C55	30.08(12)	C63-K1-C65-C105	82.59(12)
C43-K1-C65-C55	8.23(11)	Co2-K1-C65-C105	-80.05(10)
C45-K1-C65-C55	30.03(10)	Co1-K1-C65-C105	-11.44(15)
C23-K1-C65-C55	31.42(15)	K2-K1-C65-C105	-53.16(11)
C35-K1-C65-C55	62.52(11)	C35-C25-C75-C85	64.3(2)
C53-K1-C65-C55	-17.43(12)	C15-C25-C75-C85	-116.05(19)
C15-K1-C65-C55	122.74(15)	K1-C25-C75-C85	151.51(14)
C13-K1-C65-C55	-19.25(16)	C35-C25-C75-C95	-59.2(2)
C25-K1-C65-C55	94.00(11)	C15-C25-C75-C95	120.53(19)
C63-K1-C65-C55	-33.21(12)	K1-C25-C75-C95	28.1(2)
Co2-K1-C65-C55	164.15(11)	C55-C65-C105-C125	-52.7(2)
Co1-K1-C65-C55	-127.24(10)	C15-C65-C105-C125	128.84(17)
K2-K1-C65-C55	-168.96(10)	K1-C65-C105-C125	-136.21(13)
C33-K1-C65-C15	-92.65(10)	C55-C65-C105-C115	70.9(2)
C55-K1-C65-C15	-122.74(15)	C15-C65-C105-C115	-107.50(18)
C43-K1-C65-C15	-114.51(10)	K1-C65-C105-C115	-12.55(17)
C45-K1-C65-C15	-92.71(11)	C44-N24-C16-C66	-101.9(2)
C23-K1-C65-C15	-91.32(12)	Co2-N24-C16-C66	80.12(15)
C35-K1-C65-C15	-60.21(10)	C44-N24-C16-C26	84.6(2)
C53-K1-C65-C15	-140.17(9)	Co2-N24-C16-C26	-93.40(14)
C13-K1-C65-C15	-141.99(11)	C44-N24-C16-K2	161.43(13)
C25-K1-C65-C15	-28.74(9)	Co2-N24-C16-K2	-16.56(11)
C63-K1-C65-C15	-155.94(9)	C36-K2-C16-C66	92.33(11)
Co2-K1-C65-C15	41.42(8)	C52-K2-C16-C66	53.81(11)
Co1-K1-C65-C15	110.03(10)	C62-K2-C16-C66	35.92(12)

C26-K2-C16-C66	125.15(14)	N24-C16-C26-C36	174.95(14)
C46-K2-C16-C66	58.88(10)	K2-C16-C26-C36	71.19(13)
C42-K2-C16-C66	80.28(10)	C66-C16-C26-C76	-176.75(14)
C12-K2-C16-C66	62.47(18)	N24-C16-C26-C76	-3.2(2)
C32-K2-C16-C66	103.08(10)	K2-C16-C26-C76	-106.98(14)
C22-K2-C16-C66	111.62(11)	C66-C16-C26-K2	-69.77(14)
C56-K2-C16-C66	28.03(9)	N24-C16-C26-K2	103.76(13)
Co1-K2-C16-C66	-102.03(10)	C52-K2-C26-C36	-2.14(12)
Co2-K2-C16-C66	-108.43(10)	C62-K2-C26-C36	-3.91(13)
K1-K2-C16-C66	-109.00(9)	C46-K2-C26-C36	-30.11(10)
C36-K2-C16-C26	-32.82(9)	C42-K2-C26-C36	18.63(11)
C52-K2-C16-C26	-71.34(11)	C12-K2-C26-C36	31.20(14)
C62-K2-C16-C26	-89.23(11)	C16-K2-C26-C36	-120.70(15)
C46-K2-C16-C26	-66.28(10)	C32-K2-C26-C36	41.07(11)
C42-K2-C16-C26	-44.87(11)	C22-K2-C26-C36	50.73(12)
C12-K2-C16-C26	-62.69(18)	C56-K2-C26-C36	-61.48(11)
C32-K2-C16-C26	-22.07(11)	Co1-K2-C26-C36	137.64(10)
C22-K2-C16-C26	-13.54(14)	Co2-K2-C26-C36	-160.86(11)
C56-K2-C16-C26	-97.12(11)	K1-K2-C26-C36	179.58(10)
Co1-K2-C16-C26	132.81(9)	C36-K2-C26-C16	120.70(15)
Co2-K2-C16-C26	126.41(11)	C52-K2-C26-C16	118.56(10)
K1-K2-C16-C26	125.85(9)	C62-K2-C26-C16	116.79(10)
C36-K2-C16-N24	-147.46(14)	C46-K2-C26-C16	90.59(11)
C52-K2-C16-N24	174.02(10)	C42-K2-C26-C16	139.32(10)
C62-K2-C16-N24	156.13(10)	C12-K2-C26-C16	151.89(9)
C26-K2-C16-N24	-114.63(16)	C32-K2-C26-C16	161.76(9)
C46-K2-C16-N24	179.09(13)	C22-K2-C26-C16	171.43(9)
C42-K2-C16-N24	-159.50(10)	C56-K2-C26-C16	59.22(9)
C12-K2-C16-N24	-177.32(12)	Co1-K2-C26-C16	-101.67(12)
C32-K2-C16-N24	-136.70(10)	Co2-K2-C26-C16	-40.16(8)
C22-K2-C16-N24	-128.17(11)	K1-K2-C26-C16	-59.72(10)
C56-K2-C16-N24	148.24(14)	C36-K2-C26-C76	-117.55(16)
Co1-K2-C16-N24	18.18(15)	C52-K2-C26-C76	-119.69(10)
Co2-K2-C16-N24	11.78(8)	C62-K2-C26-C76	-121.46(10)
K1-K2-C16-N24	11.22(11)	C46-K2-C26-C76	-147.66(13)
C66-C16-C26-C36	1.4(2)	C42-K2-C26-C76	-98.93(10)

C12-K2-C26-C76	-86.36(12)	K1-K2-C36-C26	-0.57(13)
C16-K2-C26-C76	121.75(15)	C26-C36-C46-C56	0.2(3)
C32-K2-C26-C76	-76.49(11)	K2-C36-C46-C56	74.43(15)
C22-K2-C26-C76	-66.82(11)	C26-C36-C46-K2	-74.24(15)
C56-K2-C26-C76	-179.03(12)	C36-K2-C46-C56	-122.73(15)
Co1-K2-C26-C76	20.09(16)	C52-K2-C46-C56	116.77(11)
Co2-K2-C26-C76	81.59(10)	C62-K2-C46-C56	106.97(11)
K1-K2-C26-C76	62.03(10)	C26-K2-C46-C56	-91.62(11)
C16-C26-C36-C46	-1.2(2)	C42-K2-C46-C56	142.98(12)
C76-C26-C36-C46	176.99(15)	C12-K2-C46-C56	122.75(10)
K2-C26-C36-C46	77.04(15)	C16-K2-C46-C56	-58.47(10)
C16-C26-C36-K2	-78.25(13)	C32-K2-C46-C56	156.13(11)
C76-C26-C36-K2	99.95(13)	C22-K2-C46-C56	147.73(10)
C52-K2-C36-C46	54.32(10)	Co1-K2-C46-C56	99.08(12)
C62-K2-C36-C46	53.39(11)	Co2-K2-C46-C56	-49.51(10)
C26-K2-C36-C46	-123.64(16)	K1-K2-C46-C56	-36.80(14)
C42-K2-C36-C46	76.06(11)	C52-K2-C46-C36	-120.50(11)
C12-K2-C36-C46	77.30(11)	C62-K2-C46-C36	-130.30(10)
C16-K2-C36-C46	-92.20(12)	C26-K2-C46-C36	31.11(9)
C32-K2-C36-C46	96.59(11)	C42-K2-C46-C36	-94.29(11)
C22-K2-C36-C46	98.25(11)	C12-K2-C46-C36	-114.52(10)
C56-K2-C36-C46	-29.84(9)	C16-K2-C46-C36	64.26(10)
Co1-K2-C36-C46	111.62(14)	C32-K2-C46-C36	-81.14(11)
Co2-K2-C36-C46	-106.77(10)	C22-K2-C46-C36	-89.53(11)
K1-K2-C36-C46	-124.21(9)	C56-K2-C46-C36	122.73(15)
C52-K2-C36-C26	177.96(11)	Co1-K2-C46-C36	-138.19(10)
C62-K2-C36-C26	177.03(10)	Co2-K2-C46-C36	73.22(10)
C46-K2-C36-C26	123.64(16)	K1-K2-C46-C36	85.93(12)
C42-K2-C36-C26	-160.30(12)	C36-C46-C56-C66	0.6(3)
C12-K2-C36-C26	-159.06(10)	K2-C46-C56-C66	66.12(16)
C16-K2-C36-C26	31.44(9)	C36-C46-C56-K2	-65.49(14)
C32-K2-C36-C26	-139.77(11)	C36-K2-C56-C46	31.87(10)
C22-K2-C36-C26	-138.11(10)	C52-K2-C56-C46	-57.79(11)
C56-K2-C36-C26	93.81(12)	C62-K2-C56-C46	-75.44(11)
Co1-K2-C36-C26	-124.74(12)	C26-K2-C56-C46	66.49(11)
Co2-K2-C36-C26	16.87(10)	C42-K2-C56-C46	-33.70(11)

C12-K2-C56-C46	-68.27(11)
C16-K2-C56-C46	99.43(12)
C32-K2-C56-C46	-25.07(11)
C22-K2-C56-C46	-39.50(12)
Co1-K2-C56-C46	-126.92(10)
Co2-K2-C56-C46	129.26(10)
K1-K2-C56-C46	155.49(9)
C36-K2-C56-C66	-96.26(12)
C52-K2-C56-C66	174.08(11)
C62-K2-C56-C66	156.43(11)
C26-K2-C56-C66	-61.64(10)
C46-K2-C56-C66	-128.14(16)
C42-K2-C56-C66	-161.83(11)
C12-K2-C56-C66	163.60(10)
C16-K2-C56-C66	-28.71(9)
C32-K2-C56-C66	-153.21(10)
C22-K2-C56-C66	-167.64(10)
Co1-K2-C56-C66	104.95(11)
Co2-K2-C56-C66	1.13(10)
K1-K2-C56-C66	27.36(12)
C46-C56-C66-C16	-0.4(2)
K2-C56-C66-C16	59.97(14)
C46-C56-C66-C106	179.33(16)
K2-C56-C66-C106	-120.32(15)
C26-C16-C66-C56	-0.7(2)
N24-C16-C66-C56	-174.18(14)
K2-C16-C66-C56	-61.77(14)
C26-C16-C66-C106	179.64(15)
N24-C16-C66-C106	6.1(2)
K2-C16-C66-C106	118.53(15)
C36-C26-C76-C96	-79.70(19)
C16-C26-C76-C96	98.45(18)
K2-C26-C76-C96	1.86(16)
C36-C26-C76-C86	43.3(2)
C16-C26-C76-C86	-138.52(16)
K2-C26-C76-C86	124.90(13)
C56-C66-C106-C126	-56.2(2)
C16-C66-C106-C126	123.48(19)
C56-C66-C106-C116	67.2(2)
C16-C66-C106-C116	-113.07(19)
C17-C27-C37-C47	-174.4(2)
C27-C37-C47-C57	175.6(2)
C38#1-C18-C28-C38	-0.4(4)
C18-C28-C38-C18#1	0.4(4)

REFERENCE NUMBER: holkd21

CRYSTAL STRUCTURE REPORT

$C_{41}\ H_{64}\ Co\ N_2$

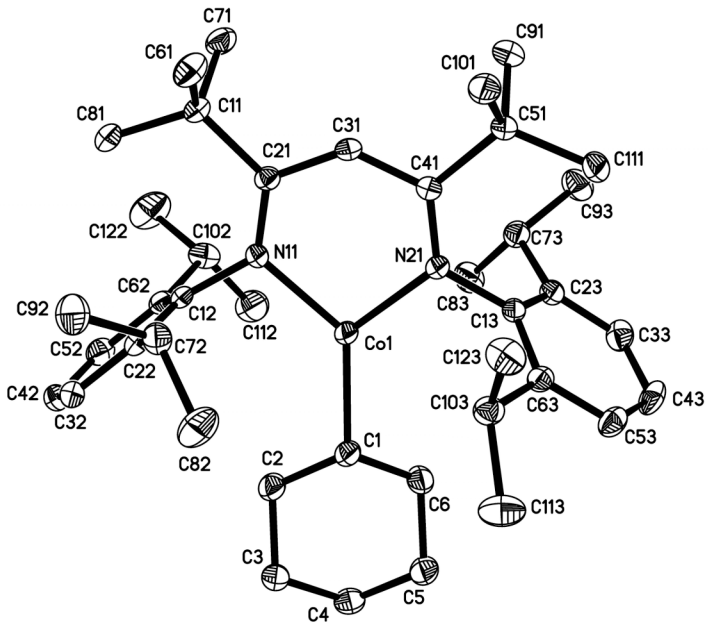
or

LCo(cyclohexyl)

Report prepared for:

K. Ding, Prof. P. Holland

December 19, 2008



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Data collection

A crystal (0.22 x 0.16 x 0.08 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART APEX II CCD Platform diffractometer for a data collection at 100.0(1) K.[1] A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 60 seconds and a detector distance of 3.97 cm. A randomly oriented region of reciprocal space was surveyed: four major sections of frames were collected with 0.50º steps in ω at four different ϕ settings and a detector position of -38º in 2θ. The intensity data were corrected for absorption.[2] Final cell constants were calculated from the xyz centroids of 3882 strong reflections from the actual data collection after integration.[3] See Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97[4] and refined using SHELXL-97.[5] The space group $P2_1/n$ was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0537$ (F^2, $I > 2\sigma(I)$) and $wR2 = 0.1310$ (F^2, all data).

Structure description

The structure is the one suggested with all atoms in general positions.

Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility, B51 Hutchison Hall, Department of Chemistry, University of Rochester. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel and the X-ray Crystallographic Facility of the Department of Chemistry at the University of Rochester.

[1] *APEX2*, version 2008.3-0; Bruker AXS: Madison, WI, 2008.

[2] Sheldrick, G. M. *SADABS*, version 2008/1; University of Göttingen: Göttingen, Germany, 2008.

[3] *SAINT*, version 7.53A; Bruker AXS: Madison, WI, 2007.

[4] Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G. L.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *SIR97: A new program for solving and refining crystal structures*; Istituto di Cristallografia, CNR: Bari, Italy, 1999.

[5] Sheldrick, G. M. *Acta. Cryst.* **2008**, *A64*, 112-122.

Some equations of interest:

$$R_{int} = \Sigma\, |F_o^2 - < F_o^2 >| \,/\, \Sigma |F_o^2|$$

$$R1 = \Sigma ||F_o| - |F_c|| \,/\, \Sigma |F_o|$$

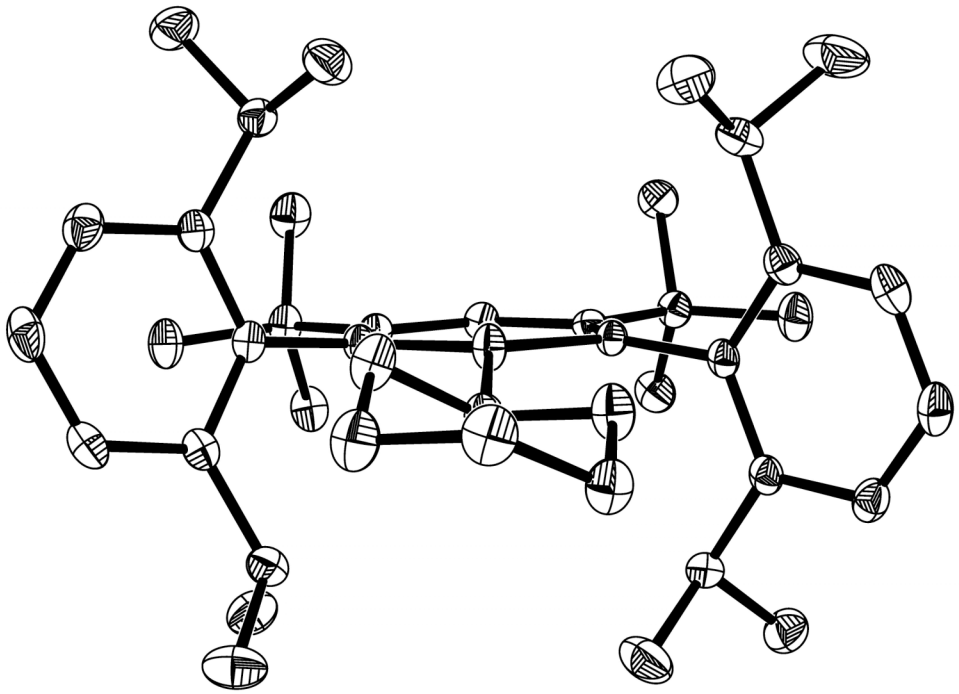
$$wR2 = [\Sigma [w(F_o^2 - F_c^2)^2] \,/\, \Sigma\, [w(F_o^2)^2]]^{1/2}$$

where $w = 1 \,/\, [\sigma^2 (F_o^2) + (aP)^2 + bP]$ and

$$P = 1/3 \text{ max } (0, F_o^2) + 2/3\, F_c^2$$

$$\text{GOF} = S = [\Sigma [w(F_o^2 - F_c^2)^2] \,/\, (m-n)]^{1/2}$$

where m = number of reflections and n = number of parameters



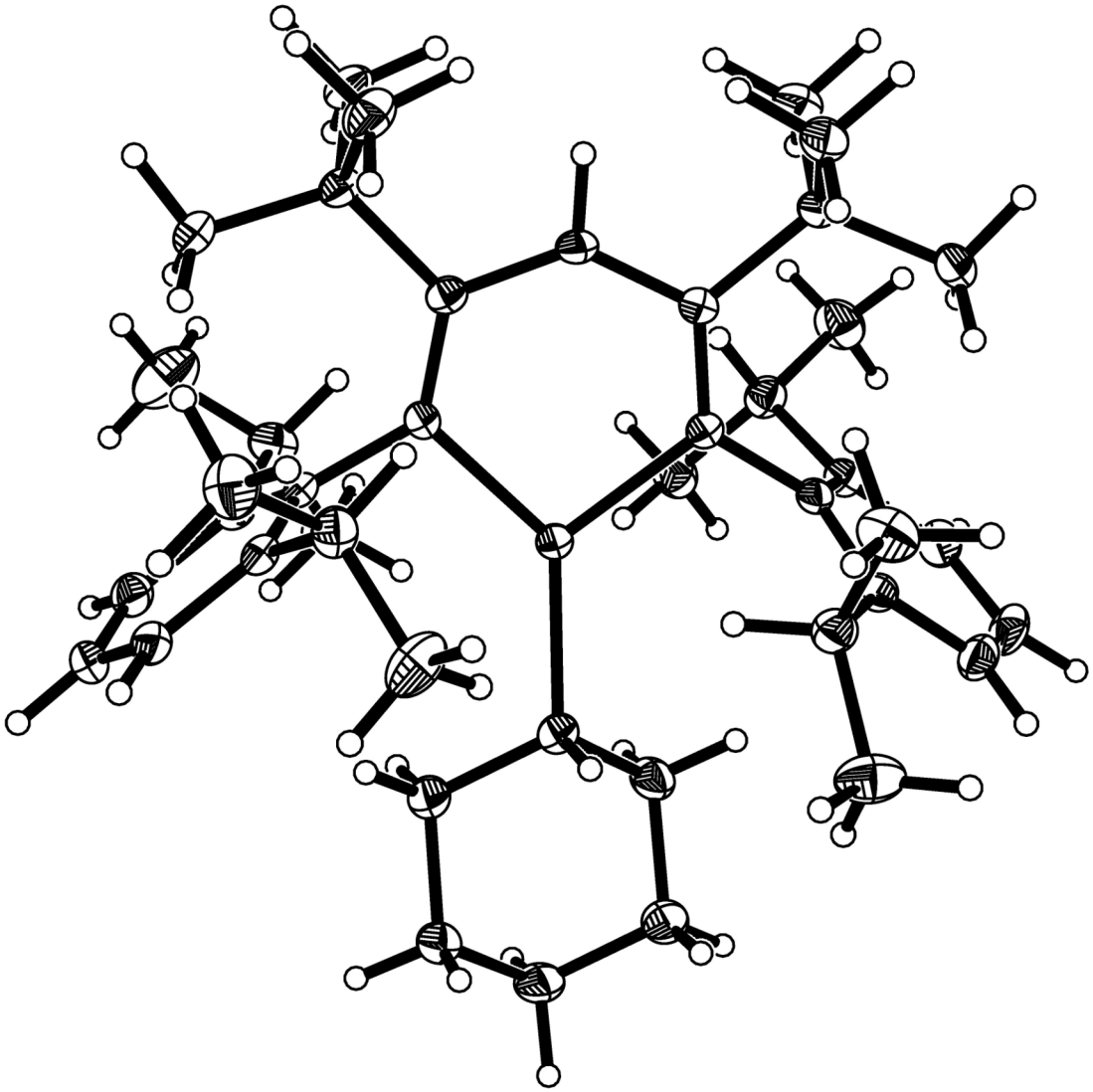


Table 1. Crystal data and structure refinement for holkd21.

Identification code	holkd21	
Empirical formula	C41 H64 Co N2	
Formula weight	643.87	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.6029(6) Å	α = 90°
	b = 17.8932(12) Å	β = 95.060(1)°
	c = 21.6988(14) Å	γ = 90°
Volume	3713.9(4) Å^3	
Z	4	
Density (calculated)	1.152 Mg/m^3	
Absorption coefficient	0.491 mm^{-1}	
F(000)	1404	
Crystal color, morphology	red-orange, block	
Crystal size	0.22 x 0.16 x 0.08 mm^3	
Theta range for data collection	1.48 to 31.77°	
Index ranges	$-14 \le h \le 14$, $-26 \le k \le 26$, $-32 \le l \le 32$	
Reflections collected	66478	
Independent reflections	12621 [R(int) = 0.0988]	
Observed reflections	8075	
Completeness to theta = 31.77°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9618 and 0.8996	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12621 / 0 / 411	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	$R1$ = 0.0537, $wR2$ = 0.1115	
R indices (all data)	$R1$ = 0.1000, $wR2$ = 0.1310	
Largest diff. peak and hole	0.455 and -0.515 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for holkd21. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	6026(1)	2434(1)	3653(1)	19(1)
N11	7225(2)	2368(1)	4419(1)	15(1)
N21	5954(2)	1369(1)	3460(1)	16(1)
C1	4617(2)	3199(1)	3330(1)	21(1)
C2	4896(2)	4000(1)	3552(1)	25(1)
C3	3706(2)	4530(1)	3331(1)	25(1)
C4	3364(2)	4496(1)	2635(1)	27(1)
C5	3082(2)	3699(1)	2420(1)	27(1)
C6	4318(2)	3189(1)	2626(1)	25(1)
C11	8860(2)	1665(1)	5219(1)	19(1)
C21	7811(2)	1734(1)	4638(1)	16(1)
C31	7530(2)	1052(1)	4330(1)	18(1)
C41	6672(2)	853(1)	3797(1)	16(1)
C51	6681(2)	-5(1)	3655(1)	20(1)
C61	8318(2)	1084(1)	5663(1)	27(1)
C71	10264(2)	1398(1)	5008(1)	25(1)
C81	9175(2)	2376(1)	5597(1)	26(1)
C91	8174(2)	-232(1)	3521(1)	28(1)
C101	6281(2)	-436(1)	4231(1)	25(1)
C111	5691(2)	-288(1)	3110(1)	26(1)
C12	7251(2)	3090(1)	4706(1)	16(1)
C22	6240(2)	3260(1)	5117(1)	18(1)
C32	6120(2)	3996(1)	5307(1)	22(1)
C42	6970(2)	4552(1)	5103(1)	24(1)
C52	7973(2)	4373(1)	4711(1)	24(1)
C62	8134(2)	3644(1)	4502(1)	19(1)
C72	5289(2)	2665(1)	5347(1)	22(1)
C82	3787(2)	2784(2)	5072(1)	36(1)
C92	5344(2)	2643(1)	6055(1)	30(1)
C102	9259(2)	3461(1)	4081(1)	24(1)
C112	8926(3)	3787(1)	3430(1)	35(1)

C122	10697(2)	3728(2)	4340(1)	44(1)
C13	5176(2)	1265(1)	2873(1)	17(1)
C23	5901(2)	1255(1)	2336(1)	19(1)
C33	5127(2)	1192(1)	1767(1)	24(1)
C43	3683(2)	1164(1)	1723(1)	26(1)
C53	2991(2)	1227(1)	2253(1)	23(1)
C63	3706(2)	1287(1)	2837(1)	18(1)
C73	7470(2)	1360(1)	2370(1)	22(1)
C83	7808(2)	2178(1)	2253(1)	30(1)
C93	8180(2)	852(1)	1926(1)	31(1)
C103	2927(2)	1406(1)	3409(1)	22(1)
C113	1491(2)	1765(1)	3261(1)	35(1)
C123	2781(2)	700(1)	3789(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for holkd21.

Co(1)-N(11)	1.9412(15)	C(51)-C(101)	1.545(3)
Co(1)-N(21)	1.9501(15)	C(61)-H(61A)	0.9800
Co(1)-C(1)	2.0077(19)	C(61)-H(61B)	0.9800
N(11)-C(21)	1.334(2)	C(61)-H(61C)	0.9800
N(11)-C(12)	1.433(2)	C(71)-H(71A)	0.9800
N(21)-C(41)	1.331(2)	C(71)-H(71B)	0.9800
N(21)-C(13)	1.432(2)	C(71)-H(71C)	0.9800
C(1)-C(2)	1.528(3)	C(81)-H(81A)	0.9800
C(1)-C(6)	1.528(3)	C(81)-H(81B)	0.9800
C(1)-H(1)	1.0000	C(81)-H(81C)	0.9800
C(2)-C(3)	1.529(3)	C(91)-H(91A)	0.9800
C(2)-H(2A)	0.9900	C(91)-H(91B)	0.9800
C(2)-H(2B)	0.9900	C(91)-H(91C)	0.9800
C(3)-C(4)	1.518(3)	C(101)-H(10A)	0.9800
C(3)-H(3A)	0.9900	C(101)-H(10B)	0.9800
C(3)-H(3B)	0.9900	C(101)-H(10C)	0.9800
C(4)-C(5)	1.519(3)	C(111)-H(11A)	0.9800
C(4)-H(4A)	0.9900	C(111)-H(11B)	0.9800
C(4)-H(4B)	0.9900	C(111)-H(11C)	0.9800
C(5)-C(6)	1.532(3)	C(12)-C(62)	1.401(3)
C(5)-H(5A)	0.9900	C(12)-C(22)	1.409(3)
C(5)-H(5B)	0.9900	C(22)-C(32)	1.388(3)
C(6)-H(6A)	0.9900	C(22)-C(72)	1.516(3)
C(6)-H(6B)	0.9900	C(32)-C(42)	1.383(3)
C(11)-C(81)	1.529(3)	C(32)-H(32)	0.9500
C(11)-C(71)	1.537(3)	C(42)-C(52)	1.378(3)
C(11)-C(61)	1.539(3)	C(42)-H(42)	0.9500
C(11)-C(21)	1.548(2)	C(52)-C(62)	1.394(3)
C(21)-C(31)	1.407(2)	C(52)-H(52)	0.9500
C(31)-C(41)	1.405(2)	C(62)-C(102)	1.513(3)
C(31)-H(31)	0.9500	C(72)-C(82)	1.527(3)
C(41)-C(51)	1.565(2)	C(72)-C(92)	1.532(3)
C(51)-C(111)	1.536(3)	C(72)-H(72)	1.0000
C(51)-C(91)	1.542(3)	C(82)-H(82A)	0.9800

C(82)-H(82B)	0.9800	C(103)-H(10E)	1.0000
C(82)-H(82C)	0.9800	C(113)-H(11G)	0.9800
C(92)-H(92A)	0.9800	C(113)-H(11H)	0.9800
C(92)-H(92B)	0.9800	C(113)-H(11I)	0.9800
C(92)-H(92C)	0.9800	C(123)-H(12D)	0.9800
C(102)-C(122)	1.522(3)	C(123)-H(12E)	0.9800
C(102)-C(112)	1.535(3)	C(123)-H(12F)	0.9800
C(102)-H(10D)	1.0000	N(11)-Co(1)-N(21)	97.54(6)
C(112)-H(11D)	0.9800	N(11)-Co(1)-C(1)	132.16(7)
C(112)-H(11E)	0.9800	N(21)-Co(1)-C(1)	125.56(7)
C(112)-H(11F)	0.9800	C(21)-N(11)-C(12)	128.46(15)
C(122)-H(12A)	0.9800	C(21)-N(11)-Co(1)	123.75(12)
C(122)-H(12B)	0.9800	C(12)-N(11)-Co(1)	107.63(11)
C(122)-H(12C)	0.9800	C(41)-N(21)-C(13)	127.01(15)
C(13)-C(63)	1.407(3)	C(41)-N(21)-Co(1)	123.64(12)
C(13)-C(23)	1.409(3)	C(13)-N(21)-Co(1)	108.87(11)
C(23)-C(33)	1.388(3)	C(2)-C(1)-C(6)	109.74(16)
C(23)-C(73)	1.513(3)	C(2)-C(1)-Co(1)	115.84(13)
C(33)-C(43)	1.383(3)	C(6)-C(1)-Co(1)	113.74(13)
C(33)-H(33)	0.9500	C(2)-C(1)-H(1)	105.5
C(43)-C(53)	1.384(3)	C(6)-C(1)-H(1)	105.5
C(43)-H(43)	0.9500	Co(1)-C(1)-H(1)	105.5
C(53)-C(63)	1.391(3)	C(1)-C(2)-C(3)	112.21(16)
C(53)-H(53)	0.9500	C(1)-C(2)-H(2A)	109.2
C(63)-C(103)	1.519(3)	C(3)-C(2)-H(2A)	109.2
C(73)-C(83)	1.526(3)	C(1)-C(2)-H(2B)	109.2
C(73)-C(93)	1.527(3)	C(3)-C(2)-H(2B)	109.2
C(73)-H(73)	1.0000	H(2A)-C(2)-H(2B)	107.9
C(83)-H(83B)	0.9800	C(4)-C(3)-C(2)	112.15(17)
C(83)-H(83C)	0.9800	C(4)-C(3)-H(3A)	109.2
C(83)-H(83D)	0.9800	C(2)-C(3)-H(3A)	109.2
C(93)-H(93A)	0.9800	C(4)-C(3)-H(3B)	109.2
C(93)-H(93B)	0.9800	C(2)-C(3)-H(3B)	109.2
C(93)-H(93C)	0.9800	H(3A)-C(3)-H(3B)	107.9
C(103)-C(123)	1.523(3)	C(3)-C(4)-C(5)	111.14(16)
C(103)-C(113)	1.529(3)	C(3)-C(4)-H(4A)	109.4

C(5)-C(4)-H(4A)	109.4	C(101)-C(51)-C(41)	108.93(15)
C(3)-C(4)-H(4B)	109.4	C(11)-C(61)-H(61A)	109.5
C(5)-C(4)-H(4B)	109.4	C(11)-C(61)-H(61B)	109.5
H(4A)-C(4)-H(4B)	108.0	H(61A)-C(61)-H(61B)	109.5
C(4)-C(5)-C(6)	110.91(17)	C(11)-C(61)-H(61C)	109.5
C(4)-C(5)-H(5A)	109.5	H(61A)-C(61)-H(61C)	109.5
C(6)-C(5)-H(5A)	109.5	H(61B)-C(61)-H(61C)	109.5
C(4)-C(5)-H(5B)	109.5	C(11)-C(71)-H(71A)	109.5
C(6)-C(5)-H(5B)	109.5	C(11)-C(71)-H(71B)	109.5
H(5A)-C(5)-H(5B)	108.0	H(71A)-C(71)-H(71B)	109.5
C(1)-C(6)-C(5)	110.99(16)	C(11)-C(71)-H(71C)	109.5
C(1)-C(6)-H(6A)	109.4	H(71A)-C(71)-H(71C)	109.5
C(5)-C(6)-H(6A)	109.4	H(71B)-C(71)-H(71C)	109.5
C(1)-C(6)-H(6B)	109.4	C(11)-C(81)-H(81A)	109.5
C(5)-C(6)-H(6B)	109.4	C(11)-C(81)-H(81B)	109.5
H(6A)-C(6)-H(6B)	108.0	H(81A)-C(81)-H(81B)	109.5
C(81)-C(11)-C(71)	106.36(16)	C(11)-C(81)-H(81C)	109.5
C(81)-C(11)-C(61)	106.73(16)	H(81A)-C(81)-H(81C)	109.5
C(71)-C(11)-C(61)	109.29(16)	H(81B)-C(81)-H(81C)	109.5
C(81)-C(11)-C(21)	117.04(15)	C(51)-C(91)-H(91A)	109.5
C(71)-C(11)-C(21)	107.87(15)	C(51)-C(91)-H(91B)	109.5
C(61)-C(11)-C(21)	109.36(15)	H(91A)-C(91)-H(91B)	109.5
N(11)-C(21)-C(31)	120.79(16)	C(51)-C(91)-H(91C)	109.5
N(11)-C(21)-C(11)	125.49(16)	H(91A)-C(91)-H(91C)	109.5
C(31)-C(21)-C(11)	113.70(15)	H(91B)-C(91)-H(91C)	109.5
C(41)-C(31)-C(21)	133.22(16)	C(51)-C(101)-H(10A)	109.5
C(41)-C(31)-H(31)	113.4	C(51)-C(101)-H(10B)	109.5
C(21)-C(31)-H(31)	113.4	H(10A)-C(101)-H(10B)	109.5
N(21)-C(41)-C(31)	120.85(16)	C(51)-C(101)-H(10C)	109.5
N(21)-C(41)-C(51)	125.78(16)	H(10A)-C(101)-H(10C)	109.5
C(31)-C(41)-C(51)	113.36(15)	H(10B)-C(101)-H(10C)	109.5
C(111)-C(51)-C(91)	106.88(16)	C(51)-C(111)-H(11A)	109.5
C(111)-C(51)-C(101)	106.04(16)	C(51)-C(111)-H(11B)	109.5
C(91)-C(51)-C(101)	108.80(16)	H(11A)-C(111)-H(11B)	109.5
C(111)-C(51)-C(41)	117.45(15)	C(51)-C(111)-H(11C)	109.5
C(91)-C(51)-C(41)	108.47(16)	H(11A)-C(111)-H(11C)	109.5

H(11B)-C(111)-H(11C)	109.5	H(92B)-C(92)-H(92C)	109.5
C(62)-C(12)-C(22)	121.10(17)	C(62)-C(102)-C(122)	112.38(18)
C(62)-C(12)-N(11)	119.28(16)	C(62)-C(102)-C(112)	111.83(17)
C(22)-C(12)-N(11)	118.91(16)	C(122)-C(102)-C(112)	109.24(18)
C(32)-C(22)-C(12)	118.19(17)	C(62)-C(102)-H(10D)	107.7
C(32)-C(22)-C(72)	120.12(17)	C(122)-C(102)-H(10D)	107.7
C(12)-C(22)-C(72)	121.68(16)	C(112)-C(102)-H(10D)	107.7
C(42)-C(32)-C(22)	121.40(18)	C(102)-C(112)-H(11D)	109.5
C(42)-C(32)-H(32)	119.3	C(102)-C(112)-H(11E)	109.5
C(22)-C(32)-H(32)	119.3	H(11D)-C(112)-H(11E)	109.5
C(52)-C(42)-C(32)	119.65(18)	C(102)-C(112)-H(11F)	109.5
C(52)-C(42)-H(42)	120.2	H(11D)-C(112)-H(11F)	109.5
C(32)-C(42)-H(42)	120.2	H(11E)-C(112)-H(11F)	109.5
C(42)-C(52)-C(62)	121.43(18)	C(102)-C(122)-H(12A)	109.5
C(42)-C(52)-H(52)	119.3	C(102)-C(122)-H(12B)	109.5
C(62)-C(52)-H(52)	119.3	H(12A)-C(122)-H(12B)	109.5
C(52)-C(62)-C(12)	118.20(18)	C(102)-C(122)-H(12C)	109.5
C(52)-C(62)-C(102)	120.36(17)	H(12A)-C(122)-H(12C)	109.5
C(12)-C(62)-C(102)	121.42(17)	H(12B)-C(122)-H(12C)	109.5
C(22)-C(72)-C(82)	110.39(17)	C(63)-C(13)-C(23)	121.43(16)
C(22)-C(72)-C(92)	112.28(16)	C(63)-C(13)-N(21)	119.17(16)
C(82)-C(72)-C(92)	110.12(18)	C(23)-C(13)-N(21)	118.71(17)
C(22)-C(72)-H(72)	108.0	C(33)-C(23)-C(13)	118.11(18)
C(82)-C(72)-H(72)	108.0	C(33)-C(23)-C(73)	120.37(18)
C(92)-C(72)-H(72)	108.0	C(13)-C(23)-C(73)	121.41(16)
C(72)-C(82)-H(82A)	109.5	C(43)-C(33)-C(23)	121.32(19)
C(72)-C(82)-H(82B)	109.5	C(43)-C(33)-H(33)	119.3
H(82A)-C(82)-H(82B)	109.5	C(23)-C(33)-H(33)	119.3
C(72)-C(82)-H(82C)	109.5	C(33)-C(43)-C(53)	119.45(18)
H(82A)-C(82)-H(82C)	109.5	C(33)-C(43)-H(43)	120.3
H(82B)-C(82)-H(82C)	109.5	C(53)-C(43)-H(43)	120.3
C(72)-C(92)-H(92A)	109.5	C(43)-C(53)-C(63)	121.93(19)
C(72)-C(92)-H(92B)	109.5	C(43)-C(53)-H(53)	119.0
H(92A)-C(92)-H(92B)	109.5	C(63)-C(53)-H(53)	119.0
C(72)-C(92)-H(92C)	109.5	C(53)-C(63)-C(13)	117.40(17)
H(92A)-C(92)-H(92C)	109.5	C(53)-C(63)-C(103)	121.00(17)

C(13)-C(63)-C(103)	121.54(16)	H(12E)-C(123)-H(12F)	109.
C(23)-C(73)-C(83)	109.64(16)		
C(23)-C(73)-C(93)	113.22(16)		
C(83)-C(73)-C(93)	110.64(17)		
C(23)-C(73)-H(73)	107.7		
C(83)-C(73)-H(73)	107.7		
C(93)-C(73)-H(73)	107.7		
C(73)-C(83)-H(83B)	109.5		
C(73)-C(83)-H(83C)	109.5		
H(83B)-C(83)-H(83C)	109.5		
C(73)-C(83)-H(83D)	109.5		
H(83B)-C(83)-H(83D)	109.5		
H(83C)-C(83)-H(83D)	109.5		
C(73)-C(93)-H(93A)	109.5		
C(73)-C(93)-H(93B)	109.5		
H(93A)-C(93)-H(93B)	109.5		
C(73)-C(93)-H(93C)	109.5		
H(93A)-C(93)-H(93C)	109.5		
H(93B)-C(93)-H(93C)	109.5		
C(63)-C(103)-C(123)	113.62(16)		
C(63)-C(103)-C(113)	112.81(17)		
C(123)-C(103)-C(113)	109.73(17)		
C(63)-C(103)-H(10E)	106.7		
C(123)-C(103)-H(10E)	106.7		
C(113)-C(103)-H(10E)	106.7		
C(103)-C(113)-H(11G)	109.5		
C(103)-C(113)-H(11H)	109.5		
H(11G)-C(113)-H(11H)	109.5		
C(103)-C(113)-H(11I)	109.5		
H(11G)-C(113)-H(11I)	109.5		
H(11H)-C(113)-H(11I)	109.5		
C(103)-C(123)-H(12D)	109.5		
C(103)-C(123)-H(12E)	109.5		
H(12D)-C(123)-H(12E)	109.5		
C(103)-C(123)-H(12F)	109.5		
H(12D)-C(123)-H(12F)	109.5		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for holkd21. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	22(1)	15(1)	18(1)	-1(1)	-6(1)	3(1)
N11	17(1)	14(1)	16(1)	-1(1)	1(1)	0(1)
N21	17(1)	16(1)	16(1)	0(1)	-2(1)	1(1)
C1	22(1)	20(1)	20(1)	0(1)	-3(1)	1(1)
C2	29(1)	20(1)	24(1)	0(1)	-6(1)	2(1)
C3	27(1)	21(1)	25(1)	-1(1)	-2(1)	4(1)
C4	30(1)	24(1)	25(1)	5(1)	-3(1)	6(1)
C5	34(1)	24(1)	21(1)	2(1)	-5(1)	4(1)
C6	34(1)	20(1)	20(1)	0(1)	-2(1)	5(1)
C11	19(1)	21(1)	16(1)	1(1)	-2(1)	2(1)
C21	14(1)	19(1)	15(1)	1(1)	2(1)	1(1)
C31	19(1)	16(1)	17(1)	2(1)	-2(1)	4(1)
C41	17(1)	15(1)	18(1)	0(1)	1(1)	2(1)
C51	24(1)	16(1)	20(1)	0(1)	-4(1)	4(1)
C61	27(1)	32(1)	20(1)	5(1)	-3(1)	-3(1)
C71	17(1)	33(1)	25(1)	-1(1)	-3(1)	4(1)
C81	26(1)	27(1)	23(1)	-4(1)	-10(1)	4(1)
C91	29(1)	23(1)	32(1)	-3(1)	-1(1)	9(1)
C101	31(1)	18(1)	25(1)	4(1)	-4(1)	0(1)
C111	34(1)	16(1)	26(1)	-2(1)	-5(1)	1(1)
C12	14(1)	18(1)	16(1)	-1(1)	-4(1)	1(1)
C22	16(1)	20(1)	17(1)	-2(1)	-4(1)	0(1)
C32	21(1)	24(1)	20(1)	-5(1)	-2(1)	4(1)
C42	27(1)	17(1)	26(1)	-5(1)	-6(1)	3(1)
C52	24(1)	18(1)	29(1)	2(1)	-5(1)	-4(1)
C62	16(1)	20(1)	21(1)	1(1)	-3(1)	0(1)
C72	18(1)	25(1)	23(1)	-4(1)	4(1)	-2(1)
C82	22(1)	50(1)	36(1)	3(1)	-2(1)	-8(1)
C92	35(1)	34(1)	24(1)	-1(1)	6(1)	-2(1)
C102	19(1)	21(1)	32(1)	4(1)	5(1)	0(1)
C112	32(1)	44(1)	30(1)	1(1)	6(1)	4(1)

C122	20(1)	69(2)	44(2)	6(1)	5(1)	-5(1)
C13	21(1)	13(1)	15(1)	0(1)	-2(1)	2(1)
C23	21(1)	16(1)	20(1)	0(1)	0(1)	0(1)
C33	31(1)	23(1)	17(1)	2(1)	1(1)	-2(1)
C43	31(1)	28(1)	18(1)	5(1)	-9(1)	-7(1)
C53	20(1)	22(1)	26(1)	4(1)	-4(1)	-5(1)
C63	19(1)	14(1)	20(1)	3(1)	-2(1)	-1(1)
C73	19(1)	25(1)	21(1)	-2(1)	2(1)	1(1)
C83	25(1)	25(1)	41(1)	-4(1)	6(1)	-4(1)
C93	30(1)	30(1)	34(1)	-6(1)	10(1)	4(1)
C103	19(1)	22(1)	25(1)	0(1)	2(1)	0(1)
C113	25(1)	40(1)	42(1)	10(1)	9(1)	8(1)
C123	37(1)	28(1)	24(1)	6(1)	9(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for holkd21.

	x	y	z	U(eq)
H1	3720	3051	3497	25
H2A	5775	4180	3396	30
H2B	5020	4006	4009	30
H3A	2862	4398	3539	30
H3B	3973	5048	3452	30
H4A	4156	4703	2427	32
H4B	2530	4808	2518	32
H5A	2919	3689	1963	32
H5B	2229	3511	2593	32
H6A	4105	2672	2486	30
H6B	5158	3359	2432	30
H31	8021	640	4521	21
H61A	8970	1048	6035	40
H61B	8242	596	5457	40
H61C	7396	1238	5778	40
H71A	10948	1351	5368	38
H71B	10601	1762	4718	38
H71C	10136	912	4803	38
H81A	9861	2265	5946	39
H81B	8312	2561	5753	39
H81C	9553	2758	5334	39
H91A	8207	-773	3451	42
H91B	8831	-99	3876	42
H91C	8432	31	3152	42
H10A	6303	-974	4150	38
H10B	5338	-290	4324	38
H10C	6948	-316	4585	38
H11A	5737	-835	3093	38
H11B	5972	-78	2724	38
H11C	4732	-133	3168	38

H32	5441	4122	5583	26
H42	6862	5055	5232	29
H52	8568	4755	4580	28
H72	5611	2169	5202	27
H82A	3757	2778	4619	54
H82B	3446	3267	5209	54
H82C	3192	2383	5211	54
H92A	6305	2544	6226	46
H92B	4728	2246	6183	46
H92C	5035	3125	6209	46
H10D	9300	2905	4040	28
H11D	8019	3598	3254	53
H11E	9655	3638	3165	53
H11F	8892	4333	3455	53
H12A	11410	3523	4092	66
H12B	10877	3559	4770	66
H12C	10729	4276	4327	66
H33	5600	1168	1401	29
H43	3170	1101	1331	32
H53	1997	1230	2218	28
H73	7857	1233	2800	26
H83B	7382	2493	2555	45
H83C	7436	2318	1834	45
H83D	8824	2249	2296	45
H93A	7905	333	1990	47
H93B	9197	899	2004	47
H93C	7894	1000	1498	47
H10E	3494	1766	3680	26
H11G	1127	1933	3646	53
H11H	849	1397	3057	53
H11I	1577	2193	2986	53
H12D	2282	816	4152	44
H12E	3712	504	3924	44
H12F	2257	324	3535	44