

SUPPORTING INFORMATION FOR

Naphthalene and Anthracene Cobaltates(1-): Useful Storable Sources of Atomic Cobalt Anion

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Single Crystal X-ray Crystallography

Crystal Structure Reports for structures 1a, 1b, 2, 3, 4, 5, 8, 9, 10a, 10b, 13, 14, 15, 16, R&D1, R&D2, R&D3

Single Crystal X-ray Crystallography

Data collection and structure solution were conducted at the X-ray Crystallographic Laboratory, 160 Kolthoff Hall, Chemistry Department, University of Minnesota.

Crystals were placed onto the tips glass capillary tubes or fibers and mounted on a Siemens or Bruker SMART CCD Platform diffractometer for data collection.¹ For each crystal a preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. Full data collections were carried out using MoK α radiation (0.71073 Å, graphite monochromator) with frame times ranging from 5 to 60 seconds and at a detector distance of approximately five cm. Randomly oriented regions of reciprocal space were surveyed: three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption.² Final cell constants were calculated from the xyz centroids of about 4000 strong reflections from the actual data collections after integration.³ See Table 1 for additional crystal and refinement information.

Structures were solved using SIR97⁴ and refined using SHELXL-97.⁵ Space groups were determined based on systematic absences, intensity statistics, or both. Direct-methods solutions were 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. When possible, hydrogen atoms on metal-coordinated carbon atoms were found from the difference Fourier map, and their positional and isotropic displacement parameters were refined independently from those of their bonded carbon atoms. All other hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

Full matrix least squares refinements on F^2 were run to convergence.

Structure **3** is a three-dimensional network of potassium cations and $[\text{Co}(\text{PF}_3)_4]^-$ anions. The formula unit is bisected by a crystallographic mirror plane that contains atoms K1, Co1, P2, and F4. One PF_3 ligand arm (P3, F6, F7, F8) is modeled as disordered over the crystallographic mirror plane (50:50), with all three P-F bond lengths restrained to be similar. The asymmetric unit of **5** contains the $[\text{Co}(\text{P}(\text{OiPr})_3)_4]^-$ anion, with all atoms in general positions, and two independent cation sites, with the potassium metals in crystallographic inversion centers. The anions are well separated from the cations. Both independent potassium-coordinated THF solvent molecules are modeled as disordered, one over two positions (77:23) and one over three positions (44:35:21). Bond lengths in the THF molecules were restrained to ideal values and anisotropic displacement parameters of spatially close atoms were constrained to be equivalent. All atoms in **8** lie in general positions and the cation and anion are well separated. In **9** the cation and anion well separated and both lie along crystallographic two-fold axes; thus one half of each is unique. The cation and anion of **14** are in general positions, and are weakly coordinated via atoms C3 and C4 of the butadiene ligand and via atom C9 of the cyclooctadiene ligand, creating a pseudo polymeric structure in one dimension parallel to the *b*-axis. Likewise in **15** the cation and anion are in general positions and are in contact with each other via atoms of the cyclooctadiene ligand, also producing a pseudo polymeric structure in one dimension. The bipyridine ligand does not associate with the cation.

Structure **16** was run at a higher temperature than usual (223 K versus 173 K) to avoid data that appeared to be between twinned monoclinic and orthorhombic, neither which offered a satisfactory model. The cations and anions are well separated. The cobalt anion is bisected by a crystallographic mirror plane that contains atoms Co1, C6, N2, C7, C9, C10, N3, and C11. The

ligand containing N1 and the methyl groups of the ligand containing N3 are modeled as disordered over the mirror plane (50:50). The charge is balanced by two independent potassium 18-crown-6 bis(THF) cations in which the potassium atoms lie in crystallographic 2/m positions (four-fold multiplicity). These THF solvent molecules are modeled as doubly disordered, over the mirror plane and over two general positions (50:50, 61:39 and 50:50, 63:37). There was an additional uncoordinated co-crystallized THF solvent molecule that was highly disordered over a crystallographic mirror plane and that could not be modeled satisfactorily. The reflection contribution from this solvent were removed using program *PLATON*, function *Squeeze*,⁶ which determined there to be 152 electrons in 599.6 Å³ removed per unit cell (approximately one THF per cobalt anion). Since the identity of the removed solvent molecule was known, it was included in the molecular formula.

For additional details and for structures introduced in the Results and Discussion section of the article, see the individual reports below.

Crystallographic information files (CIFs) are also available from the Cambridge Crystallographic Data Centre (CCDC) with reference codes CCDC 885955-885971.

¹ *SMART*, version 5.629; Bruker AXS: Madison, WI, 2003.

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

³ *SAINT*, version 7.06A; Bruker AXS: Madison, WI, 2003.

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.

⁶ Spek, A. L. *PLATON*, version 300106; *J. Appl. Cryst.* **2003**, *36*, 7-13.

REFERENCE NUMBER: 01168 [**1a**]

CRYSTAL STRUCTURE REPORT

$\text{C}_{51} \text{H}_{61} \text{Co K O}_8$

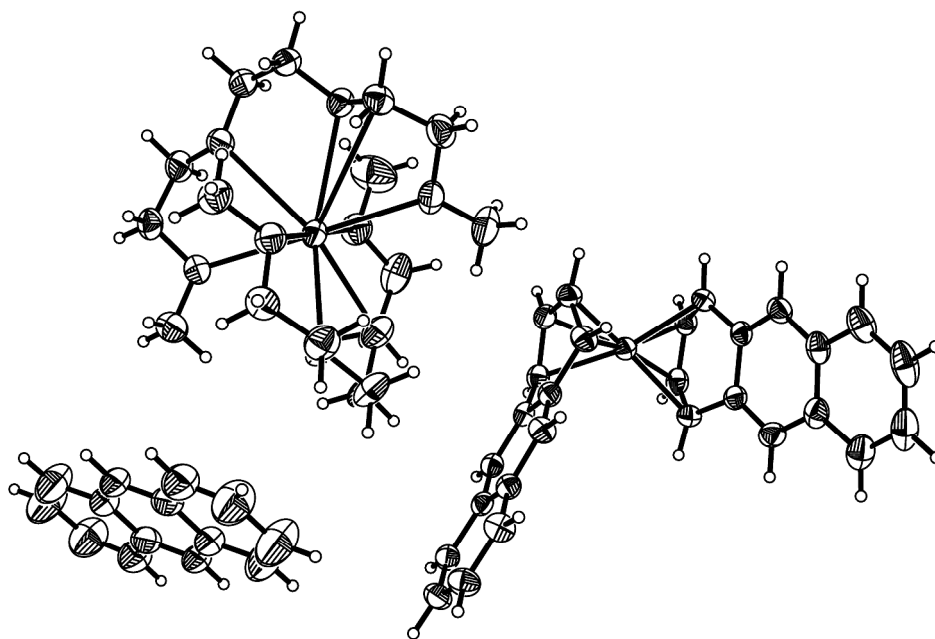
or

$[\text{K}(\text{triglyme})_2][\text{Co}(\text{C}_{14}\text{H}_{10})_2] \cdot \frac{1}{2} \text{C}_{14}\text{H}_{10}$

Report prepared for:

W. Brennessel, Prof. J. Ellis

May 26, 2001



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Data collection

A crystal (0.31 x 0.28 x 0.23 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Siemens SMART Platform CCD diffractometer for a data collection at 173(2) 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 MoK α radiation (graphite monochromator) with a frame time of 20 seconds and a detector distance of 4.88 cm. A randomly oriented region of reciprocal space was surveyed: three major sections of frames were collected with 0.30° steps in ω at three different ω settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption.² Final cell constants were calculated from the xyz centroids of 6246 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 SHELXS-97⁴ and refined using SHELXL-97.⁴ The space group $P2_1/c$ was determined based on systematic absences. 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. Hydrogen atoms on metal-coordinated carbon atoms were found from the difference Fourier map, and their positional and isotropic displacement parameters were refined independently from those of their respective bonded atoms. All other 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 $R1 = 0.0320$ (F^2 , $I > 2\sigma(I)$) and $wR2 = 0.0780$ (F^2 , all data).

Structure description

The structure is a greatly improved repeat of structure 01005. Per formula unit are one cobalt anion, one bis(triglyme) potassium cation, and one half of an anthracene molecule (uncoordinated) that lies in a crystallographic inversion center. The cobalt-centroid distances (centroids C1-C2-C13-C14 and C15-C16-C27-C28) are 1.64 Å; the centroid-Co-centroid angle is 170°. The fold angles are 29.0° and 29.3°, respectively. The coordinated anthracene containing C2 through C13 is twisted with respect to itself by 9.5° (see figure below).

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

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using SGI INDY R4400-SC or Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young,

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- ¹ *APEX2*, version 2011.4-1; Bruker AXS: Madison, WI, 2011.
² Sheldrick, G. M. *SADABS*, version 2008/1; University of Göttingen: Göttingen, Germany, 2008.
³ *SAINT*, version 7.68A; Bruker AXS: Madison, WI, 2009.
⁴ Sheldrick, G. M. *Acta. Cryst.* **2008**, *A64*, 112-122.

Some equations of interest:

$$R_{\text{int}} = \frac{\sum |F_o|^2 - \langle F_o^2 \rangle}{\sum |F_o|^2}$$

$$R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$$

$$wR2 = \left[\frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)^2]} \right]^{1/2}$$

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

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

$$\text{GOF} = S = \left[\frac{\sum [w(F_o^2 - F_c^2)^2]}{(m-n)} \right]^{1/2}$$

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

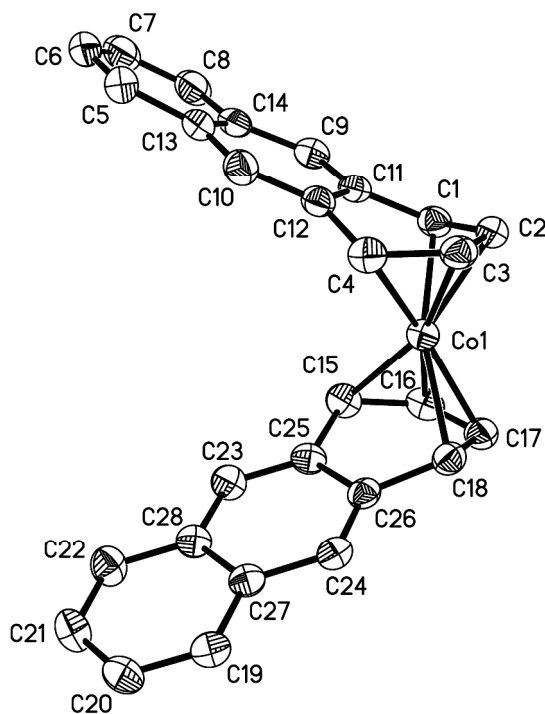


Table 1. Crystal data and structure refinement for 168.

Identification code	01168	
Empirical formula	C ₅₁ H ₆₁ Co K O ₈	
Formula weight	900.03	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 12.5111(12) Å	∠ = 90°
	<i>b</i> = 28.183(3) Å	∠ = 105.816(2)°
	<i>c</i> = 14.0234(13) Å	∠ = 90°
Volume	4757.5(8) Å ³	
<i>Z</i>	4	
Density (calculated)	1.257 Mg/m ³	
Absorption coefficient	0.500 mm ⁻¹	
<i>F</i> (000)	1908	
Crystal color, morphology	black, block	
Crystal size	0.31 x 0.28 x 0.23 mm ³	
Theta range for data collection	1.45 to 25.08°	
Index ranges	-14 ≤ <i>h</i> ≤ 14, -33 ≤ <i>k</i> ≤ 33, -16 ≤ <i>l</i> ≤ 16	
Reflections collected	35034	
Independent reflections	8427 [<i>R</i> (int) = 0.0443]	
Observed reflections	6341	
Completeness to theta = 25.08°	99.8%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8937 and 0.8605	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	8427 / 0 / 586	
Goodness-of-fit on <i>F</i> ²	1.014	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0320, <i>wR</i> 2 = 0.0725	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0531, <i>wR</i> 2 = 0.0780	
Largest diff. peak and hole	0.207 and -0.218 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 168. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	1415(1)	768(1)	58(1)	28(1)
C1	-152(2)	1076(1)	-561(1)	32(1)
C2	-139(2)	576(1)	-672(1)	33(1)
C3	650(2)	398(1)	-1134(1)	33(1)
C4	1311(2)	733(1)	-1482(1)	32(1)
C5	899(2)	2209(1)	-3547(2)	48(1)
C6	523(2)	2669(1)	-3718(2)	58(1)
C7	-50(2)	2883(1)	-3109(2)	58(1)
C8	-281(2)	2626(1)	-2355(2)	47(1)
C9	-238(2)	1857(1)	-1448(1)	34(1)
C10	1110(2)	1468(1)	-2539(1)	37(1)
C11	111(1)	1396(1)	-1284(1)	30(1)
C12	861(1)	1201(1)	-1814(1)	30(1)
C13	702(2)	1940(1)	-2761(1)	38(1)
C14	60(2)	2148(1)	-2169(1)	37(1)
C15	2469(2)	1294(1)	882(2)	34(1)
C16	1830(2)	1032(1)	1410(1)	35(1)
C17	1974(2)	533(1)	1457(1)	33(1)
C18	2738(2)	346(1)	963(1)	31(1)
C19	6651(1)	539(1)	726(1)	32(1)
C20	7486(2)	833(1)	615(1)	37(1)
C21	7310(2)	1323(1)	509(2)	40(1)
C22	6307(2)	1517(1)	531(2)	37(1)
C23	4401(2)	1414(1)	724(1)	32(1)
C24	4716(1)	430(1)	862(1)	28(1)
C25	3555(1)	1130(1)	847(1)	29(1)
C26	3716(1)	621(1)	908(1)	28(1)
C27	5602(1)	723(1)	748(1)	28(1)
C28	5432(1)	1224(1)	661(1)	30(1)
K1	5151(1)	1376(1)	5479(1)	34(1)
C29	3011(2)	1823(1)	3298(2)	62(1)

O1	3574(1)	1968(1)	4284(1)	48(1)
C30	2880(2)	2235(1)	4731(2)	47(1)
C31	3446(2)	2301(1)	5807(2)	42(1)
O2	3557(1)	1849(1)	6293(1)	37(1)
C32	3858(2)	1888(1)	7350(1)	40(1)
C33	4298(2)	1419(1)	7789(2)	42(1)
O3	5314(1)	1334(1)	7540(1)	39(1)
C34	5838(2)	897(1)	7929(2)	42(1)
C35	6976(2)	888(1)	7769(2)	43(1)
O4	6871(1)	881(1)	6731(1)	42(1)
C36	7932(2)	864(1)	6537(2)	54(1)
C37	6860(2)	2300(1)	6994(2)	51(1)
O5	6517(1)	2182(1)	5968(1)	43(1)
C38	7410(2)	2220(1)	5523(2)	44(1)
C39	6986(2)	2095(1)	4450(2)	52(1)
O6	6682(1)	1606(1)	4374(1)	46(1)
C40	6340(2)	1441(1)	3371(2)	59(1)
C41	6035(2)	925(1)	3390(2)	59(1)
O7	5066(1)	891(1)	3738(1)	50(1)
C42	4663(2)	417(1)	3719(2)	60(1)
C43	3583(2)	420(1)	3977(2)	60(1)
O8	3749(1)	585(1)	4960(1)	53(1)
C44	2733(2)	588(1)	5236(2)	89(1)
C45	9767(2)	1001(1)	5036(2)	67(1)
C46	9445(3)	1248(1)	4186(2)	88(1)
C47	9181(3)	1011(1)	3259(2)	99(1)
C48	9273(3)	530(1)	3224(2)	83(1)
C49	9640(2)	254(1)	4106(2)	53(1)
C50	9881(2)	497(1)	5036(2)	50(1)
C51	10234(2)	236(1)	5904(2)	53(1)

Table 3. Bond lengths [Å] and angles [°] for 168.

Co(1)-C(16)	1.9692(19)	C(15)-C(16)	1.434(3)
Co(1)-C(3)	1.9823(19)	C(15)-C(25)	1.448(2)
Co(1)-C(17)	2.0067(19)	C(15)-H(15)	0.928(18)
Co(1)-C(2)	2.0093(19)	C(16)-C(17)	1.414(3)
Co(1)-C(1)	2.1020(18)	C(16)-H(16)	0.968(18)
Co(1)-C(15)	2.1067(19)	C(17)-C(18)	1.427(3)
Co(1)-C(4)	2.1297(19)	C(17)-H(17)	0.966(18)
Co(1)-C(18)	2.1504(19)	C(18)-C(26)	1.468(2)
C(1)-C(2)	1.416(3)	C(18)-H(18)	0.958(18)
C(1)-C(11)	1.460(2)	C(19)-C(20)	1.375(2)
C(1)-H(1)	0.940(18)	C(19)-C(27)	1.419(2)
C(2)-C(3)	1.413(3)	C(19)-H(19)	0.9500
C(2)-H(2)	0.938(18)	C(20)-C(21)	1.400(3)
C(3)-C(4)	1.426(3)	C(20)-H(20)	0.9500
C(3)-H(3)	0.998(18)	C(21)-C(22)	1.377(3)
C(4)-C(12)	1.459(3)	C(21)-H(21)	0.9500
C(4)-H(4)	0.943(17)	C(22)-C(28)	1.422(2)
C(5)-C(6)	1.378(3)	C(22)-H(22)	0.9500
C(5)-C(13)	1.412(3)	C(23)-C(25)	1.375(2)
C(5)-H(5)	0.9500	C(23)-C(28)	1.422(2)
C(6)-C(7)	1.393(3)	C(23)-H(23)	0.9500
C(6)-H(6)	0.9500	C(24)-C(26)	1.380(2)
C(7)-C(8)	1.376(3)	C(24)-C(27)	1.426(2)
C(7)-H(7)	0.9500	C(24)-H(24)	0.9500
C(8)-C(14)	1.415(3)	C(25)-C(26)	1.449(2)
C(8)-H(8)	0.9500	C(27)-C(28)	1.427(2)
C(9)-C(11)	1.371(2)	K(1)-O(4)	2.7566(14)
C(9)-C(14)	1.428(3)	K(1)-O(1)	2.7713(14)
C(9)-H(9)	0.9500	K(1)-O(7)	2.7761(14)
C(10)-C(12)	1.368(2)	K(1)-O(8)	2.8082(15)
C(10)-C(13)	1.429(3)	K(1)-O(5)	2.8118(14)
C(10)-H(10)	0.9500	K(1)-O(3)	2.8440(14)
C(11)-C(12)	1.454(2)	K(1)-O(6)	2.8463(14)
C(13)-C(14)	1.429(3)	K(1)-O(2)	2.8797(13)

K(1)-C(31)	3.477(2)	C(38)-H(38A)	0.9900
C(29)-O(1)	1.429(2)	C(38)-H(38B)	0.9900
C(29)-H(29A)	0.9800	C(39)-O(6)	1.426(2)
C(29)-H(29B)	0.9800	C(39)-H(39A)	0.9900
C(29)-H(29C)	0.9800	C(39)-H(39B)	0.9900
O(1)-C(30)	1.418(2)	O(6)-C(40)	1.431(2)
C(30)-C(31)	1.494(3)	C(40)-C(41)	1.505(3)
C(30)-H(30A)	0.9900	C(40)-H(40A)	0.9900
C(30)-H(30B)	0.9900	C(40)-H(40B)	0.9900
C(31)-O(2)	1.434(2)	C(41)-O(7)	1.428(3)
C(31)-H(31A)	0.9900	C(41)-H(41A)	0.9900
C(31)-H(31B)	0.9900	C(41)-H(41B)	0.9900
O(2)-C(32)	1.431(2)	O(7)-C(42)	1.426(2)
C(32)-C(33)	1.497(3)	C(42)-C(43)	1.491(3)
C(32)-H(32A)	0.9900	C(42)-H(42A)	0.9900
C(32)-H(32B)	0.9900	C(42)-H(42B)	0.9900
C(33)-O(3)	1.428(2)	C(43)-O(8)	1.416(2)
C(33)-H(33A)	0.9900	C(43)-H(43A)	0.9900
C(33)-H(33B)	0.9900	C(43)-H(43B)	0.9900
O(3)-C(34)	1.432(2)	O(8)-C(44)	1.426(3)
C(34)-C(35)	1.501(3)	C(44)-H(44A)	0.9800
C(34)-H(34A)	0.9900	C(44)-H(44B)	0.9800
C(34)-H(34B)	0.9900	C(44)-H(44C)	0.9800
C(35)-O(4)	1.426(2)	C(45)-C(46)	1.344(4)
C(35)-H(35A)	0.9900	C(45)-C(50)	1.427(3)
C(35)-H(35B)	0.9900	C(45)-H(45)	0.9500
O(4)-C(36)	1.427(2)	C(46)-C(47)	1.418(4)
C(36)-H(36A)	0.9800	C(46)-H(46)	0.9500
C(36)-H(36B)	0.9800	C(47)-C(48)	1.361(4)
C(36)-H(36C)	0.9800	C(47)-H(47)	0.9500
C(37)-O(5)	1.424(2)	C(48)-C(49)	1.429(3)
C(37)-H(37A)	0.9800	C(48)-H(48)	0.9500
C(37)-H(37B)	0.9800	C(49)-C(51)#1	1.390(3)
C(37)-H(37C)	0.9800	C(49)-C(50)	1.431(3)
O(5)-C(38)	1.425(2)	C(50)-C(51)	1.387(3)
C(38)-C(39)	1.496(3)	C(51)-C(49)#1	1.390(3)

C(51)-H(51)	0.9500	C(3)-C(2)-Co(1)	68.25(11)
C(16)-Co(1)-C(3)	161.90(8)	C(1)-C(2)-Co(1)	73.41(11)
C(16)-Co(1)-C(17)	41.67(8)	C(3)-C(2)-H(2)	120.6(11)
C(3)-Co(1)-C(17)	127.59(8)	C(1)-C(2)-H(2)	123.5(11)
C(16)-Co(1)-C(2)	123.84(8)	Co(1)-C(2)-H(2)	124.9(11)
C(3)-Co(1)-C(2)	41.46(7)	C(2)-C(3)-C(4)	117.58(17)
C(17)-Co(1)-C(2)	116.11(8)	C(2)-C(3)-Co(1)	70.29(11)
C(16)-Co(1)-C(1)	102.35(8)	C(4)-C(3)-Co(1)	75.38(11)
C(3)-Co(1)-C(1)	71.78(8)	C(2)-C(3)-H(3)	120.4(10)
C(17)-Co(1)-C(1)	125.21(7)	C(4)-C(3)-H(3)	121.9(10)
C(2)-Co(1)-C(1)	40.22(7)	Co(1)-C(3)-H(3)	122.4(10)
C(16)-Co(1)-C(15)	41.03(7)	C(3)-C(4)-C(12)	119.94(16)
C(3)-Co(1)-C(15)	156.80(8)	C(3)-C(4)-Co(1)	64.25(10)
C(17)-Co(1)-C(15)	72.36(8)	C(12)-C(4)-Co(1)	101.17(12)
C(2)-Co(1)-C(15)	147.46(8)	C(3)-C(4)-H(4)	116.6(11)
C(1)-Co(1)-C(15)	108.08(7)	C(12)-C(4)-H(4)	119.4(11)
C(16)-Co(1)-C(4)	157.06(8)	Co(1)-C(4)-H(4)	122.1(11)
C(3)-Co(1)-C(4)	40.37(7)	C(6)-C(5)-C(13)	121.1(2)
C(17)-Co(1)-C(4)	152.19(8)	C(6)-C(5)-H(5)	119.5
C(2)-Co(1)-C(4)	71.76(7)	C(13)-C(5)-H(5)	119.5
C(1)-Co(1)-C(4)	78.92(7)	C(5)-C(6)-C(7)	120.6(2)
C(15)-Co(1)-C(4)	116.43(7)	C(5)-C(6)-H(6)	119.7
C(16)-Co(1)-C(18)	71.46(8)	C(7)-C(6)-H(6)	119.7
C(3)-Co(1)-C(18)	108.83(8)	C(8)-C(7)-C(6)	119.6(2)
C(17)-Co(1)-C(18)	39.97(7)	C(8)-C(7)-H(7)	120.2
C(2)-Co(1)-C(18)	129.34(8)	C(6)-C(7)-H(7)	120.2
C(1)-Co(1)-C(18)	162.39(7)	C(7)-C(8)-C(14)	121.8(2)
C(15)-Co(1)-C(18)	78.47(8)	C(7)-C(8)-H(8)	119.1
C(4)-Co(1)-C(18)	113.39(7)	C(14)-C(8)-H(8)	119.1
C(2)-C(1)-C(11)	121.69(17)	C(11)-C(9)-C(14)	121.95(17)
C(2)-C(1)-Co(1)	66.36(10)	C(11)-C(9)-H(9)	119.0
C(11)-C(1)-Co(1)	100.39(11)	C(14)-C(9)-H(9)	119.0
C(2)-C(1)-H(1)	118.3(11)	C(12)-C(10)-C(13)	122.36(17)
C(11)-C(1)-H(1)	115.8(11)	C(12)-C(10)-H(10)	118.8
Co(1)-C(1)-H(1)	123.2(11)	C(13)-C(10)-H(10)	118.8
C(3)-C(2)-C(1)	115.76(17)	C(9)-C(11)-C(12)	119.59(16)

C(9)-C(11)-C(1)	125.45(17)	C(20)-C(19)-H(19)	119.4
C(12)-C(11)-C(1)	114.86(16)	C(27)-C(19)-H(19)	119.4
C(10)-C(12)-C(11)	118.74(17)	C(19)-C(20)-C(21)	120.28(17)
C(10)-C(12)-C(4)	126.10(17)	C(19)-C(20)-H(20)	119.9
C(11)-C(12)-C(4)	115.12(15)	C(21)-C(20)-H(20)	119.9
C(5)-C(13)-C(10)	122.76(19)	C(22)-C(21)-C(20)	120.40(17)
C(5)-C(13)-C(14)	118.67(19)	C(22)-C(21)-H(21)	119.8
C(10)-C(13)-C(14)	118.57(17)	C(20)-C(21)-H(21)	119.8
C(8)-C(14)-C(9)	123.54(19)	C(21)-C(22)-C(28)	120.72(17)
C(8)-C(14)-C(13)	118.11(18)	C(21)-C(22)-H(22)	119.6
C(9)-C(14)-C(13)	118.31(17)	C(28)-C(22)-H(22)	119.6
C(16)-C(15)-C(25)	120.86(17)	C(25)-C(23)-C(28)	122.12(16)
C(16)-C(15)-Co(1)	64.33(10)	C(25)-C(23)-H(23)	118.9
C(25)-C(15)-Co(1)	102.13(12)	C(28)-C(23)-H(23)	118.9
C(16)-C(15)-H(15)	119.8(10)	C(26)-C(24)-C(27)	121.55(16)
C(25)-C(15)-H(15)	115.5(11)	C(26)-C(24)-H(24)	119.2
Co(1)-C(15)-H(15)	122.0(11)	C(27)-C(24)-H(24)	119.2
C(17)-C(16)-C(15)	117.04(17)	C(23)-C(25)-C(15)	125.53(16)
C(17)-C(16)-Co(1)	70.59(11)	C(23)-C(25)-C(26)	118.95(15)
C(15)-C(16)-Co(1)	74.63(11)	C(15)-C(25)-C(26)	115.47(15)
C(17)-C(16)-H(16)	122.9(11)	C(24)-C(26)-C(25)	119.76(15)
C(15)-C(16)-H(16)	119.9(11)	C(24)-C(26)-C(18)	125.14(16)
Co(1)-C(16)-H(16)	121.2(11)	C(25)-C(26)-C(18)	115.02(15)
C(16)-C(17)-C(18)	116.02(17)	C(19)-C(27)-C(24)	122.93(16)
C(16)-C(17)-Co(1)	67.75(11)	C(19)-C(27)-C(28)	118.44(16)
C(18)-C(17)-Co(1)	75.44(11)	C(24)-C(27)-C(28)	118.63(15)
C(16)-C(17)-H(17)	121.3(11)	C(22)-C(28)-C(23)	122.11(16)
C(18)-C(17)-H(17)	122.6(11)	C(22)-C(28)-C(27)	118.92(16)
Co(1)-C(17)-H(17)	122.9(11)	C(23)-C(28)-C(27)	118.95(15)
C(17)-C(18)-C(26)	120.48(17)	O(4)-K(1)-O(1)	173.31(4)
C(17)-C(18)-Co(1)	64.59(10)	O(4)-K(1)-O(7)	98.43(4)
C(26)-C(18)-Co(1)	101.21(12)	O(1)-K(1)-O(7)	85.07(4)
C(17)-C(18)-H(18)	119.3(10)	O(4)-K(1)-O(8)	94.98(4)
C(26)-C(18)-H(18)	116.3(11)	O(1)-K(1)-O(8)	91.70(5)
Co(1)-C(18)-H(18)	122.8(11)	O(7)-K(1)-O(8)	60.57(4)
C(20)-C(19)-C(27)	121.21(17)	O(4)-K(1)-O(5)	86.37(4)

O(1)-K(1)-O(5)	86.95(4)	C(30)-O(1)-K(1)	118.24(11)
O(7)-K(1)-O(5)	119.18(4)	C(29)-O(1)-K(1)	119.65(12)
O(8)-K(1)-O(5)	178.65(5)	O(1)-C(30)-C(31)	109.50(16)
O(4)-K(1)-O(3)	60.30(4)	O(1)-C(30)-H(30A)	109.8
O(1)-K(1)-O(3)	118.81(4)	C(31)-C(30)-H(30A)	109.8
O(7)-K(1)-O(3)	148.05(4)	O(1)-C(30)-H(30B)	109.8
O(8)-K(1)-O(3)	95.59(4)	C(31)-C(30)-H(30B)	109.8
O(5)-K(1)-O(3)	85.14(4)	H(30A)-C(30)-H(30B)	108.2
O(4)-K(1)-O(6)	86.41(4)	O(2)-C(31)-C(30)	109.09(16)
O(1)-K(1)-O(6)	90.44(4)	O(2)-C(31)-K(1)	54.05(8)
O(7)-K(1)-O(6)	60.21(4)	C(30)-C(31)-K(1)	84.94(11)
O(8)-K(1)-O(6)	120.28(4)	O(2)-C(31)-H(31A)	109.9
O(5)-K(1)-O(6)	59.68(4)	C(30)-C(31)-H(31A)	109.9
O(3)-K(1)-O(6)	133.64(4)	K(1)-C(31)-H(31A)	74.4
O(4)-K(1)-O(2)	119.12(4)	O(2)-C(31)-H(31B)	109.9
O(1)-K(1)-O(2)	60.37(4)	C(30)-C(31)-H(31B)	109.9
O(7)-K(1)-O(2)	135.38(4)	K(1)-C(31)-H(31B)	162.1
O(8)-K(1)-O(2)	91.10(4)	H(31A)-C(31)-H(31B)	108.3
O(5)-K(1)-O(2)	88.31(4)	C(32)-O(2)-C(31)	112.89(14)
O(3)-K(1)-O(2)	58.82(4)	C(32)-O(2)-K(1)	115.52(10)
O(6)-K(1)-O(2)	138.76(4)	C(31)-O(2)-K(1)	102.17(10)
O(4)-K(1)-C(31)	134.11(5)	O(2)-C(32)-C(33)	108.82(15)
O(1)-K(1)-C(31)	42.91(4)	O(2)-C(32)-H(32A)	109.9
O(7)-K(1)-C(31)	127.43(5)	C(33)-C(32)-H(32A)	109.9
O(8)-K(1)-C(31)	105.50(5)	O(2)-C(32)-H(32B)	109.9
O(5)-K(1)-C(31)	73.54(4)	C(33)-C(32)-H(32B)	109.9
O(3)-K(1)-C(31)	76.92(4)	H(32A)-C(32)-H(32B)	108.3
O(6)-K(1)-C(31)	115.46(4)	O(3)-C(33)-C(32)	107.41(15)
O(2)-K(1)-C(31)	23.78(4)	O(3)-C(33)-H(33A)	110.2
O(1)-C(29)-H(29A)	109.5	C(32)-C(33)-H(33A)	110.2
O(1)-C(29)-H(29B)	109.5	O(3)-C(33)-H(33B)	110.2
H(29A)-C(29)-H(29B)	109.5	C(32)-C(33)-H(33B)	110.2
O(1)-C(29)-H(29C)	109.5	H(33A)-C(33)-H(33B)	108.5
H(29A)-C(29)-H(29C)	109.5	C(33)-O(3)-C(34)	113.33(14)
H(29B)-C(29)-H(29C)	109.5	C(33)-O(3)-K(1)	114.80(11)
C(30)-O(1)-C(29)	112.27(17)	C(34)-O(3)-K(1)	108.77(11)

O(3)-C(34)-C(35)	108.17(15)	O(6)-C(39)-C(38)	108.53(17)
O(3)-C(34)-H(34A)	110.1	O(6)-C(39)-H(39A)	110.0
C(35)-C(34)-H(34A)	110.1	C(38)-C(39)-H(39A)	110.0
O(3)-C(34)-H(34B)	110.1	O(6)-C(39)-H(39B)	110.0
C(35)-C(34)-H(34B)	110.1	C(38)-C(39)-H(39B)	110.0
H(34A)-C(34)-H(34B)	108.4	H(39A)-C(39)-H(39B)	108.4
O(4)-C(35)-C(34)	109.03(16)	C(39)-O(6)-C(40)	112.79(16)
O(4)-C(35)-H(35A)	109.9	C(39)-O(6)-K(1)	112.62(11)
C(34)-C(35)-H(35A)	109.9	C(40)-O(6)-K(1)	113.38(12)
O(4)-C(35)-H(35B)	109.9	O(6)-C(40)-C(41)	107.71(17)
C(34)-C(35)-H(35B)	109.9	O(6)-C(40)-H(40A)	110.2
H(35A)-C(35)-H(35B)	108.3	C(41)-C(40)-H(40A)	110.2
C(35)-O(4)-C(36)	111.32(15)	O(6)-C(40)-H(40B)	110.2
C(35)-O(4)-K(1)	118.80(10)	C(41)-C(40)-H(40B)	110.2
C(36)-O(4)-K(1)	120.09(12)	H(40A)-C(40)-H(40B)	108.5
O(4)-C(36)-H(36A)	109.5	O(7)-C(41)-C(40)	108.35(18)
O(4)-C(36)-H(36B)	109.5	O(7)-C(41)-H(41A)	110.0
H(36A)-C(36)-H(36B)	109.5	C(40)-C(41)-H(41A)	110.0
O(4)-C(36)-H(36C)	109.5	O(7)-C(41)-H(41B)	110.0
H(36A)-C(36)-H(36C)	109.5	C(40)-C(41)-H(41B)	110.0
H(36B)-C(36)-H(36C)	109.5	H(41A)-C(41)-H(41B)	108.4
O(5)-C(37)-H(37A)	109.5	C(42)-O(7)-C(41)	112.74(16)
O(5)-C(37)-H(37B)	109.5	C(42)-O(7)-K(1)	113.98(12)
H(37A)-C(37)-H(37B)	109.5	C(41)-O(7)-K(1)	115.73(12)
O(5)-C(37)-H(37C)	109.5	O(7)-C(42)-C(43)	109.27(19)
H(37A)-C(37)-H(37C)	109.5	O(7)-C(42)-H(42A)	109.8
H(37B)-C(37)-H(37C)	109.5	C(43)-C(42)-H(42A)	109.8
C(37)-O(5)-C(38)	111.64(15)	O(7)-C(42)-H(42B)	109.8
C(37)-O(5)-K(1)	115.48(11)	C(43)-C(42)-H(42B)	109.8
C(38)-O(5)-K(1)	116.85(11)	H(42A)-C(42)-H(42B)	108.3
O(5)-C(38)-C(39)	108.48(16)	O(8)-C(43)-C(42)	109.60(19)
O(5)-C(38)-H(38A)	110.0	O(8)-C(43)-H(43A)	109.8
C(39)-C(38)-H(38A)	110.0	C(42)-C(43)-H(43A)	109.8
O(5)-C(38)-H(38B)	110.0	O(8)-C(43)-H(43B)	109.8
C(39)-C(38)-H(38B)	110.0	C(42)-C(43)-H(43B)	109.8
H(38A)-C(38)-H(38B)	108.4	H(43A)-C(43)-H(43B)	108.2

C(43)-O(8)-C(44)	111.18(19)
C(43)-O(8)-K(1)	115.45(12)
C(44)-O(8)-K(1)	117.67(14)
O(8)-C(44)-H(44A)	109.5
O(8)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
O(8)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(46)-C(45)-C(50)	121.4(3)
C(46)-C(45)-H(45)	119.3
C(50)-C(45)-H(45)	119.3
C(45)-C(46)-C(47)	120.5(3)
C(45)-C(46)-H(46)	119.7
C(47)-C(46)-H(46)	119.7
C(48)-C(47)-C(46)	120.0(3)
C(48)-C(47)-H(47)	120.0
C(46)-C(47)-H(47)	120.0
C(47)-C(48)-C(49)	121.5(3)
C(47)-C(48)-H(48)	119.2
C(49)-C(48)-H(48)	119.2
C(51)#1-C(49)-C(48)	122.9(2)
C(51)#1-C(49)-C(50)	119.3(2)
C(48)-C(49)-C(50)	117.8(2)
C(51)-C(50)-C(45)	122.3(2)
C(51)-C(50)-C(49)	118.9(2)
C(45)-C(50)-C(49)	118.7(2)
C(50)-C(51)-C(49)#1	121.8(2)
C(50)-C(51)-H(51)	119.1
C(49)#1-C(51)-H(51)	119.1

Symmetry transformations used to generate equivalent atoms:

#1 $-x+2, -y, -z+1$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 168. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	27(1)	30(1)	28(1)	-1(1)	7(1)	0(1)
C1	24(1)	40(1)	31(1)	0(1)	9(1)	2(1)
C2	28(1)	38(1)	31(1)	5(1)	5(1)	-3(1)
C3	36(1)	30(1)	30(1)	-1(1)	2(1)	-1(1)
C4	32(1)	36(1)	31(1)	-3(1)	11(1)	5(1)
C5	38(1)	58(2)	45(1)	14(1)	6(1)	-12(1)
C6	37(1)	68(2)	59(2)	31(1)	-2(1)	-16(1)
C7	35(1)	45(1)	79(2)	24(1)	-6(1)	-8(1)
C8	32(1)	38(1)	63(2)	7(1)	2(1)	-2(1)
C9	27(1)	38(1)	35(1)	-2(1)	5(1)	2(1)
C10	31(1)	45(1)	34(1)	0(1)	11(1)	-4(1)
C11	24(1)	36(1)	26(1)	0(1)	2(1)	-1(1)
C12	26(1)	37(1)	26(1)	-2(1)	5(1)	-3(1)
C13	28(1)	46(1)	35(1)	6(1)	1(1)	-9(1)
C14	26(1)	38(1)	40(1)	4(1)	-2(1)	-5(1)
C15	34(1)	26(1)	40(1)	-5(1)	9(1)	3(1)
C16	30(1)	42(1)	32(1)	-9(1)	8(1)	3(1)
C17	30(1)	42(1)	27(1)	3(1)	6(1)	-2(1)
C18	33(1)	28(1)	30(1)	2(1)	6(1)	1(1)
C19	34(1)	31(1)	29(1)	-2(1)	7(1)	4(1)
C20	28(1)	42(1)	41(1)	-3(1)	10(1)	4(1)
C21	34(1)	40(1)	48(1)	-4(1)	15(1)	-7(1)
C22	38(1)	27(1)	46(1)	-4(1)	13(1)	-3(1)
C23	34(1)	23(1)	38(1)	-5(1)	9(1)	1(1)
C24	33(1)	25(1)	25(1)	-1(1)	7(1)	2(1)
C25	29(1)	30(1)	26(1)	-5(1)	4(1)	1(1)
C26	31(1)	28(1)	21(1)	0(1)	4(1)	-1(1)
C27	31(1)	30(1)	20(1)	-3(1)	5(1)	1(1)
C28	32(1)	29(1)	27(1)	-5(1)	6(1)	-1(1)
K1	36(1)	36(1)	29(1)	-1(1)	6(1)	0(1)
C29	69(2)	68(2)	39(2)	5(1)	-3(1)	4(1)

O1	49(1)	53(1)	35(1)	1(1)	1(1)	9(1)
C30	46(1)	45(1)	49(2)	11(1)	9(1)	9(1)
C31	46(1)	32(1)	49(1)	5(1)	14(1)	5(1)
O2	45(1)	31(1)	34(1)	2(1)	8(1)	2(1)
C32	40(1)	46(1)	36(1)	-4(1)	12(1)	0(1)
C33	39(1)	52(1)	36(1)	6(1)	13(1)	2(1)
O3	39(1)	42(1)	38(1)	10(1)	13(1)	6(1)
C34	46(1)	42(1)	39(1)	12(1)	10(1)	5(1)
C35	43(1)	45(1)	37(1)	10(1)	4(1)	5(1)
O4	35(1)	52(1)	39(1)	3(1)	8(1)	4(1)
C36	44(1)	66(2)	54(2)	6(1)	16(1)	6(1)
C37	49(1)	58(1)	47(2)	-9(1)	13(1)	-12(1)
O5	38(1)	48(1)	41(1)	-7(1)	10(1)	-7(1)
C38	41(1)	39(1)	52(2)	-1(1)	14(1)	-6(1)
C39	58(1)	52(1)	48(2)	8(1)	20(1)	-7(1)
O6	62(1)	49(1)	30(1)	-3(1)	14(1)	-9(1)
C40	75(2)	71(2)	33(1)	-4(1)	20(1)	-14(1)
C41	82(2)	65(2)	34(1)	-15(1)	20(1)	-3(1)
O7	69(1)	42(1)	38(1)	-5(1)	14(1)	-6(1)
C42	105(2)	40(1)	38(1)	-4(1)	22(1)	-5(1)
C43	77(2)	48(1)	47(2)	-1(1)	1(1)	-20(1)
O8	49(1)	57(1)	51(1)	-10(1)	10(1)	-10(1)
C44	59(2)	94(2)	121(3)	-26(2)	36(2)	-21(2)
C45	68(2)	75(2)	58(2)	-12(2)	18(1)	-1(1)
C46	116(3)	80(2)	69(2)	4(2)	25(2)	11(2)
C47	150(3)	88(2)	57(2)	5(2)	24(2)	23(2)
C48	116(3)	85(2)	47(2)	-4(2)	18(2)	18(2)
C49	48(1)	72(2)	40(1)	-4(1)	13(1)	1(1)
C50	42(1)	63(2)	49(2)	-10(1)	16(1)	-2(1)
C51	49(1)	73(2)	37(1)	-16(1)	12(1)	-1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 168.

	x	y	z	U(eq)
H1	-590(15)	1205(6)	-177(13)	32(5)
H2	-586(15)	369(6)	-426(13)	39(5)
H3	756(14)	49(7)	-1185(12)	35(5)
H4	1892(14)	609(6)	-1716(12)	32(5)
H5	1297	2070	-3964	58
H6	656	2842	-4256	69
H7	-280	3204	-3214	69
H8	-681	2773	-1949	56
H9	-692	1987	-1070	41
H10	1571	1336	-2908	44
H15	2333(14)	1615(6)	762(13)	32(5)
H16	1291(16)	1193(6)	1674(13)	38(5)
H17	1537(15)	334(6)	1767(13)	39(5)
H18	2783(15)	9(7)	886(13)	38(5)
H19	6779	207	791	38
H20	8186	703	610	44
H21	7887	1524	420	48
H22	6198	1850	460	44
H23	4294	1748	679	38
H24	4816	96	908	34
H29A	3516	1636	3024	93
H29B	2767	2104	2885	93
H29C	2363	1630	3311	93
H30A	2166	2067	4651	57
H30B	2720	2548	4403	57
H31A	4188	2444	5889	51
H31B	3004	2518	6106	51
H32A	3200	1978	7574	48
H32B	4432	2136	7571	48
H33A	4431	1426	8518	50

H33B	3756	1164	7517	50
H34A	5394	626	7587	51
H34B	5894	874	8646	51
H35A	7399	1172	8073	51
H35B	7383	603	8086	51
H36A	7835	876	5820	81
H36B	8309	568	6803	81
H36C	8380	1135	6854	81
H37A	6239	2252	7284	77
H37B	7095	2633	7071	77
H37C	7482	2096	7332	77
H38A	8019	2002	5854	53
H38B	7705	2548	5593	53
H39A	6333	2293	4132	62
H39B	7569	2153	4107	62
H40A	6952	1480	3054	70
H40B	5692	1626	2987	70
H41A	5885	789	2716	71
H41B	6655	747	3835	71
H42A	5208	220	4201	73
H42B	4560	279	3051	73
H43A	3049	629	3513	72
H43B	3270	95	3916	72
H44A	2877	692	5926	133
H44B	2417	268	5167	133
H44C	2208	807	4805	133
H45	9923	1165	5650	80
H46	9393	1583	4206	106
H47	8940	1188	2662	119
H48	9090	376	2598	100
H51	10394	397	6523	64

Table 6. Torsion angles [°] for 168.

C16-Co1-C1-C2	-128.60(12)	C15-Co1-C3-C2	-126.24(19)
C3-Co1-C1-C2	33.63(11)	C4-Co1-C3-C2	-126.99(16)
C17-Co1-C1-C2	-89.99(13)	C18-Co1-C3-C2	128.73(11)
C15-Co1-C1-C2	-170.80(11)	C16-Co1-C3-C4	167.9(2)
C4-Co1-C1-C2	74.79(11)	C17-Co1-C3-C4	-144.87(11)
C18-Co1-C1-C2	-61.3(3)	C2-Co1-C3-C4	126.99(16)
C16-Co1-C1-C11	111.21(12)	C1-Co1-C3-C4	94.29(12)
C3-Co1-C1-C11	-86.55(13)	C15-Co1-C3-C4	0.8(2)
C17-Co1-C1-C11	149.82(11)	C18-Co1-C3-C4	-104.28(11)
C2-Co1-C1-C11	-120.18(17)	C2-C3-C4-C12	-30.3(3)
C15-Co1-C1-C11	69.02(13)	Co1-C3-C4-C12	-88.30(16)
C4-Co1-C1-C11	-45.39(12)	C2-C3-C4-Co1	58.03(15)
C18-Co1-C1-C11	178.5(2)	C16-Co1-C4-C3	-170.39(18)
C11-C1-C2-C3	32.7(3)	C17-Co1-C4-C3	77.80(19)
Co1-C1-C2-C3	-55.03(15)	C2-Co1-C4-C3	-33.84(11)
C11-C1-C2-Co1	87.77(16)	C1-Co1-C4-C3	-74.84(12)
C16-Co1-C2-C3	-165.82(11)	C15-Co1-C4-C3	-179.67(11)
C17-Co1-C2-C3	-118.12(12)	C18-Co1-C4-C3	91.95(12)
C1-Co1-C2-C3	127.38(16)	C16-Co1-C4-C12	-52.4(2)
C15-Co1-C2-C3	143.79(14)	C3-Co1-C4-C12	118.01(17)
C4-Co1-C2-C3	33.00(11)	C17-Co1-C4-C12	-164.20(14)
C18-Co1-C2-C3	-72.69(13)	C2-Co1-C4-C12	84.17(12)
C16-Co1-C2-C1	66.80(14)	C1-Co1-C4-C12	43.17(12)
C3-Co1-C2-C1	-127.38(16)	C15-Co1-C4-C12	-61.66(13)
C17-Co1-C2-C1	114.50(12)	C18-Co1-C4-C12	-150.05(11)
C15-Co1-C2-C1	16.41(19)	C13-C5-C6-C7	0.8(3)
C4-Co1-C2-C1	-94.38(12)	C5-C6-C7-C8	-2.6(3)
C18-Co1-C2-C1	159.93(11)	C6-C7-C8-C14	0.9(3)
C1-C2-C3-C4	-3.0(3)	C14-C9-C11-C12	3.7(3)
Co1-C2-C3-C4	-60.69(15)	C14-C9-C11-C1	179.71(17)
C1-C2-C3-Co1	57.73(15)	C2-C1-C11-C9	155.71(19)
C16-Co1-C3-C2	40.9(3)	Co1-C1-C11-C9	-135.76(17)
C17-Co1-C3-C2	88.14(13)	C2-C1-C11-C12	-28.1(2)
C1-Co1-C3-C2	-32.70(11)	Co1-C1-C11-C12	40.42(17)

C13-C10-C12-C11	3.0(3)	Co1-C15-C16-C17	58.18(15)
C13-C10-C12-C4	-174.62(18)	C25-C15-C16-Co1	-89.11(17)
C9-C11-C12-C10	-6.6(3)	C3-Co1-C16-C17	61.0(3)
C1-C11-C12-C10	176.97(17)	C2-Co1-C16-C17	92.50(13)
C9-C11-C12-C4	171.28(17)	C1-Co1-C16-C17	129.92(11)
C1-C11-C12-C4	-5.1(2)	C15-Co1-C16-C17	-126.64(16)
C3-C4-C12-C10	-148.33(19)	C4-Co1-C16-C17	-139.35(18)
Co1-C4-C12-C10	145.09(17)	C18-Co1-C16-C17	-32.96(11)
C3-C4-C12-C11	34.0(2)	C3-Co1-C16-C15	-172.3(2)
Co1-C4-C12-C11	-32.62(17)	C17-Co1-C16-C15	126.64(16)
C6-C5-C13-C10	-177.81(19)	C2-Co1-C16-C15	-140.86(11)
C6-C5-C13-C14	2.7(3)	C1-Co1-C16-C15	-103.44(11)
C12-C10-C13-C5	-176.06(18)	C4-Co1-C16-C15	-12.7(2)
C12-C10-C13-C14	3.4(3)	C18-Co1-C16-C15	93.68(12)
C7-C8-C14-C9	-174.79(19)	C15-C16-C17-C18	-0.4(3)
C7-C8-C14-C13	2.6(3)	Co1-C16-C17-C18	59.87(15)
C11-C9-C14-C8	-179.81(18)	C15-C16-C17-Co1	-60.31(16)
C11-C9-C14-C13	2.8(3)	C3-Co1-C17-C16	-159.94(11)
C5-C13-C14-C8	-4.3(3)	C2-Co1-C17-C16	-112.47(12)
C10-C13-C14-C8	176.15(17)	C1-Co1-C17-C16	-66.48(13)
C5-C13-C14-C9	173.22(17)	C15-Co1-C17-C16	33.56(11)
C10-C13-C14-C9	-6.3(3)	C4-Co1-C17-C16	147.03(15)
C3-Co1-C15-C16	173.96(18)	C18-Co1-C17-C16	126.59(16)
C17-Co1-C15-C16	-34.04(11)	C16-Co1-C17-C18	-126.59(16)
C2-Co1-C15-C16	77.07(18)	C3-Co1-C17-C18	73.47(14)
C1-Co1-C15-C16	88.14(12)	C2-Co1-C17-C18	120.95(11)
C4-Co1-C15-C16	174.51(11)	C1-Co1-C17-C18	166.93(10)
C18-Co1-C15-C16	-74.94(12)	C15-Co1-C17-C18	-93.03(12)
C16-Co1-C15-C25	118.61(18)	C4-Co1-C17-C18	20.4(2)
C3-Co1-C15-C25	-67.4(2)	C16-C17-C18-C26	32.5(3)
C17-Co1-C15-C25	84.57(13)	Co1-C17-C18-C26	88.28(16)
C2-Co1-C15-C25	-164.32(13)	C16-C17-C18-Co1	-55.79(15)
C1-Co1-C15-C25	-153.26(12)	C16-Co1-C18-C17	34.27(11)
C4-Co1-C15-C25	-66.89(14)	C3-Co1-C18-C17	-126.62(12)
C18-Co1-C15-C25	43.67(12)	C2-Co1-C18-C17	-84.72(14)
C25-C15-C16-C17	-30.9(3)	C1-Co1-C18-C17	-37.6(3)

C15-Co1-C18-C17	76.23(12)	C19-C27-C28-C22	1.6(3)
C4-Co1-C18-C17	-169.77(11)	C24-C27-C28-C22	-179.07(16)
C16-Co1-C18-C26	-84.32(12)	C19-C27-C28-C23	-177.31(16)
C3-Co1-C18-C26	114.80(12)	C24-C27-C28-C23	2.0(3)
C17-Co1-C18-C26	-118.58(17)	O4-K1-O1-C30	-80.8(4)
C2-Co1-C18-C26	156.70(11)	O7-K1-O1-C30	157.27(14)
C1-Co1-C18-C26	-156.2(2)	O8-K1-O1-C30	97.00(14)
C15-Co1-C18-C26	-42.35(12)	O5-K1-O1-C30	-83.08(14)
C4-Co1-C18-C26	71.65(13)	O3-K1-O1-C30	-0.32(15)
C27-C19-C20-C21	-0.7(3)	O6-K1-O1-C30	-142.68(14)
C19-C20-C21-C22	1.1(3)	O2-K1-O1-C30	6.71(13)
C20-C21-C22-C28	-0.1(3)	C31-K1-O1-C30	-14.14(13)
C28-C23-C25-C15	-177.63(17)	O4-K1-O1-C29	136.0(3)
C28-C23-C25-C26	-0.4(3)	O7-K1-O1-C29	14.09(15)
C16-C15-C25-C23	-153.21(19)	O8-K1-O1-C29	-46.18(15)
Co1-C15-C25-C23	139.60(17)	O5-K1-O1-C29	133.73(15)
C16-C15-C25-C26	29.5(2)	O3-K1-O1-C29	-143.51(14)
Co1-C15-C25-C26	-37.67(18)	O6-K1-O1-C29	74.13(15)
C27-C24-C26-C25	-0.5(3)	O2-K1-O1-C29	-136.47(16)
C27-C24-C26-C18	175.98(16)	C31-K1-O1-C29	-157.33(17)
C23-C25-C26-C24	1.3(3)	C29-O1-C30-C31	170.01(17)
C15-C25-C26-C24	178.76(16)	K1-O1-C30-C31	24.3(2)
C23-C25-C26-C18	-175.49(16)	O1-C30-C31-O2	-66.0(2)
C15-C25-C26-C18	2.0(2)	O1-C30-C31-K1	-16.83(14)
C17-C18-C26-C24	150.27(18)	O4-K1-C31-O2	-58.70(13)
Co1-C18-C26-C24	-142.74(16)	O1-K1-C31-O2	129.86(13)
C17-C18-C26-C25	-33.1(2)	O7-K1-C31-O2	119.07(10)
Co1-C18-C26-C25	33.84(17)	O8-K1-C31-O2	54.52(11)
C20-C19-C27-C24	-179.97(17)	O5-K1-C31-O2	-126.47(11)
C20-C19-C27-C28	-0.7(3)	O3-K1-C31-O2	-37.73(10)
C26-C24-C27-C19	178.10(16)	O6-K1-C31-O2	-170.11(10)
C26-C24-C27-C28	-1.2(3)	O4-K1-C31-C30	-176.73(11)
C21-C22-C28-C23	177.65(18)	O1-K1-C31-C30	11.83(11)
C21-C22-C28-C27	-1.2(3)	O7-K1-C31-C30	1.04(14)
C25-C23-C28-C22	179.91(18)	O8-K1-C31-C30	-63.50(12)
C25-C23-C28-C27	-1.2(3)	O5-K1-C31-C30	115.50(12)

O3-K1-C31-C30	-155.76(12)	O7-K1-O3-C34	23.90(15)
O6-K1-C31-C30	71.86(12)	O8-K1-O3-C34	63.01(11)
O2-K1-C31-C30	-118.03(17)	O5-K1-O3-C34	-118.13(11)
C30-C31-O2-C32	-166.78(16)	O6-K1-O3-C34	-79.49(12)
K1-C31-O2-C32	124.71(14)	O2-K1-O3-C34	150.90(12)
C30-C31-O2-K1	68.51(16)	C31-K1-O3-C34	167.66(12)
O4-K1-O2-C32	12.44(13)	C33-O3-C34-C35	-170.56(16)
O1-K1-O2-C32	-159.91(12)	K1-O3-C34-C35	60.46(17)
O7-K1-O2-C32	155.89(11)	O3-C34-C35-O4	-64.7(2)
O8-K1-O2-C32	108.75(12)	C34-C35-O4-C36	-178.97(16)
O5-K1-O2-C32	-72.46(11)	C34-C35-O4-K1	35.05(19)
O3-K1-O2-C32	12.88(11)	O1-K1-O4-C35	80.5(4)
O6-K1-O2-C32	-109.35(12)	O7-K1-O4-C35	-158.25(12)
C31-K1-O2-C32	-122.95(17)	O8-K1-O4-C35	-97.31(13)
O4-K1-O2-C31	135.39(11)	O5-K1-O4-C35	82.77(13)
O1-K1-O2-C31	-36.96(11)	O3-K1-O4-C35	-3.71(12)
O7-K1-O2-C31	-81.16(12)	O6-K1-O4-C35	142.58(13)
O8-K1-O2-C31	-128.29(11)	O2-K1-O4-C35	-3.27(14)
O5-K1-O2-C31	50.49(11)	C31-K1-O4-C35	19.96(15)
O3-K1-O2-C31	135.84(12)	O1-K1-O4-C36	-62.5(4)
O6-K1-O2-C31	13.60(13)	O7-K1-O4-C36	58.79(14)
C31-O2-C32-C33	-162.39(15)	O8-K1-O4-C36	119.73(14)
K1-O2-C32-C33	-45.31(17)	O5-K1-O4-C36	-60.19(14)
O2-C32-C33-O3	66.3(2)	O3-K1-O4-C36	-146.67(15)
C32-C33-O3-C34	179.16(16)	O6-K1-O4-C36	-0.38(14)
C32-C33-O3-K1	-55.01(17)	O2-K1-O4-C36	-146.23(13)
O4-K1-O3-C33	-157.70(13)	C31-K1-O4-C36	-123.00(14)
O1-K1-O3-C33	29.89(13)	O4-K1-O5-C37	-58.88(13)
O7-K1-O3-C33	-104.25(13)	O1-K1-O5-C37	120.86(13)
O8-K1-O3-C33	-65.15(12)	O7-K1-O5-C37	-156.52(12)
O5-K1-O3-C33	113.71(12)	O8-K1-O5-C37	124.4(18)
O6-K1-O3-C33	152.35(11)	O3-K1-O5-C37	1.59(13)
O2-K1-O3-C33	22.74(11)	O6-K1-O5-C37	-146.84(14)
C31-K1-O3-C33	39.50(12)	O2-K1-O5-C37	60.44(13)
O4-K1-O3-C34	-29.55(11)	C31-K1-O5-C37	79.37(13)
O1-K1-O3-C34	158.05(11)	O4-K1-O5-C38	75.48(13)

O1-K1-O5-C38	-104.79(13)	O5-K1-O7-C42	160.35(14)
O7-K1-O5-C38	-22.16(14)	O3-K1-O7-C42	24.93(19)
O8-K1-O5-C38	-101.2(19)	O6-K1-O7-C42	150.72(16)
O3-K1-O5-C38	135.95(13)	O2-K1-O7-C42	-78.47(16)
O6-K1-O5-C38	-12.49(12)	C31-K1-O7-C42	-108.58(15)
O2-K1-O5-C38	-165.21(13)	O4-K1-O7-C41	-63.36(14)
C31-K1-O5-C38	-146.28(13)	O1-K1-O7-C41	110.91(14)
C37-O5-C38-C39	-179.66(17)	O8-K1-O7-C41	-154.34(15)
K1-O5-C38-C39	44.33(19)	O5-K1-O7-C41	27.19(15)
O5-C38-C39-O6	-65.9(2)	O3-K1-O7-C41	-108.22(15)
C38-C39-O6-C40	-175.69(17)	O6-K1-O7-C41	17.57(13)
C38-C39-O6-K1	54.42(19)	O2-K1-O7-C41	148.37(13)
O4-K1-O6-C39	-110.34(13)	C31-K1-O7-C41	118.26(14)
O1-K1-O6-C39	63.75(13)	C41-O7-C42-C43	-173.34(18)
O7-K1-O6-C39	147.82(14)	K1-O7-C42-C43	52.1(2)
O8-K1-O6-C39	155.99(13)	O7-C42-C43-O8	-63.7(2)
O5-K1-O6-C39	-22.45(12)	C42-C43-O8-C44	-179.4(2)
O3-K1-O6-C39	-68.56(14)	C42-C43-O8-K1	43.2(2)
O2-K1-O6-C39	21.58(16)	O4-K1-O8-C43	-109.32(15)
C31-K1-O6-C39	27.61(14)	O1-K1-O8-C43	70.93(15)
O4-K1-O6-C40	120.07(14)	O7-K1-O8-C43	-12.44(14)
O1-K1-O6-C40	-65.84(14)	O5-K1-O8-C43	67.4(19)
O7-K1-O6-C40	18.23(13)	O3-K1-O8-C43	-169.90(14)
O8-K1-O6-C40	26.40(15)	O6-K1-O8-C43	-20.58(16)
O5-K1-O6-C40	-152.04(15)	O2-K1-O8-C43	131.32(14)
O3-K1-O6-C40	161.85(13)	C31-K1-O8-C43	112.15(14)
O2-K1-O6-C40	-108.01(14)	O4-K1-O8-C44	116.13(18)
C31-K1-O6-C40	-101.98(14)	O1-K1-O8-C44	-63.61(18)
C39-O6-C40-C41	-179.60(19)	O7-K1-O8-C44	-146.98(19)
K1-O6-C40-C41	-50.1(2)	O5-K1-O8-C44	-67.2(19)
O6-C40-C41-O7	66.8(2)	O3-K1-O8-C44	55.55(18)
C40-C41-O7-C42	176.00(18)	O6-K1-O8-C44	-155.12(17)
C40-C41-O7-K1	-50.3(2)	O2-K1-O8-C44	-3.22(18)
O4-K1-O7-C42	69.80(15)	C31-K1-O8-C44	-22.39(18)
O1-K1-O7-C42	-115.94(15)	C50-C45-C46-C47	1.5(4)
O8-K1-O7-C42	-21.18(14)	C45-C46-C47-C48	-1.2(5)

C46-C47-C48-C49	-0.4(5)	C48-C49-C50-C51	179.7(2)
C47-C48-C49-C51#1	-178.6(3)	C51#1-C49-C50-C45	178.9(2)
C47-C48-C49-C50	1.6(4)	C48-C49-C50-C45	-1.3(3)
C46-C45-C50-C51	178.7(3)	C45-C50-C51-C49#1	-178.8(2)
C46-C45-C50-C49	-0.2(4)	C49-C50-C51-C49#1	0.1(4)
C51#1-C49-C50-C51	-0.1(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

REFERENCE NUMBER: 99325 [**1b**]

CRYSTAL STRUCTURE REPORT

$C_{44} H_{52} Co K O_4$

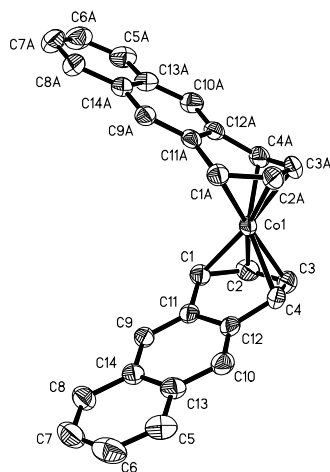
or

$[K(THF)_4][Co(C_{14}H_{10})_2]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

November 07, 1999



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Data collection

A crystal (approximate dimensions 0.34 x 0.26 x 0.20 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 99 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 30 seconds and a detector distance of 4.91 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 6246 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SHELXS-97⁴ and refined using SHELXL-97.⁴ The space group *C2/c* 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. Hydrogen atoms on carbon atoms C1, C2, C3, and C4 were found from the difference map and refined with individual isotropic displacement parameters. The remaining 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 $R1 = 0.0476$ and $wR2 = 0.1410$ (F^2 , all data).

Structure description

The structure is the one suggested. The cobalt and potassium atoms lie on a two fold axis; thus, one half of the molecule is unique. The cobalt anion is coordinated by two tetrahapto-anthracene ligands. The potassium cation is surrounded by four THF (tetrahydrofuran) molecules occupying four approximate positions of an octahedron. The other two positions are "occupied" by C11, C12, C13 C11A, C12A, C13A of the anthracene ligands at a distance that varies from 3.1 to 3.4 Å. The cobalt-potassium distance is 4.0 Å and the dihedral (fold) angle is 30.8°. Both unique THF molecules were modeled as disordered over two positions (74:26 and 78:22).

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
⁴ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

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

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2 (F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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

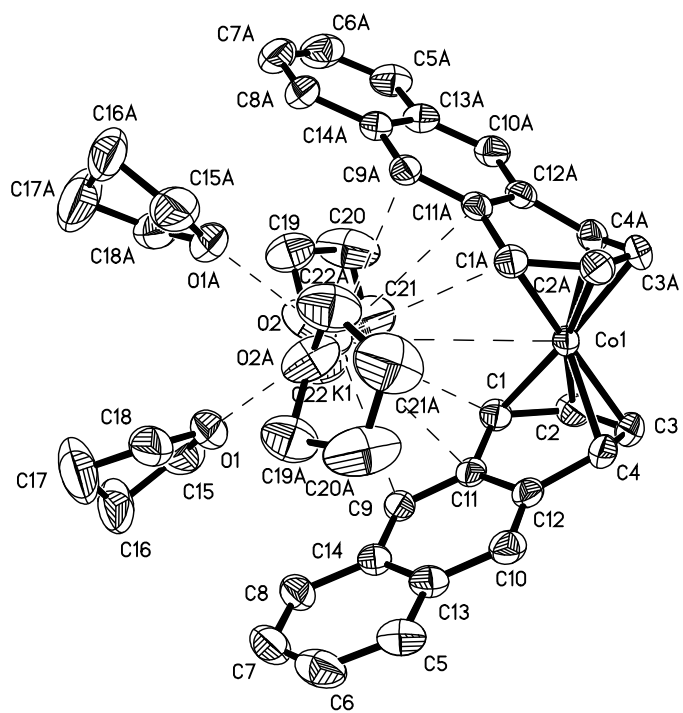
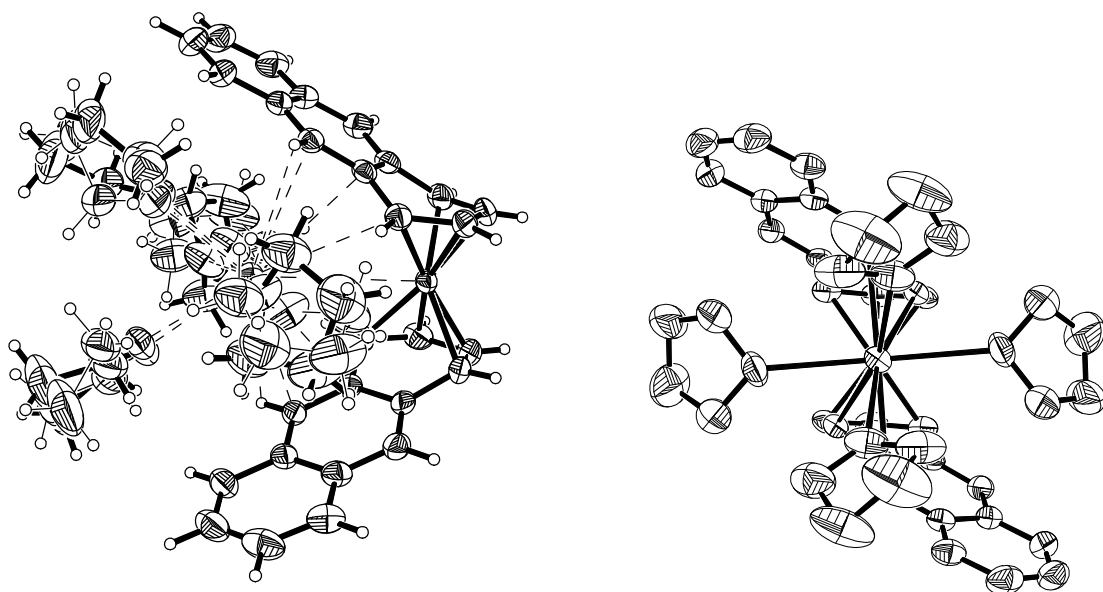


Table 1. Crystal data and structure refinement for 99325.

Identification code	99325	
Empirical formula	C ₄₄ H ₅₂ Co K O ₄	
Formula weight	742.89	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	<i>C</i> 2/ <i>c</i>	
Unit cell dimensions	<i>a</i> = 20.170(2) Å	$\alpha = 90^\circ$
	<i>b</i> = 16.421(2) Å	$\beta = 120.527(2)^\circ$
	<i>c</i> = 13.2241(15) Å	$\gamma = 90^\circ$
Volume	3772.8(7) Å ³	
<i>Z</i>	4	
Density (calculated)	1.308 Mg/m ³	
Absorption coefficient	0.607 mm ⁻¹	
<i>F</i> (000)	1576	
Crystal color, morphology	red-black, block	
Crystal size	0.34 x 0.26 x 0.20 mm ³	
Theta range for data collection	1.71 to 27.61°	
Index ranges	-20 ≤ <i>h</i> ≤ 26, -19 ≤ <i>k</i> ≤ 21, -17 ≤ <i>l</i> ≤ 16	
Reflections collected	11816	
Independent reflections	4298 [<i>R</i> (int) = 0.0317]	
Observed reflections	3577	
Completeness to theta = 27.61°	98.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8882 and 0.8201	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	4298 / 54 / 275	
Goodness-of-fit on <i>F</i> ²	1.038	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0476, <i>wR</i> 2 = 0.1343	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0561, <i>wR</i> 2 = 0.1410	
Largest diff. peak and hole	0.685 and -0.718 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 99325. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	0	361(1)	7500	30(1)
C1	906(1)	1017(1)	8921(2)	34(1)
C2	878(1)	159(2)	9084(2)	41(1)
C3	925(1)	-354(1)	8273(3)	45(1)
C4	973(1)	29(1)	7361(2)	39(1)
C5	2407(2)	2143(2)	6522(2)	48(1)
C6	2707(2)	2921(2)	6709(3)	57(1)
C7	2704(2)	3416(2)	7560(3)	54(1)
C8	2392(1)	3143(2)	8205(2)	44(1)
C9	1702(1)	2073(1)	8639(2)	32(1)
C10	1744(1)	1056(1)	6983(2)	38(1)
C11	1350(1)	1324(1)	8412(2)	30(1)
C12	1379(1)	796(1)	7562(2)	33(1)
C13	2077(1)	1839(2)	7169(2)	38(1)
C14	2063(1)	2357(1)	8025(2)	35(1)
K1	0	2775(1)	7500	35(1)
O1	993(10)	4092(7)	8471(10)	59(2)
C15	1415(10)	4411(9)	9624(9)	72(2)
C16	1892(6)	5100(5)	9543(8)	95(2)
C17	1353(7)	5441(5)	8324(9)	121(4)
C18	1014(5)	4668(5)	7673(8)	73(2)
O1'	920(30)	4150(20)	8440(30)	59(2)
C15'	1500(30)	4420(30)	9570(20)	72(2)
C16'	1760(20)	5241(17)	9380(20)	95(2)
C17'	1583(15)	5182(16)	8120(30)	121(4)
C18'	813(11)	4768(19)	7600(20)	73(2)
O2	121(2)	3052(2)	9618(2)	61(1)
C19	-533(2)	3248(3)	9754(3)	66(1)
C20	-480(3)	2578(5)	10622(4)	93(2)
C21	330(3)	2348(4)	11258(5)	98(2)
C22	711(3)	2889(3)	10758(4)	75(1)

O2'	-79(7)	2696(7)	9491(6)	61(1)
C19'	29(9)	2051(8)	10232(11)	66(1)
C20'	-266(13)	2379(12)	11007(17)	93(2)
C21'	-192(14)	3253(11)	10983(17)	98(2)
C22'	157(9)	3405(9)	10184(13)	75(1)

Table 3. Bond lengths [Å] and angles [°] for 99325.

Co(1)-C(2)#1	1.966(2)	C(10)-H(10A)	0.9500
Co(1)-C(2)	1.967(2)	C(11)-C(12)	1.445(3)
Co(1)-C(3)#1	1.991(2)	C(11)-K(1)	3.348(2)
Co(1)-C(3)	1.991(2)	C(13)-C(14)	1.427(3)
Co(1)-C(1)	2.131(2)	K(1)-O(2')	2.721(4)
Co(1)-C(1)#1	2.131(2)	K(1)-O(2')#1	2.721(4)
Co(1)-C(4)#1	2.132(2)	K(1)-O(2)	2.724(2)
Co(1)-C(4)	2.132(2)	K(1)-O(2)#1	2.724(2)
Co(1)-K(1)	3.9638(8)	K(1)-O(1)#1	2.779(2)
C(1)-C(2)	1.431(3)	K(1)-O(1)	2.779(2)
C(1)-C(11)	1.458(3)	K(1)-O(1')	2.779(4)
C(1)-K(1)	3.422(2)	K(1)-O(1')#1	2.779(4)
C(1)-H(1)	1.04(2)	K(1)-C(9)#1	3.182(2)
C(2)-C(3)	1.403(4)	K(1)-C(11)#1	3.348(2)
C(2)-H(2)	0.97(3)	O(1)-C(15)	1.416(8)
C(3)-C(4)	1.407(4)	O(1)-C(18)	1.434(7)
C(3)-H(3)	0.86(3)	C(15)-C(16)	1.524(8)
C(4)-C(12)	1.452(3)	C(15)-H(15A)	0.9900
C(4)-H(4)	0.97(3)	C(15)-H(15B)	0.9900
C(5)-C(6)	1.382(4)	C(16)-C(17)	1.522(10)
C(5)-C(13)	1.416(3)	C(16)-H(16A)	0.9900
C(5)-H(5A)	0.9500	C(16)-H(16B)	0.9900
C(6)-C(7)	1.391(5)	C(17)-C(18)	1.490(9)
C(6)-H(6A)	0.9500	C(17)-H(17A)	0.9900
C(7)-C(8)	1.366(4)	C(17)-H(17B)	0.9900
C(7)-H(7A)	0.9500	C(18)-H(18A)	0.9900
C(8)-C(14)	1.416(3)	C(18)-H(18B)	0.9900
C(8)-H(8A)	0.9500	O(1')-C(15')	1.427(14)
C(9)-C(11)	1.375(3)	O(1')-C(18')	1.437(14)
C(9)-C(14)	1.418(3)	C(15')-C(16')	1.510(15)
C(9)-K(1)	3.183(2)	C(15')-H(15C)	0.9900
C(9)-H(9A)	0.9500	C(15')-H(15D)	0.9900
C(10)-C(12)	1.371(3)	C(16')-C(17')	1.528(18)
C(10)-C(13)	1.413(3)	C(16')-H(16C)	0.9900

C(16')-H(16D)	0.9900	C(2)-Co(1)-C(3)	41.52(11)
C(17')-C(18')	1.505(15)	C(3)#1-Co(1)-C(3)	107.72(14)
C(17')-H(17C)	0.9900	C(2)#1-Co(1)-C(1)	158.37(10)
C(17')-H(17D)	0.9900	C(2)-Co(1)-C(1)	40.64(9)
C(18')-H(18C)	0.9900	C(3)#1-Co(1)-C(1)	155.61(11)
C(18')-H(18D)	0.9900	C(3)-Co(1)-C(1)	71.68(10)
O(2)-C(22)	1.392(5)	C(2)#1-Co(1)-C(1)#1	40.64(9)
O(2)-C(19)	1.455(5)	C(2)-Co(1)-C(1)#1	158.37(10)
C(19)-C(20)	1.554(7)	C(3)#1-Co(1)-C(1)#1	71.69(10)
C(19)-H(19A)	0.9900	C(3)-Co(1)-C(1)#1	155.61(11)
C(19)-H(19B)	0.9900	C(1)-Co(1)-C(1)#1	119.25(12)
C(20)-C(21)	1.457(7)	C(2)#1-Co(1)-C(4)#1	71.22(10)
C(20)-H(20A)	0.9900	C(2)-Co(1)-C(4)#1	103.62(10)
C(20)-H(20B)	0.9900	C(3)#1-Co(1)-C(4)#1	39.71(11)
C(21)-C(22)	1.528(7)	C(3)-Co(1)-C(4)#1	117.85(10)
C(21)-H(21A)	0.9900	C(1)-Co(1)-C(4)#1	117.87(9)
C(21)-H(21B)	0.9900	C(1)#1-Co(1)-C(4)#1	77.97(9)
C(22)-H(22A)	0.9900	C(2)#1-Co(1)-C(4)	103.62(10)
C(22)-H(22B)	0.9900	C(2)-Co(1)-C(4)	71.22(10)
O(2')-C(19')	1.383(12)	C(3)#1-Co(1)-C(4)	117.85(10)
O(2')-C(22')	1.408(13)	C(3)-Co(1)-C(4)	39.71(11)
C(19')-C(20')	1.521(15)	C(1)-Co(1)-C(4)	77.97(9)
C(19')-H(19C)	0.9900	C(1)#1-Co(1)-C(4)	117.87(9)
C(19')-H(19D)	0.9900	C(4)#1-Co(1)-C(4)	150.32(12)
C(20')-C(21')	1.445(18)	C(2)#1-Co(1)-K(1)	99.72(7)
C(20')-H(20C)	0.9900	C(2)-Co(1)-K(1)	99.72(7)
C(20')-H(20D)	0.9900	C(3)#1-Co(1)-K(1)	126.14(7)
C(21')-C(22')	1.559(14)	C(3)-Co(1)-K(1)	126.14(7)
C(21')-H(21C)	0.9900	C(1)-Co(1)-K(1)	59.62(6)
C(21')-H(21D)	0.9900	C(1)#1-Co(1)-K(1)	59.62(6)
C(22')-H(22C)	0.9900	C(4)#1-Co(1)-K(1)	104.84(6)
C(22')-H(22D)	0.9900	C(4)-Co(1)-K(1)	104.84(6)
C(2)#1-Co(1)-C(2)	160.56(14)	C(2)-C(1)-C(11)	119.3(2)
C(2)#1-Co(1)-C(3)#1	41.52(11)	C(2)-C(1)-Co(1)	63.50(12)
C(2)-Co(1)-C(3)#1	123.33(11)	C(11)-C(1)-Co(1)	102.74(13)
C(2)#1-Co(1)-C(3)	123.33(11)	C(2)-C(1)-K(1)	149.64(15)

C(11)-C(1)-K(1)	74.75(11)	C(11)-C(9)-C(14)	121.81(19)
Co(1)-C(1)-K(1)	87.88(6)	C(11)-C(9)-K(1)	84.71(12)
C(2)-C(1)-H(1)	115.5(13)	C(14)-C(9)-K(1)	110.77(13)
C(11)-C(1)-H(1)	119.9(14)	C(11)-C(9)-H(9A)	119.1
Co(1)-C(1)-H(1)	122.6(14)	C(14)-C(9)-H(9A)	119.1
K(1)-C(1)-H(1)	70.3(13)	K(1)-C(9)-H(9A)	74.4
C(3)-C(2)-C(1)	117.0(2)	C(12)-C(10)-C(13)	121.9(2)
C(3)-C(2)-Co(1)	70.18(14)	C(12)-C(10)-H(10A)	119.0
C(1)-C(2)-Co(1)	75.86(13)	C(13)-C(10)-H(10A)	119.0
C(3)-C(2)-H(2)	118.0(18)	C(9)-C(11)-C(12)	119.1(2)
C(1)-C(2)-H(2)	124.8(18)	C(9)-C(11)-C(1)	125.36(19)
Co(1)-C(2)-H(2)	119.3(18)	C(12)-C(11)-C(1)	115.44(18)
C(2)-C(3)-C(4)	116.6(2)	C(9)-C(11)-K(1)	71.17(11)
C(2)-C(3)-Co(1)	68.30(13)	C(12)-C(11)-K(1)	119.60(12)
C(4)-C(3)-Co(1)	75.56(13)	C(1)-C(11)-K(1)	80.42(11)
C(2)-C(3)-H(3)	122.9(19)	C(10)-C(12)-C(11)	119.50(19)
C(4)-C(3)-H(3)	120.2(19)	C(10)-C(12)-C(4)	125.6(2)
Co(1)-C(3)-H(3)	120.7(19)	C(11)-C(12)-C(4)	114.9(2)
C(3)-C(4)-C(12)	120.6(2)	C(10)-C(13)-C(5)	122.9(2)
C(3)-C(4)-Co(1)	64.73(13)	C(10)-C(13)-C(14)	118.7(2)
C(12)-C(4)-Co(1)	102.76(14)	C(5)-C(13)-C(14)	118.3(2)
C(3)-C(4)-H(4)	120.2(16)	C(8)-C(14)-C(9)	122.4(2)
C(12)-C(4)-H(4)	114.2(17)	C(8)-C(14)-C(13)	118.8(2)
Co(1)-C(4)-H(4)	124.1(18)	C(9)-C(14)-C(13)	118.8(2)
C(6)-C(5)-C(13)	121.0(3)	O(2')-K(1)-O(2')#1	174.5(5)
C(6)-C(5)-H(5A)	119.5	O(2')-K(1)-O(2)	14.4(2)
C(13)-C(5)-H(5A)	119.5	O(2')#1-K(1)-O(2)	169.9(3)
C(5)-C(6)-C(7)	120.2(2)	O(2')-K(1)-O(2)#1	169.9(3)
C(5)-C(6)-H(6A)	119.9	O(2')#1-K(1)-O(2)#1	14.4(2)
C(7)-C(6)-H(6A)	119.9	O(2)-K(1)-O(2)#1	160.78(15)
C(8)-C(7)-C(6)	120.5(2)	O(2')-K(1)-O(1)#1	95.8(5)
C(8)-C(7)-H(7A)	119.8	O(2')#1-K(1)-O(1)#1	88.4(4)
C(6)-C(7)-H(7A)	119.8	O(2)-K(1)-O(1)#1	90.7(3)
C(7)-C(8)-C(14)	121.2(3)	O(2)#1-K(1)-O(1)#1	74.2(4)
C(7)-C(8)-H(8A)	119.4	O(2')-K(1)-O(1)	88.4(4)
C(14)-C(8)-H(8A)	119.4	O(2')#1-K(1)-O(1)	95.8(5)

O(2)-K(1)-O(1)	74.2(4)	O(2)#1-K(1)-C(11)#1	96.70(8)
O(2)#1-K(1)-O(1)	90.7(3)	O(1)#1-K(1)-C(11)#1	97.1(5)
O(1)#1-K(1)-O(1)	77.8(8)	O(1)-K(1)-C(11)#1	169.6(5)
O(2')-K(1)-O(1')	87.8(11)	O(1')-K(1)-C(11)#1	167.0(15)
O(2')#1-K(1)-O(1')	96.7(11)	O(1')#1-K(1)-C(11)#1	100.3(14)
O(2)-K(1)-O(1')	73.4(11)	C(9)#1-K(1)-C(11)#1	24.13(5)
O(2)#1-K(1)-O(1')	90.8(9)	C(9)-K(1)-C(11)#1	113.40(6)
O(1)#1-K(1)-O(1')	74.8(9)	O(2')-K(1)-C(11)	93.1(3)
O(1)-K(1)-O(1')	3(2)	O(2')#1-K(1)-C(11)	83.0(2)
O(2')-K(1)-O(1')#1	96.7(11)	O(2)-K(1)-C(11)	96.70(8)
O(2')#1-K(1)-O(1')#1	87.8(11)	O(2)#1-K(1)-C(11)	96.95(7)
O(2)-K(1)-O(1')#1	90.8(9)	O(1)#1-K(1)-C(11)	169.6(5)
O(2)#1-K(1)-O(1')#1	73.4(11)	O(1)-K(1)-C(11)	97.1(5)
O(1)#1-K(1)-O(1')#1	3(2)	O(1')-K(1)-C(11)	100.3(14)
O(1)-K(1)-O(1')#1	74.8(9)	O(1')#1-K(1)-C(11)	167.0(15)
O(1')-K(1)-O(1')#1	72(3)	C(9)#1-K(1)-C(11)	113.41(6)
O(2')-K(1)-C(9)#1	82.0(2)	C(9)-K(1)-C(11)	24.13(5)
O(2')#1-K(1)-C(9)#1	96.0(3)	C(11)#1-K(1)-C(11)	89.28(7)
O(2)-K(1)-C(9)#1	93.39(7)	C(15)-O(1)-C(18)	108.8(5)
O(2)#1-K(1)-C(9)#1	93.55(8)	C(15)-O(1)-K(1)	133.1(8)
O(1)#1-K(1)-C(9)#1	73.3(5)	C(18)-O(1)-K(1)	117.2(6)
O(1)-K(1)-C(9)#1	148.4(5)	O(1)-C(15)-C(16)	104.8(7)
O(1')-K(1)-C(9)#1	145.2(15)	O(1)-C(15)-H(15A)	110.8
O(1')#1-K(1)-C(9)#1	76.5(14)	C(16)-C(15)-H(15A)	110.8
O(2')-K(1)-C(9)	96.0(3)	O(1)-C(15)-H(15B)	110.8
O(2')#1-K(1)-C(9)	82.0(2)	C(16)-C(15)-H(15B)	110.8
O(2)-K(1)-C(9)	93.55(8)	H(15A)-C(15)-H(15B)	108.9
O(2)#1-K(1)-C(9)	93.39(7)	C(17)-C(16)-C(15)	102.1(8)
O(1)#1-K(1)-C(9)	148.4(5)	C(17)-C(16)-H(16A)	111.3
O(1)-K(1)-C(9)	73.3(5)	C(15)-C(16)-H(16A)	111.3
O(1')-K(1)-C(9)	76.5(14)	C(17)-C(16)-H(16B)	111.3
O(1')#1-K(1)-C(9)	145.2(15)	C(15)-C(16)-H(16B)	111.3
C(9)#1-K(1)-C(9)	137.53(8)	H(16A)-C(16)-H(16B)	109.2
O(2')-K(1)-C(11)#1	83.0(2)	C(18)-C(17)-C(16)	99.8(7)
O(2')#1-K(1)-C(11)#1	93.1(3)	C(18)-C(17)-H(17A)	111.8
O(2)-K(1)-C(11)#1	96.95(7)	C(16)-C(17)-H(17A)	111.8

C(18)-C(17)-H(17B)	111.8	C(22)-O(2)-C(19)	103.8(3)
C(16)-C(17)-H(17B)	111.8	C(22)-O(2)-K(1)	131.5(3)
H(17A)-C(17)-H(17B)	109.5	C(19)-O(2)-K(1)	123.4(2)
O(1)-C(18)-C(17)	108.2(7)	O(2)-C(19)-C(20)	102.0(4)
O(1)-C(18)-H(18A)	110.1	O(2)-C(19)-H(19A)	111.4
C(17)-C(18)-H(18A)	110.1	C(20)-C(19)-H(19A)	111.4
O(1)-C(18)-H(18B)	110.1	O(2)-C(19)-H(19B)	111.4
C(17)-C(18)-H(18B)	110.1	C(20)-C(19)-H(19B)	111.4
H(18A)-C(18)-H(18B)	108.4	H(19A)-C(19)-H(19B)	109.2
C(15')-O(1')-C(18')	107.8(14)	C(21)-C(20)-C(19)	104.3(4)
C(15')-O(1')-K(1)	137(2)	C(21)-C(20)-H(20A)	110.9
C(18')-O(1')-K(1)	115.2(16)	C(19)-C(20)-H(20A)	110.9
O(1')-C(15')-C(16')	106.0(14)	C(21)-C(20)-H(20B)	110.9
O(1')-C(15')-H(15C)	110.5	C(19)-C(20)-H(20B)	110.9
C(16')-C(15')-H(15C)	110.5	H(20A)-C(20)-H(20B)	108.9
O(1')-C(15')-H(15D)	110.5	C(20)-C(21)-C(22)	105.2(4)
C(16')-C(15')-H(15D)	110.5	C(20)-C(21)-H(21A)	110.7
H(15C)-C(15')-H(15D)	108.7	C(22)-C(21)-H(21A)	110.7
C(15')-C(16')-C(17')	102.6(16)	C(20)-C(21)-H(21B)	110.7
C(15')-C(16')-H(16C)	111.2	C(22)-C(21)-H(21B)	110.7
C(17')-C(16')-H(16C)	111.2	H(21A)-C(21)-H(21B)	108.8
C(15')-C(16')-H(16D)	111.2	O(2)-C(22)-C(21)	103.9(4)
C(17')-C(16')-H(16D)	111.2	O(2)-C(22)-H(22A)	111.0
H(16C)-C(16')-H(16D)	109.2	C(21)-C(22)-H(22A)	111.0
C(18')-C(17')-C(16')	97.8(16)	O(2)-C(22)-H(22B)	111.0
C(18')-C(17')-H(17C)	112.2	C(21)-C(22)-H(22B)	111.0
C(16')-C(17')-H(17C)	112.2	H(22A)-C(22)-H(22B)	109.0
C(18')-C(17')-H(17D)	112.2	C(19')-O(2')-C(22')	107.1(9)
C(16')-C(17')-H(17D)	112.2	C(19')-O(2')-K(1)	131.0(8)
H(17C)-C(17')-H(17D)	109.8	C(22')-O(2')-K(1)	115.0(7)
O(1')-C(18')-C(17')	104.8(17)	O(2')-C(19')-C(20')	103.3(10)
O(1')-C(18')-H(18C)	110.8	O(2')-C(19')-H(19C)	111.1
C(17')-C(18')-H(18C)	110.8	C(20')-C(19')-H(19C)	111.1
O(1')-C(18')-H(18D)	110.8	O(2')-C(19')-H(19D)	111.1
C(17')-C(18')-H(18D)	110.8	C(20')-C(19')-H(19D)	111.1
H(18C)-C(18')-H(18D)	108.9	H(19C)-C(19')-H(19D)	109.1

C(21')-C(20')-C(19')	104.9(11)	C(20')-C(21')-H(21D)	110.7
C(21')-C(20')-H(20C)	110.8	C(22')-C(21')-H(21D)	110.7
C(19')-C(20')-H(20C)	110.8	H(21C)-C(21')-H(21D)	108.8
C(21')-C(20')-H(20D)	110.8	O(2')-C(22')-C(21')	100.8(11)
C(19')-C(20')-H(20D)	110.8	O(2')-C(22')-H(22C)	111.6
H(20C)-C(20')-H(20D)	108.8	C(21')-C(22')-H(22C)	111.6
C(20')-C(21')-C(22')	105.2(11)	O(2')-C(22')-H(22D)	111.6
C(20')-C(21')-H(21C)	110.7	C(21')-C(22')-H(22D)	111.6
C(22')-C(21')-H(21C)	110.7	H(22C)-C(22')-H(22D)	109.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 99325. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	28(1)	22(1)	34(1)	0	11(1)	0
C1	32(1)	34(1)	30(1)	-1(1)	12(1)	0(1)
C2	34(1)	40(1)	39(1)	13(1)	10(1)	2(1)
C3	37(1)	25(1)	62(2)	8(1)	18(1)	7(1)
C4	35(1)	27(1)	50(1)	-9(1)	18(1)	2(1)
C5	38(1)	64(2)	44(1)	3(1)	22(1)	2(1)
C6	43(1)	71(2)	58(2)	17(1)	26(1)	-5(1)
C7	43(1)	48(2)	66(2)	8(1)	24(1)	-10(1)
C8	36(1)	38(1)	50(1)	-1(1)	15(1)	-6(1)
C9	27(1)	31(1)	31(1)	-4(1)	10(1)	0(1)
C10	34(1)	41(1)	38(1)	-9(1)	17(1)	1(1)
C11	24(1)	29(1)	27(1)	-1(1)	6(1)	3(1)
C12	25(1)	31(1)	36(1)	-4(1)	10(1)	4(1)
C13	29(1)	45(1)	36(1)	-1(1)	14(1)	0(1)
C14	27(1)	35(1)	36(1)	1(1)	11(1)	1(1)
K1	34(1)	34(1)	32(1)	0	12(1)	0
O1	45(4)	43(2)	72(1)	-7(1)	17(2)	-9(3)
C15	55(4)	71(2)	77(2)	-20(2)	24(2)	-4(2)
C16	72(5)	43(4)	103(4)	-5(3)	-4(3)	-15(3)
C17	114(7)	54(4)	134(6)	12(4)	18(5)	-29(4)
C18	45(4)	61(3)	94(3)	20(2)	21(3)	-1(3)
O1'	45(4)	43(2)	72(1)	-7(1)	17(2)	-9(3)
C15'	55(4)	71(2)	77(2)	-20(2)	24(2)	-4(2)
C16'	72(5)	43(4)	103(4)	-5(3)	-4(3)	-15(3)
C17'	114(7)	54(4)	134(6)	12(4)	18(5)	-29(4)
C18'	45(4)	61(3)	94(3)	20(2)	21(3)	-1(3)
O2	60(2)	90(2)	30(1)	-11(1)	20(1)	-26(2)
C19	55(2)	86(3)	49(2)	10(2)	19(2)	14(2)
C20	61(3)	153(6)	57(3)	28(3)	24(3)	-11(3)
C21	98(4)	124(5)	89(3)	51(3)	58(3)	27(3)
C22	59(2)	107(4)	57(2)	12(2)	27(2)	11(2)

O2'	60(2)	90(2)	30(1)	-11(1)	20(1)	-26(2)
C19'	55(2)	86(3)	49(2)	10(2)	19(2)	14(2)
C20'	61(3)	153(6)	57(3)	28(3)	24(3)	-11(3)
C21'	98(4)	124(5)	89(3)	51(3)	58(3)	27(3)
C22'	59(2)	107(4)	57(2)	12(2)	27(2)	11(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 99325.

	x	y	z	U(eq)
H1	815(15)	1385(14)	9480(20)	35(6)
H2	788(17)	-90(18)	9670(30)	48(7)
H3	877(16)	-871(19)	8280(20)	48(7)
H4	942(17)	-293(16)	6720(30)	49(8)
H5A	2423	1806	5949	58
H6A	2916	3119	6254	69
H7A	2920	3946	7694	65
H8A	2396	3488	8785	53
H9A	1703	2410	9224	38
H10A	1773	699	6442	46
H15A	1752	3988	10184	87
H15B	1064	4620	9882	87
H16A	2020	5515	10158	114
H16B	2374	4892	9612	114
H17A	956	5801	8315	145
H17B	1636	5738	8010	145
H18A	487	4767	7008	87
H18B	1330	4452	7356	87
H15C	1935	4035	9930	87
H15D	1285	4476	10098	87
H16C	2317	5325	9935	114
H16D	1468	5690	9477	114
H17C	1545	5724	7765	145
H17D	1965	4844	8048	145
H18C	411	5159	7507	87
H18D	661	4526	6830	87
H19A	-1023	3212	8996	80
H19B	-483	3799	10089	80
H20A	-640	2793	11164	112
H20B	-809	2106	10193	112

H21A	392	1765	11131	118
H21B	559	2444	12111	118
H22A	908	3398	11218	90
H22B	1142	2601	10757	90
H19C	580	1901	10705	80
H19D	-270	1568	9784	80
H20C	-810	2222	10693	112
H20D	46	2168	11818	112
H21C	154	3467	11784	118
H21D	-700	3520	10653	118
H22C	-58	3902	9700	90
H22D	725	3449	10650	90

Table 6. Torsion angles [°] for 99325.

C2#1-Co1-C1-C2	-171.73(14)	C2#1-Co1-C2-C1	170.84(14)
C3#1-Co1-C1-C2	58.3(3)	C3#1-Co1-C2-C1	-155.14(14)
C3-Co1-C1-C2	-34.39(16)	C3-Co1-C2-C1	126.0(2)
C1#1-Co1-C1-C2	169.53(16)	C1#1-Co1-C2-C1	-25.5(4)
C4#1-Co1-C1-C2	78.05(16)	C4#1-Co1-C2-C1	-117.15(14)
C4-Co1-C1-C2	-75.10(15)	C4-Co1-C2-C1	93.33(15)
K1-Co1-C1-C2	169.53(16)	K1-Co1-C2-C1	-9.16(14)
C2#1-Co1-C1-C11	-55.1(3)	C1-C2-C3-C4	-1.6(3)
C2-Co1-C1-C11	116.6(2)	Co1-C2-C3-C4	60.05(19)
C3#1-Co1-C1-C11	174.89(19)	C1-C2-C3-Co1	-61.66(18)
C3-Co1-C1-C11	82.24(15)	C2#1-Co1-C3-C2	-163.69(13)
C1#1-Co1-C1-C11	-73.84(12)	C3#1-Co1-C3-C2	-120.63(17)
C4#1-Co1-C1-C11	-165.33(13)	C1-Co1-C3-C2	33.71(14)
C4-Co1-C1-C11	41.52(14)	C1#1-Co1-C3-C2	154.8(2)
K1-Co1-C1-C11	-73.85(12)	C4#1-Co1-C3-C2	-78.75(16)
C2#1-Co1-C1-K1	18.7(3)	C4-Co1-C3-C2	126.9(2)
C2-Co1-C1-K1	-169.53(16)	K1-Co1-C3-C2	59.38(17)
C3#1-Co1-C1-K1	-111.3(2)	C2#1-Co1-C3-C4	69.46(17)
C3-Co1-C1-K1	156.08(10)	C2-Co1-C3-C4	-126.9(2)
C1#1-Co1-C1-K1	0.0	C3#1-Co1-C3-C4	112.52(16)
C4#1-Co1-C1-K1	-91.48(8)	C1-Co1-C3-C4	-93.14(14)
C4-Co1-C1-K1	115.37(8)	C1#1-Co1-C3-C4	27.9(3)
C11-C1-C2-C3	-31.5(3)	C4#1-Co1-C3-C4	154.39(12)
Co1-C1-C2-C3	58.63(18)	K1-Co1-C3-C4	-67.48(16)
K1-C1-C2-C3	79.7(4)	C2-C3-C4-C12	34.0(3)
C11-C1-C2-Co1	-90.15(18)	Co1-C3-C4-C12	90.26(19)
K1-C1-C2-Co1	21.1(3)	C2-C3-C4-Co1	-56.23(18)
C2#1-Co1-C2-C3	44.83(13)	C2#1-Co1-C4-C3	-126.39(16)
C3#1-Co1-C2-C3	78.8(2)	C2-Co1-C4-C3	34.07(15)
C1-Co1-C2-C3	-126.0(2)	C3#1-Co1-C4-C3	-84.4(2)
C1#1-Co1-C2-C3	-151.5(2)	C1-Co1-C4-C3	75.74(15)
C4#1-Co1-C2-C3	116.84(15)	C1#1-Co1-C4-C3	-167.36(14)
C4-Co1-C2-C3	-32.68(14)	C4#1-Co1-C4-C3	-50.51(13)
K1-Co1-C2-C3	-135.17(13)	K1-Co1-C4-C3	129.49(13)

C2#1-Co1-C4-C12	115.54(16)	C12-C10-C13-C5	-175.3(2)
C2-Co1-C4-C12	-84.00(16)	C12-C10-C13-C14	2.9(3)
C3#1-Co1-C4-C12	157.52(15)	C6-C5-C13-C10	178.1(2)
C3-Co1-C4-C12	-118.1(2)	C6-C5-C13-C14	-0.1(4)
C1-Co1-C4-C12	-42.33(15)	C7-C8-C14-C9	-176.8(2)
C1#1-Co1-C4-C12	74.57(17)	C7-C8-C14-C13	1.5(3)
C4#1-Co1-C4-C12	-168.58(16)	C11-C9-C14-C8	176.6(2)
K1-Co1-C4-C12	11.42(16)	K1-C9-C14-C8	79.8(2)
C13-C5-C6-C7	1.4(4)	C11-C9-C14-C13	-1.6(3)
C5-C6-C7-C8	-1.2(4)	K1-C9-C14-C13	-98.49(19)
C6-C7-C8-C14	-0.2(4)	C10-C13-C14-C8	-179.5(2)
C14-C9-C11-C12	2.8(3)	C5-C13-C14-C8	-1.3(3)
K1-C9-C11-C12	114.04(16)	C10-C13-C14-C9	-1.2(3)
C14-C9-C11-C1	-173.96(19)	C5-C13-C14-C9	177.1(2)
K1-C9-C11-C1	-62.76(19)	C11-C9-K1-O2'	84.3(3)
C14-C9-C11-K1	-111.20(19)	C14-C9-K1-O2'	-153.7(3)
C2-C1-C11-C9	-150.6(2)	C11-C9-K1-O2'#1	-90.6(3)
Co1-C1-C11-C9	142.79(17)	C14-C9-K1-O2'#1	31.5(3)
K1-C1-C11-C9	58.58(18)	C11-C9-K1-O2	98.48(14)
C2-C1-C11-C12	32.5(3)	C14-C9-K1-O2	-139.44(15)
Co1-C1-C11-C12	-34.11(19)	C11-C9-K1-O2#1	-99.46(14)
K1-C1-C11-C12	-118.32(16)	C14-C9-K1-O2#1	22.62(16)
C2-C1-C11-K1	150.77(19)	C11-C9-K1-O1#1	-164.3(6)
Co1-C1-C11-K1	84.21(8)	C14-C9-K1-O1#1	-42.3(6)
C13-C10-C12-C11	-1.8(3)	C11-C9-K1-O1	170.8(4)
C13-C10-C12-C4	175.2(2)	C14-C9-K1-O1	-67.1(4)
C9-C11-C12-C10	-1.1(3)	C11-C9-K1-O1'	170.5(10)
C1-C11-C12-C10	175.96(18)	C14-C9-K1-O1'	-67.4(10)
K1-C11-C12-C10	82.6(2)	C11-C9-K1-O1'#1	-164.9(14)
C9-C11-C12-C4	-178.37(18)	C14-C9-K1-O1'#1	-42.9(14)
C1-C11-C12-C4	-1.3(3)	C11-C9-K1-C9#1	-0.46(11)
K1-C11-C12-C4	-94.60(19)	C14-C9-K1-C9#1	121.62(15)
C3-C4-C12-C10	150.9(2)	C11-C9-K1-C11#1	-0.66(16)
Co1-C4-C12-C10	-141.11(19)	C14-C9-K1-C11#1	121.42(14)
C3-C4-C12-C11	-32.1(3)	C14-C9-K1-C11	122.1(2)
Co1-C4-C12-C11	35.9(2)	C9-C11-K1-O2'	-97.7(3)

C12-C11-K1-O2'	148.9(3)	O1'-K1-O1-C15	92(22)
C1-C11-K1-O2'	35.0(3)	O1'#1-K1-O1-C15	111.7(15)
C9-C11-K1-O2'#1	86.2(3)	C9#1-K1-O1-C15	86.4(19)
C12-C11-K1-O2'#1	-27.3(3)	C9-K1-O1-C15	-82.4(19)
C1-C11-K1-O2'#1	-141.2(3)	C11#1-K1-O1-C15	49(3)
C9-C11-K1-O2	-83.69(14)	C11-K1-O1-C15	-79(2)
C12-C11-K1-O2	162.87(16)	O2'-K1-O1-C18	-153.3(14)
C1-C11-K1-O2	48.97(13)	O2'#1-K1-O1-C18	30.1(15)
C9-C11-K1-O2#1	82.73(14)	O2-K1-O1-C18	-151.3(15)
C12-C11-K1-O2#1	-30.71(17)	O2#1-K1-O1-C18	16.6(14)
C1-C11-K1-O2#1	-144.60(13)	O1#1-K1-O1-C18	-57.0(11)
C9-C11-K1-O1#1	51.4(17)	O1'-K1-O1-C18	-75(21)
C12-C11-K1-O1#1	-62.0(17)	O1'#1-K1-O1-C18	-56(2)
C1-C11-K1-O1#1	-175.9(17)	C9#1-K1-O1-C18	-81.3(17)
C9-C11-K1-O1	-8.9(4)	C9-K1-O1-C18	109.9(15)
C12-C11-K1-O1	-122.3(4)	C11#1-K1-O1-C18	-118.9(13)
C1-C11-K1-O1	123.8(4)	C11-K1-O1-C18	113.7(14)
C9-C11-K1-O1'	-9.4(10)	C18-O1-C15-C16	-16(2)
C12-C11-K1-O1'	-122.8(10)	K1-O1-C15-C16	175.4(15)
C1-C11-K1-O1'	123.3(10)	O1-C15-C16-C17	35.1(19)
C9-C11-K1-O1'#1	41(4)	C15-C16-C17-C18	-39.1(17)
C12-C11-K1-O1'#1	-72(4)	C15-O1-C18-C17	-10(2)
C1-C11-K1-O1'#1	174(4)	K1-O1-C18-C17	160.8(11)
C9-C11-K1-C9#1	179.66(8)	C16-C17-C18-O1	30.9(18)
C12-C11-K1-C9#1	66.22(17)	O2'-K1-O1'-C15'	36(7)
C1-C11-K1-C9#1	-47.67(12)	O2'#1-K1-O1'-C15'	-141(7)
C12-C11-K1-C9	-113.4(2)	O2-K1-O1'-C15'	37(6)
C1-C11-K1-C9	132.66(18)	O2#1-K1-O1'-C15'	-154(7)
C9-C11-K1-C11#1	179.40(15)	O1#1-K1-O1'-C15'	132(7)
C12-C11-K1-C11#1	65.96(15)	O1-K1-O1'-C15'	-66(19)
C1-C11-K1-C11#1	-47.94(10)	O1'#1-K1-O1'-C15'	133(8)
O2'-K1-O1-C15	14(2)	C9#1-K1-O1'-C15'	108(6)
O2'#1-K1-O1-C15	-162(2)	C9-K1-O1'-C15'	-61(7)
O2-K1-O1-C15	16.4(19)	C11#1-K1-O1'-C15'	80(9)
O2#1-K1-O1-C15	-176(2)	C11-K1-O1'-C15'	-57(7)
O1#1-K1-O1-C15	111(2)	O2'-K1-O1'-C18'	-144(4)

O2#1-K1-O1'-C18'	39(4)	C9-K1-O2-C19	-168.1(3)
O2-K1-O1'-C18'	-143(4)	C11#1-K1-O2-C19	-54.0(3)
O2#1-K1-O1'-C18'	26(4)	C11-K1-O2-C19	-144.1(3)
O1#1-K1-O1'-C18'	-48(4)	C22-O2-C19-C20	-43.8(5)
O1-K1-O1'-C18'	114(24)	K1-O2-C19-C20	124.6(3)
O1#1-K1-O1'-C18'	-46(3)	O2-C19-C20-C21	25.2(6)
C9#1-K1-O1'-C18'	-72(5)	C19-C20-C21-C22	0.7(7)
C9-K1-O1'-C18'	119(4)	C19-O2-C22-C21	44.8(5)
C11#1-K1-O1'-C18'	-100(4)	K1-O2-C22-C21	-122.2(4)
C11-K1-O1'-C18'	123(4)	C20-C21-C22-O2	-27.8(6)
C18'-O1'-C15'-C16'	-2(6)	O2#1-K1-O2'-C19'	12.8(12)
K1-O1'-C15'-C16'	178(5)	O2-K1-O2'-C19'	-136(2)
O1'-C15'-C16'-C17'	-26(6)	O2#1-K1-O2'-C19'	146.2(13)
C15'-C16'-C17'-C18'	42(4)	O1#1-K1-O2'-C19'	153.9(13)
C15'-O1'-C18'-C17'	30(6)	O1-K1-O2'-C19'	-128.5(13)
K1-O1'-C18'-C17'	-151(3)	O1'-K1-O2'-C19'	-131.6(18)
C16'-C17'-C18'-O1'	-44(4)	O1#1-K1-O2'-C19'	157.1(18)
O2'-K1-O2-C22	97.0(13)	C9#1-K1-O2'-C19'	81.8(12)
O2#1-K1-O2-C22	-66.8(16)	C9-K1-O2'-C19'	-55.5(12)
O2#1-K1-O2-C22	-114.2(4)	C11#1-K1-O2'-C19'	57.5(12)
O1#1-K1-O2-C22	-151.9(6)	C11-K1-O2'-C19'	-31.4(12)
O1-K1-O2-C22	-74.8(6)	O2#1-K1-O2'-C22'	159.6(11)
O1'-K1-O2-C22	-78.0(15)	O2-K1-O2'-C22'	10.3(9)
O1#1-K1-O2-C22	-148.7(15)	O2#1-K1-O2'-C22'	-67(2)
C9#1-K1-O2-C22	134.8(4)	O1#1-K1-O2'-C22'	-59.3(11)
C9-K1-O2-C22	-3.3(4)	O1-K1-O2'-C22'	18.3(11)
C11#1-K1-O2-C22	110.8(4)	O1'-K1-O2'-C22'	15.1(17)
C11-K1-O2-C22	20.7(4)	O1#1-K1-O2'-C22'	-56.2(17)
O2'-K1-O2-C19	-67.8(12)	C9#1-K1-O2'-C22'	-131.5(11)
O2#1-K1-O2-C19	128.4(13)	C9-K1-O2'-C22'	91.3(11)
O2#1-K1-O2-C19	81.0(3)	C11#1-K1-O2'-C22'	-155.8(11)
O1#1-K1-O2-C19	43.3(6)	C11-K1-O2'-C22'	115.3(11)
O1-K1-O2-C19	120.4(6)	C22'-O2'-C19'-C20'	43.0(16)
O1'-K1-O2-C19	117.1(14)	K1-O2'-C19'-C20'	-168.3(11)
O1#1-K1-O2-C19	46.5(15)	O2'-C19'-C20'-C21'	-25(2)
C9#1-K1-O2-C19	-30.0(3)	C19'-C20'-C21'-C22'	0(2)

C19'-O2'-C22'-C21'	-42.2(16)	C20'-C21'-C22'-O2'	25(2)
K1-O2'-C22'-C21'	163.4(10)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2

REFERENCE NUMBER: 05319 [2]

CRYSTAL STRUCTURE REPORT

$C_{20} H_{36} Co K O_6$

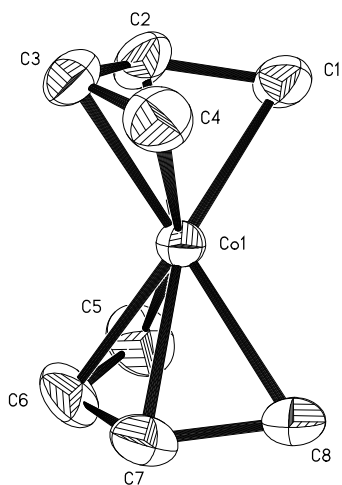
or

$[K(18\text{-crown-6})][Co(C_4H_6)_2]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

October 31, 2005



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X-Ray Crystallographic Laboratory
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Data collection

A crystal (approximate dimensions $0.50 \times 0.25 \times 0.18 \text{ mm}^3$) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 122 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 10 seconds and a detector distance of 4.98 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 2932 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ 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. The butadiene ligand hydrogen atoms were found from the difference map and refined with individual isotropic displacement parameters. All remaining 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 $R1 = 0.0357$ and $wR2 = 0.0816$ (F^2 , all data).

Structure description

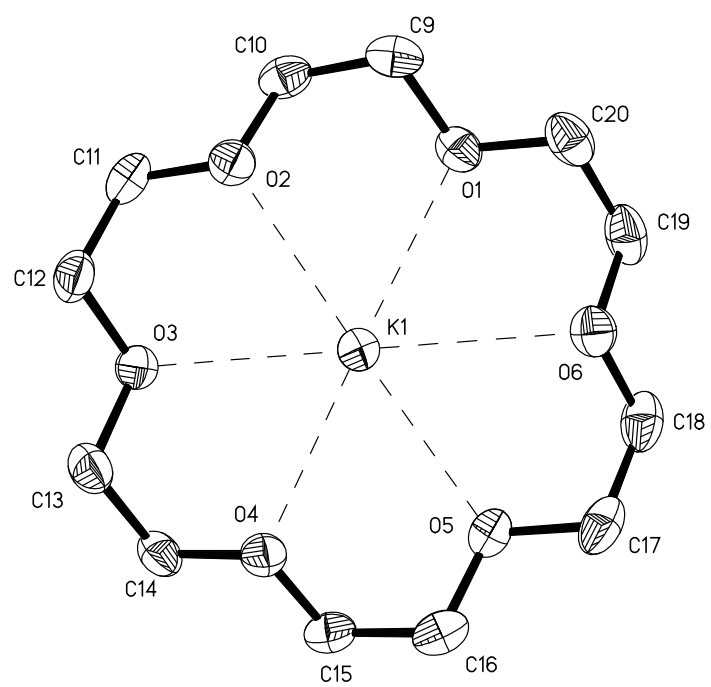
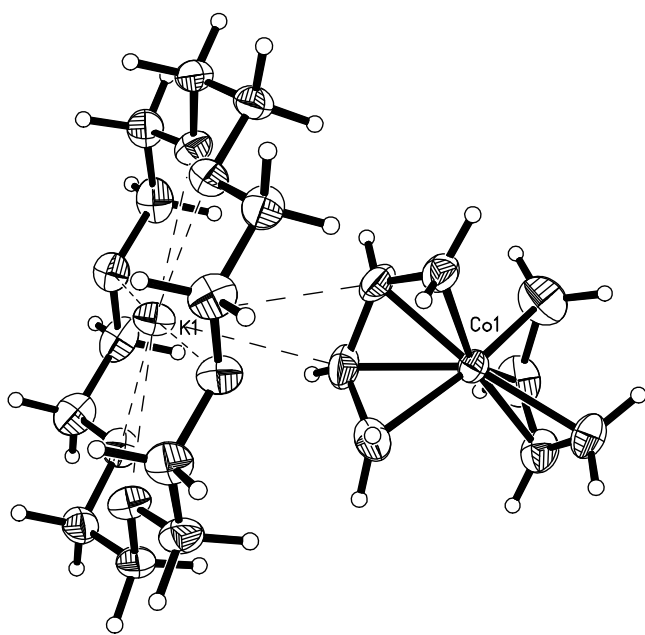
The structure is the one suggested. All atoms lie on general positions. The butadiene ligands occupy the axial positions of the potassium 18-crown-6 cations, thus forming one dimensional chains (see diagram). The angle between the planes of the butadiene ligands is 14.23(18) degrees. The twist angle of 62.1 degrees means that the geometry is closer to tetrahedral than to square planar.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
 - ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
 - ³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
 - ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
 - ⁵ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

$$\begin{aligned}
 R_{\text{int}} &= \Sigma |F_o|^2 - \langle F_o|^2 \rangle / \Sigma |F_o|^2 \\
 R_1 &= \Sigma ||F_o| - |F_c|| / \Sigma |F_o| \\
 wR2 &= [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2} \\
 \text{where } w &= q / [\sigma^2(F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)] \\
 \text{GooF} = S &= [\Sigma [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}
 \end{aligned}$$



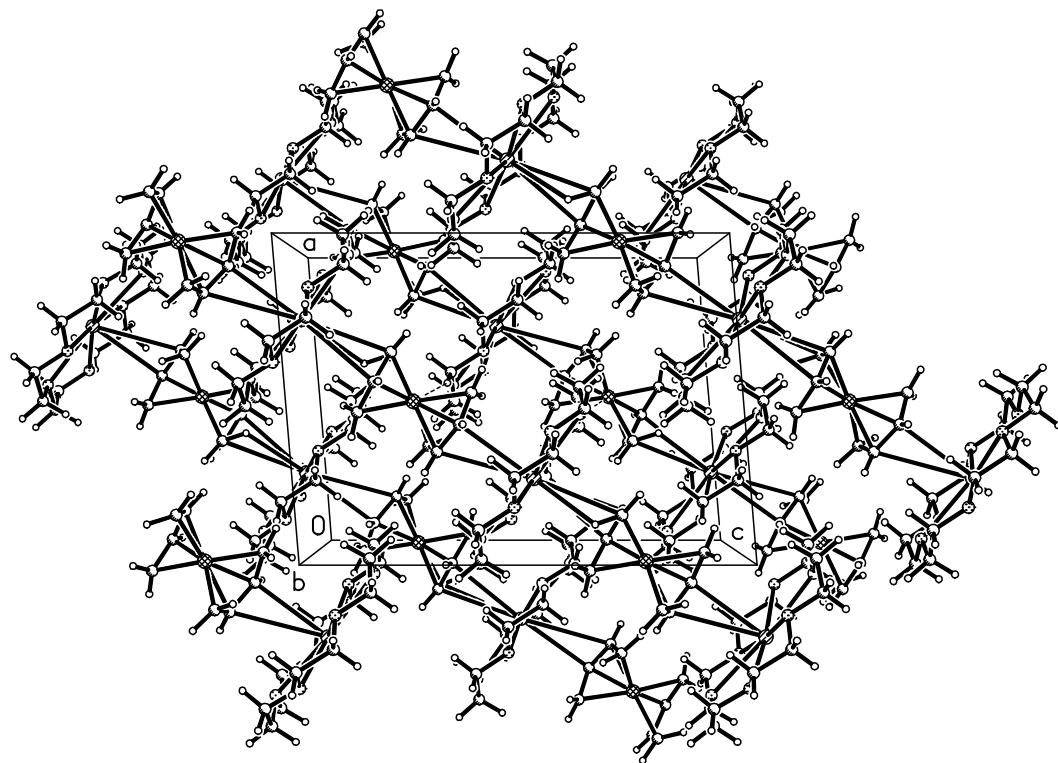
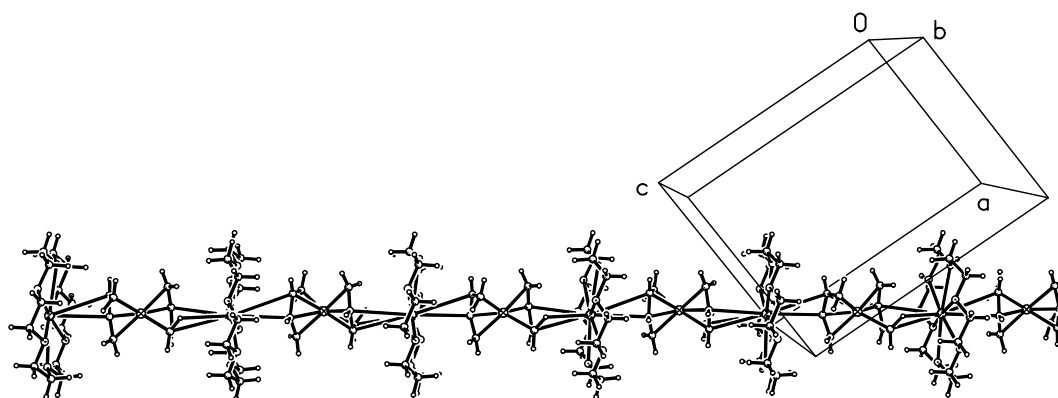


Table 1. Crystal data and structure refinement for 05319.

Identification code	05319	
Empirical formula	C ₂₀ H ₃₆ Co K O ₆	
Formula weight	470.52	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	$a = 11.1122(9)$ Å	$\alpha = 90^\circ$
	$b = 13.5440(11)$ Å	$\beta = 94.778(2)^\circ$
	$c = 15.2768(13)$ Å	$\gamma = 90^\circ$
Volume	2291.2(3) Å ³	
Z	4	
Density (calculated)	1.364 Mg/m ³	
Absorption coefficient	0.961 mm ⁻¹	
$F(000)$	1000	
Crystal color, morphology	red, block	
Crystal size	0.50 x 0.25 x 0.18 mm ³	
Theta range for data collection	2.01 to 27.51°	
Index ranges	$-13 \leq h \leq 14$, $-17 \leq k \leq 17$, $-19 \leq l \leq 19$	
Reflections collected	19531	
Independent reflections	5182 [$R(\text{int}) = 0.0367$]	
Observed reflections	3920	
Completeness to $\theta = 27.51^\circ$	98.3%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8460 and 0.6450	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5182 / 0 / 301	
Goodness-of-fit on F^2	1.049	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0357$, $wR2 = 0.0732$	
R indices (all data)	$R1 = 0.0581$, $wR2 = 0.0816$	
Largest diff. peak and hole	0.702 and -0.329 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05319. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	9931(1)	7838(1)	7669(1)	25(1)
C1	8502(2)	8722(2)	7902(2)	37(1)
C2	8328(2)	7702(2)	8113(2)	40(1)
C3	9209(2)	7236(2)	8687(2)	39(1)
C4	10204(3)	7816(2)	9019(2)	39(1)
C5	9600(3)	7396(2)	6392(2)	54(1)
C6	10556(3)	6868(2)	6844(2)	47(1)
C7	11492(2)	7433(2)	7271(2)	41(1)
C8	11411(2)	8487(2)	7198(2)	38(1)
K1	7505(1)	7423(1)	10280(1)	30(1)
O1	5619(1)	7140(1)	8949(1)	32(1)
O2	6129(1)	9036(1)	9686(1)	30(1)
O3	8406(1)	9336(1)	10628(1)	32(1)
O4	9524(1)	7657(1)	11465(1)	31(1)
O5	8998(1)	5762(1)	10728(1)	34(1)
O6	6704(1)	5459(1)	9792(1)	33(1)
C9	4784(2)	7936(2)	8888(2)	34(1)
C10	5471(2)	8881(2)	8861(1)	34(1)
C11	6750(2)	9962(2)	9719(2)	34(1)
C12	7471(2)	10051(2)	10583(2)	35(1)
C13	9105(2)	9370(2)	11458(2)	35(1)
C14	10075(2)	8605(2)	11455(2)	34(1)
C15	10369(2)	6875(2)	11476(2)	34(1)
C16	9707(2)	5921(2)	11535(2)	34(1)
C17	8357(2)	4851(2)	10721(2)	41(1)
C18	7648(2)	4748(2)	9854(2)	40(1)
C19	6009(2)	5425(2)	8967(2)	40(1)
C20	5055(2)	6202(2)	8958(2)	37(1)

Table 3. Bond lengths [Å] and angles [°] for 05319.

Co(1)-C(7)	1.964(2)	K(1)-O(1)	2.8216(15)
Co(1)-C(2)	1.966(2)	K(1)-O(5)	2.8440(16)
Co(1)-C(3)	1.983(2)	K(1)-O(6)	2.8826(15)
Co(1)-C(6)	1.986(2)	K(1)-C(7)#2	3.335(3)
Co(1)-C(1)	2.043(2)	K(1)-C(8)#2	3.489(2)
Co(1)-C(5)	2.045(3)	K(1)-C(6)#2	3.491(3)
Co(1)-C(8)	2.048(2)	O(1)-C(20)	1.417(3)
Co(1)-C(4)	2.059(2)	O(1)-C(9)	1.420(3)
C(1)-C(2)	1.435(3)	O(2)-C(10)	1.419(2)
C(1)-H(1A)	0.98(3)	O(2)-C(11)	1.430(3)
C(1)-H(1B)	0.98(2)	O(3)-C(12)	1.419(3)
C(2)-C(3)	1.408(4)	O(3)-C(13)	1.431(3)
C(2)-K(1)	3.528(3)	O(4)-C(15)	1.414(3)
C(2)-H(2)	0.97(3)	O(4)-C(14)	1.423(3)
C(3)-C(4)	1.416(4)	O(5)-C(16)	1.423(3)
C(3)-K(1)	3.216(2)	O(5)-C(17)	1.424(3)
C(3)-H(3)	0.93(2)	O(6)-C(18)	1.421(3)
C(4)-H(4A)	0.97(3)	O(6)-C(19)	1.423(3)
C(4)-H(4B)	0.96(3)	C(9)-C(10)	1.492(3)
C(5)-C(6)	1.413(4)	C(9)-H(9A)	0.9900
C(5)-H(5A)	0.97(3)	C(9)-H(9B)	0.9900
C(5)-H(5B)	1.04(3)	C(10)-H(10A)	0.9900
C(6)-C(7)	1.407(4)	C(10)-H(10B)	0.9900
C(6)-K(1)#1	3.491(3)	C(11)-C(12)	1.491(3)
C(6)-H(6)	0.96(3)	C(11)-H(11A)	0.9900
C(7)-C(8)	1.434(4)	C(11)-H(11B)	0.9900
C(7)-K(1)#1	3.336(3)	C(12)-H(12A)	0.9900
C(7)-H(7)	0.98(3)	C(12)-H(12B)	0.9900
C(8)-K(1)#1	3.489(2)	C(13)-C(14)	1.495(3)
C(8)-H(8A)	0.98(3)	C(13)-H(13B)	0.9900
C(8)-H(8B)	0.96(3)	C(13)-H(13C)	0.9900
K(1)-O(2)	2.7765(15)	C(14)-H(14A)	0.9900
K(1)-O(4)	2.7808(15)	C(14)-H(14B)	0.9900
K(1)-O(3)	2.8126(15)	C(15)-C(16)	1.494(3)

C(15)-H(15A)	0.9900	C(2)-Co(1)-C(4)	73.50(11)
C(15)-H(15B)	0.9900	C(3)-Co(1)-C(4)	40.96(11)
C(16)-H(16A)	0.9900	C(6)-Co(1)-C(4)	126.55(12)
C(16)-H(16B)	0.9900	C(1)-Co(1)-C(4)	83.46(11)
C(17)-C(18)	1.491(3)	C(5)-Co(1)-C(4)	162.00(13)
C(17)-H(17A)	0.9900	C(8)-Co(1)-C(4)	107.59(11)
C(17)-H(17B)	0.9900	C(2)-C(1)-Co(1)	66.19(13)
C(18)-H(18A)	0.9900	C(2)-C(1)-H(1A)	116.3(16)
C(18)-H(18B)	0.9900	Co(1)-C(1)-H(1A)	112.1(16)
C(19)-C(20)	1.492(3)	C(2)-C(1)-H(1B)	115.9(15)
C(19)-H(19A)	0.9900	Co(1)-C(1)-H(1B)	120.7(15)
C(19)-H(19B)	0.9900	H(1A)-C(1)-H(1B)	116(2)
C(20)-H(20A)	0.9900	C(3)-C(2)-C(1)	118.1(2)
C(20)-H(20B)	0.9900	C(3)-C(2)-Co(1)	69.75(14)
C(7)-Co(1)-C(2)	158.34(11)	C(1)-C(2)-Co(1)	71.90(14)
C(7)-Co(1)-C(3)	123.61(11)	C(3)-C(2)-K(1)	65.72(14)
C(2)-Co(1)-C(3)	41.76(10)	C(1)-C(2)-K(1)	111.34(18)
C(7)-Co(1)-C(6)	41.72(11)	Co(1)-C(2)-K(1)	130.29(11)
C(2)-Co(1)-C(6)	122.10(12)	C(3)-C(2)-H(2)	118.1(15)
C(3)-Co(1)-C(6)	114.26(12)	C(1)-C(2)-H(2)	122.8(15)
C(7)-Co(1)-C(1)	159.54(10)	Co(1)-C(2)-H(2)	119.7(15)
C(2)-Co(1)-C(1)	41.91(10)	K(1)-C(2)-H(2)	100.3(15)
C(3)-Co(1)-C(1)	74.55(10)	C(2)-C(3)-C(4)	117.1(2)
C(6)-Co(1)-C(1)	144.72(12)	C(2)-C(3)-Co(1)	68.49(14)
C(7)-Co(1)-C(5)	73.49(13)	C(4)-C(3)-Co(1)	72.41(14)
C(2)-Co(1)-C(5)	101.85(13)	C(2)-C(3)-K(1)	90.76(15)
C(3)-Co(1)-C(5)	125.11(14)	C(4)-C(3)-K(1)	100.17(16)
C(6)-Co(1)-C(5)	41.01(12)	Co(1)-C(3)-K(1)	149.65(12)
C(1)-Co(1)-C(5)	104.90(13)	C(2)-C(3)-H(3)	119.6(15)
C(7)-Co(1)-C(8)	41.81(10)	C(4)-C(3)-H(3)	122.7(15)
C(2)-Co(1)-C(8)	159.83(10)	Co(1)-C(3)-H(3)	122.4(15)
C(3)-Co(1)-C(8)	147.27(12)	K(1)-C(3)-H(3)	86.8(15)
C(6)-Co(1)-C(8)	74.15(11)	C(3)-C(4)-Co(1)	66.63(14)
C(1)-Co(1)-C(8)	117.94(10)	C(3)-C(4)-H(4A)	118.9(16)
C(5)-Co(1)-C(8)	82.88(13)	Co(1)-C(4)-H(4A)	122.0(16)
C(7)-Co(1)-C(4)	104.23(11)	C(3)-C(4)-H(4B)	119.2(16)

Co(1)-C(4)-H(4B)	109.8(15)	K(1)#1-C(8)-H(8B)	113.6(16)
H(4A)-C(4)-H(4B)	113(2)	H(8A)-C(8)-H(8B)	118(2)
C(6)-C(5)-Co(1)	67.27(15)	O(2)-K(1)-O(4)	121.03(5)
C(6)-C(5)-H(5A)	117.5(18)	O(2)-K(1)-O(3)	60.95(4)
Co(1)-C(5)-H(5A)	117.6(18)	O(4)-K(1)-O(3)	61.08(4)
C(6)-C(5)-H(5B)	117.3(18)	O(2)-K(1)-O(1)	61.00(4)
Co(1)-C(5)-H(5B)	106.8(17)	O(4)-K(1)-O(1)	174.23(5)
H(5A)-C(5)-H(5B)	119(2)	O(3)-K(1)-O(1)	119.50(5)
C(7)-C(6)-C(5)	116.6(3)	O(2)-K(1)-O(5)	174.56(5)
C(7)-C(6)-Co(1)	68.29(14)	O(4)-K(1)-O(5)	60.72(4)
C(5)-C(6)-Co(1)	71.72(15)	O(3)-K(1)-O(5)	119.44(5)
C(7)-C(6)-K(1)#1	71.98(15)	O(1)-K(1)-O(5)	116.72(5)
C(5)-C(6)-K(1)#1	90.57(19)	O(2)-K(1)-O(6)	119.47(5)
Co(1)-C(6)-K(1)#1	121.47(12)	O(4)-K(1)-O(6)	119.25(5)
C(7)-C(6)-H(6)	117.1(17)	O(3)-K(1)-O(6)	174.99(5)
C(5)-C(6)-H(6)	124.8(17)	O(1)-K(1)-O(6)	59.60(4)
Co(1)-C(6)-H(6)	118.7(17)	O(5)-K(1)-O(6)	59.61(5)
K(1)#1-C(6)-H(6)	117.1(17)	O(2)-K(1)-C(3)	99.06(6)
C(6)-C(7)-C(8)	117.8(3)	O(4)-K(1)-C(3)	90.44(6)
C(6)-C(7)-Co(1)	69.99(15)	O(3)-K(1)-C(3)	89.57(6)
C(8)-C(7)-Co(1)	72.23(14)	O(1)-K(1)-C(3)	83.85(6)
C(6)-C(7)-K(1)#1	84.38(16)	O(5)-K(1)-C(3)	75.61(6)
C(8)-C(7)-K(1)#1	83.95(15)	O(6)-K(1)-C(3)	85.43(6)
Co(1)-C(7)-K(1)#1	129.80(12)	O(2)-K(1)-C(7)#2	91.92(6)
C(6)-C(7)-H(7)	118.2(15)	O(4)-K(1)-C(7)#2	73.44(6)
C(8)-C(7)-H(7)	122.7(15)	O(3)-K(1)-C(7)#2	85.16(6)
Co(1)-C(7)-H(7)	117.6(15)	O(1)-K(1)-C(7)#2	112.21(6)
K(1)#1-C(7)-H(7)	112.5(15)	O(5)-K(1)-C(7)#2	93.52(6)
C(7)-C(8)-Co(1)	65.96(14)	O(6)-K(1)-C(7)#2	99.76(6)
C(7)-C(8)-K(1)#1	71.93(14)	C(3)-K(1)-C(7)#2	163.63(7)
Co(1)-C(8)-K(1)#1	119.34(10)	O(2)-K(1)-C(8)#2	109.36(5)
C(7)-C(8)-H(8A)	115.3(17)	O(4)-K(1)-C(8)#2	79.17(6)
Co(1)-C(8)-H(8A)	108.9(17)	O(3)-K(1)-C(8)#2	108.05(6)
K(1)#1-C(8)-H(8A)	55.0(16)	O(1)-K(1)-C(8)#2	105.51(6)
C(7)-C(8)-H(8B)	114.8(17)	O(5)-K(1)-C(8)#2	75.87(5)
Co(1)-C(8)-H(8B)	122.7(16)	O(6)-K(1)-C(8)#2	76.69(5)

C(3)-K(1)-C(8)#2	151.18(6)	C(18)-O(6)-C(19)	112.33(17)
C(7)#2-K(1)-C(8)#2	24.12(6)	C(18)-O(6)-K(1)	113.44(13)
O(2)-K(1)-C(6)#2	69.57(5)	C(19)-O(6)-K(1)	113.05(12)
O(4)-K(1)-C(6)#2	92.05(6)	O(1)-C(9)-C(10)	108.70(18)
O(3)-K(1)-C(6)#2	81.28(6)	O(1)-C(9)-H(9A)	109.9
O(1)-K(1)-C(6)#2	93.71(6)	C(10)-C(9)-H(9A)	109.9
O(5)-K(1)-C(6)#2	115.83(6)	O(1)-C(9)-H(9B)	109.9
O(6)-K(1)-C(6)#2	103.61(6)	C(10)-C(9)-H(9B)	109.9
C(3)-K(1)-C(6)#2	167.88(6)	H(9A)-C(9)-H(9B)	108.3
C(7)#2-K(1)-C(6)#2	23.65(6)	O(2)-C(10)-C(9)	109.23(18)
C(8)#2-K(1)-C(6)#2	40.79(6)	O(2)-C(10)-H(10A)	109.8
O(2)-K(1)-C(2)	77.74(5)	C(9)-C(10)-H(10A)	109.8
O(4)-K(1)-C(2)	109.90(5)	O(2)-C(10)-H(10B)	109.8
O(3)-K(1)-C(2)	87.85(6)	C(9)-C(10)-H(10B)	109.8
O(1)-K(1)-C(2)	64.76(5)	H(10A)-C(10)-H(10B)	108.3
O(5)-K(1)-C(2)	96.83(5)	O(2)-C(11)-C(12)	108.97(18)
O(6)-K(1)-C(2)	87.42(5)	O(2)-C(11)-H(11A)	109.9
C(3)-K(1)-C(2)	23.51(6)	C(12)-C(11)-H(11A)	109.9
C(7)#2-K(1)-C(2)	169.43(6)	O(2)-C(11)-H(11B)	109.9
C(8)#2-K(1)-C(2)	164.10(6)	C(12)-C(11)-H(11B)	109.9
C(6)#2-K(1)-C(2)	146.83(6)	H(11A)-C(11)-H(11B)	108.3
C(20)-O(1)-C(9)	113.26(17)	O(3)-C(12)-C(11)	108.94(18)
C(20)-O(1)-K(1)	114.67(12)	O(3)-C(12)-H(12A)	109.9
C(9)-O(1)-K(1)	112.76(12)	C(11)-C(12)-H(12A)	109.9
C(10)-O(2)-C(11)	111.91(16)	O(3)-C(12)-H(12B)	109.9
C(10)-O(2)-K(1)	113.73(12)	C(11)-C(12)-H(12B)	109.9
C(11)-O(2)-K(1)	115.30(12)	H(12A)-C(12)-H(12B)	108.3
C(12)-O(3)-C(13)	111.23(16)	O(3)-C(13)-C(14)	108.27(17)
C(12)-O(3)-K(1)	111.86(12)	O(3)-C(13)-H(13B)	110.0
C(13)-O(3)-K(1)	110.83(12)	C(14)-C(13)-H(13B)	110.0
C(15)-O(4)-C(14)	112.92(17)	O(3)-C(13)-H(13C)	110.0
C(15)-O(4)-K(1)	114.92(12)	C(14)-C(13)-H(13C)	110.0
C(14)-O(4)-K(1)	114.91(12)	H(13B)-C(13)-H(13C)	108.4
C(16)-O(5)-C(17)	112.19(17)	O(4)-C(14)-C(13)	108.32(18)
C(16)-O(5)-K(1)	111.06(12)	O(4)-C(14)-H(14A)	110.0
C(17)-O(5)-K(1)	113.73(13)	C(13)-C(14)-H(14A)	110.0

O(4)-C(14)-H(14B)	110.0	H(17A)-C(17)-H(17B)	108.4
C(13)-C(14)-H(14B)	110.0	O(6)-C(18)-C(17)	109.17(18)
H(14A)-C(14)-H(14B)	108.4	O(6)-C(18)-H(18A)	109.8
O(4)-C(15)-C(16)	108.62(18)	C(17)-C(18)-H(18A)	109.8
O(4)-C(15)-H(15A)	110.0	O(6)-C(18)-H(18B)	109.8
C(16)-C(15)-H(15A)	110.0	C(17)-C(18)-H(18B)	109.8
O(4)-C(15)-H(15B)	110.0	H(18A)-C(18)-H(18B)	108.3
C(16)-C(15)-H(15B)	110.0	O(6)-C(19)-C(20)	108.60(18)
H(15A)-C(15)-H(15B)	108.3	O(6)-C(19)-H(19A)	110.0
O(5)-C(16)-C(15)	108.55(18)	C(20)-C(19)-H(19A)	110.0
O(5)-C(16)-H(16A)	110.0	O(6)-C(19)-H(19B)	110.0
C(15)-C(16)-H(16A)	110.0	C(20)-C(19)-H(19B)	110.0
O(5)-C(16)-H(16B)	110.0	H(19A)-C(19)-H(19B)	108.3
C(15)-C(16)-H(16B)	110.0	O(1)-C(20)-C(19)	108.55(19)
H(16A)-C(16)-H(16B)	108.4	O(1)-C(20)-H(20A)	110.0
O(5)-C(17)-C(18)	108.34(19)	C(19)-C(20)-H(20A)	110.0
O(5)-C(17)-H(17A)	110.0	O(1)-C(20)-H(20B)	110.0
C(18)-C(17)-H(17A)	110.0	C(19)-C(20)-H(20B)	110.0
O(5)-C(17)-H(17B)	110.0	H(20A)-C(20)-H(20B)	108.4
C(18)-C(17)-H(17B)	110.0		

Symmetry transformations used to generate equivalent atoms:

#1 $x+1/2, -y+3/2, z-1/2$ #2 $x-1/2, -y+3/2, z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05319. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	25(1)	25(1)	25(1)	-2(1)	5(1)	-1(1)
C1	28(1)	38(1)	47(2)	10(1)	11(1)	6(1)
C2	23(1)	40(1)	57(2)	13(1)	10(1)	-3(1)
C3	40(1)	34(1)	46(1)	15(1)	18(1)	3(1)
C4	46(2)	40(1)	30(1)	5(1)	7(1)	6(1)
C5	72(2)	54(2)	35(1)	-19(1)	-2(1)	-2(2)
C6	68(2)	32(1)	44(2)	-16(1)	16(1)	8(1)
C7	39(2)	42(1)	43(1)	-2(1)	17(1)	8(1)
C8	36(2)	39(1)	40(1)	-3(1)	18(1)	0(1)
K1	29(1)	24(1)	34(1)	-3(1)	-5(1)	1(1)
O1	25(1)	34(1)	36(1)	-3(1)	2(1)	-4(1)
O2	32(1)	30(1)	29(1)	2(1)	0(1)	3(1)
O3	30(1)	28(1)	37(1)	-7(1)	0(1)	4(1)
O4	23(1)	31(1)	39(1)	-4(1)	-1(1)	2(1)
O5	38(1)	26(1)	38(1)	2(1)	4(1)	2(1)
O6	39(1)	29(1)	32(1)	-8(1)	6(1)	-1(1)
C9	23(1)	48(1)	30(1)	1(1)	0(1)	4(1)
C10	30(1)	40(1)	30(1)	4(1)	-1(1)	9(1)
C11	35(1)	26(1)	42(1)	3(1)	8(1)	7(1)
C12	36(1)	25(1)	45(1)	-6(1)	5(1)	4(1)
C13	38(1)	31(1)	37(1)	-11(1)	-2(1)	-4(1)
C14	28(1)	37(1)	36(1)	-7(1)	-3(1)	-4(1)
C15	24(1)	41(1)	36(1)	4(1)	-1(1)	8(1)
C16	33(1)	38(1)	33(1)	6(1)	4(1)	11(1)
C17	41(2)	22(1)	60(2)	4(1)	10(1)	6(1)
C18	43(2)	25(1)	55(2)	-10(1)	19(1)	-2(1)
C19	54(2)	34(1)	32(1)	-10(1)	4(1)	-15(1)
C20	35(1)	46(1)	30(1)	-4(1)	-3(1)	-17(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05319.

	x	y	z	U(eq)
H1A	8690(20)	9170(20)	8399(18)	55(8)
H1B	7970(20)	8984(18)	7417(16)	43(7)
H2	7720(20)	7292(18)	7798(16)	45(7)
H3	9180(20)	6554(19)	8769(16)	41(7)
H4A	10900(20)	7489(19)	9323(17)	51(8)
H4B	10060(20)	8460(20)	9249(17)	52(8)
H5A	8850(30)	7040(20)	6235(19)	69(10)
H5B	9830(30)	7980(20)	6000(20)	74(10)
H6	10530(20)	6180(20)	6989(17)	59(8)
H7	12070(20)	7102(18)	7697(16)	45(7)
H8A	11190(20)	8740(20)	6603(19)	61(9)
H8B	12000(20)	8840(20)	7566(17)	53(8)
H9A	4296	7932	9401	41
H9B	4231	7867	8349	41
H10A	6033	8850	8392	40
H10B	4905	9436	8729	40
H11A	6160	10510	9646	41
H11B	7290	10000	9237	41
H12A	7822	10722	10647	42
H12B	6944	9944	11066	42
H13B	8583	9236	11939	42
H13C	9470	10032	11552	42
H14A	10520	8677	10924	41
H14B	10654	8685	11979	41
H15A	10972	6947	11987	40
H15B	10799	6890	10934	40
H16A	10290	5372	11646	41
H16B	9181	5945	12026	41
H17A	7809	4842	11199	49
H17B	8932	4294	10813	49

H18A	8181	4851	9374	48
H18B	7302	4075	9794	48
H19A	5631	4767	8879	48
H19B	6535	5544	8486	48
H20A	4482	6125	8430	45
H20B	4599	6138	9484	45

Table 6. Torsion angles [°] for 05319.

C7-Co1-C1-C2	173.9(3)	C7-Co1-C3-C2	-158.63(16)
C3-Co1-C1-C2	-31.71(17)	C6-Co1-C3-C2	-111.74(18)
C6-Co1-C1-C2	78.6(2)	C1-Co1-C3-C2	31.81(17)
C5-Co1-C1-C2	91.24(19)	C5-Co1-C3-C2	-65.8(2)
C8-Co1-C1-C2	-179.00(16)	C8-Co1-C3-C2	149.78(19)
C4-Co1-C1-C2	-72.52(17)	C4-Co1-C3-C2	129.8(2)
Co1-C1-C2-C3	54.0(2)	C7-Co1-C3-C4	71.62(19)
Co1-C1-C2-K1	127.07(13)	C2-Co1-C3-C4	-129.8(2)
C7-Co1-C2-C3	55.3(4)	C6-Co1-C3-C4	118.50(17)
C6-Co1-C2-C3	91.48(19)	C1-Co1-C3-C4	-97.94(17)
C1-Co1-C2-C3	-130.5(2)	C5-Co1-C3-C4	164.48(17)
C5-Co1-C2-C3	130.34(18)	C8-Co1-C3-C4	20.0(3)
C8-Co1-C2-C3	-127.9(3)	C7-Co1-C3-K1	151.5(2)
C4-Co1-C2-C3	-31.71(16)	C2-Co1-C3-K1	-49.8(2)
C7-Co1-C2-C1	-174.2(3)	C6-Co1-C3-K1	-161.6(2)
C3-Co1-C2-C1	130.5(2)	C1-Co1-C3-K1	-18.0(2)
C6-Co1-C2-C1	-138.05(18)	C5-Co1-C3-K1	-115.6(2)
C5-Co1-C2-C1	-99.19(18)	C8-Co1-C3-K1	100.0(3)
C8-Co1-C2-C1	2.6(4)	C4-Co1-C3-K1	79.9(3)
C4-Co1-C2-C1	98.76(18)	C2-C3-C4-Co1	-53.5(2)
C7-Co1-C2-K1	82.8(3)	K1-C3-C4-Co1	-149.64(11)
C3-Co1-C2-K1	27.48(13)	C7-Co1-C4-C3	-125.38(16)
C6-Co1-C2-K1	118.95(15)	C2-Co1-C4-C3	32.28(16)
C1-Co1-C2-K1	-103.0(2)	C6-Co1-C4-C3	-85.78(19)
C5-Co1-C2-K1	157.82(14)	C1-Co1-C4-C3	73.92(16)
C8-Co1-C2-K1	-100.4(3)	C5-Co1-C4-C3	-45.1(5)
C4-Co1-C2-K1	-4.23(13)	C8-Co1-C4-C3	-168.80(15)
C1-C2-C3-C4	0.4(4)	C7-Co1-C5-C6	32.28(18)
Co1-C2-C3-C4	55.4(2)	C2-Co1-C5-C6	-125.89(19)
K1-C2-C3-C4	-101.8(2)	C3-Co1-C5-C6	-87.5(2)
C1-C2-C3-Co1	-55.1(2)	C1-Co1-C5-C6	-168.92(18)
K1-C2-C3-Co1	-157.29(10)	C8-Co1-C5-C6	73.99(19)
C1-C2-C3-K1	102.2(2)	C4-Co1-C5-C6	-53.0(5)
Co1-C2-C3-K1	157.29(10)	Co1-C5-C6-C7	-53.1(2)

Co1-C5-C6-K1#1	-123.12(10)	C1-Co1-C7-C8	9.5(4)
C2-Co1-C6-C7	-160.91(16)	C5-Co1-C7-C8	97.91(19)
C3-Co1-C6-C7	-114.00(17)	C4-Co1-C7-C8	-100.62(17)
C1-Co1-C6-C7	148.46(18)	C2-Co1-C7-K1#1	112.6(3)
C5-Co1-C6-C7	129.7(3)	C3-Co1-C7-K1#1	153.73(13)
C8-Co1-C6-C7	32.23(17)	C6-Co1-C7-K1#1	63.95(18)
C4-Co1-C6-C7	-68.2(2)	C1-Co1-C7-K1#1	-56.3(4)
C7-Co1-C6-C5	-129.7(3)	C5-Co1-C7-K1#1	32.18(15)
C2-Co1-C6-C5	69.4(2)	C8-Co1-C7-K1#1	-65.73(17)
C3-Co1-C6-C5	116.3(2)	C4-Co1-C7-K1#1	-166.35(13)
C1-Co1-C6-C5	18.8(3)	C6-C7-C8-Co1	54.9(2)
C8-Co1-C6-C5	-97.5(2)	K1#1-C7-C8-Co1	135.23(10)
C4-Co1-C6-C5	162.11(19)	C6-C7-C8-K1#1	-80.4(2)
C7-Co1-C6-K1#1	-50.64(15)	Co1-C7-C8-K1#1	-135.23(10)
C2-Co1-C6-K1#1	148.44(11)	C2-Co1-C8-C7	-178.2(3)
C3-Co1-C6-K1#1	-164.64(12)	C3-Co1-C8-C7	78.2(2)
C1-Co1-C6-K1#1	97.8(2)	C6-Co1-C8-C7	-32.17(17)
C5-Co1-C6-K1#1	79.1(2)	C1-Co1-C8-C7	-176.27(16)
C8-Co1-C6-K1#1	-18.41(12)	C5-Co1-C8-C7	-73.14(18)
C4-Co1-C6-K1#1	-118.82(14)	C4-Co1-C8-C7	91.85(18)
C5-C6-C7-C8	-1.2(4)	C7-Co1-C8-K1#1	50.18(14)
Co1-C6-C7-C8	-56.0(2)	C2-Co1-C8-K1#1	-128.0(3)
K1#1-C6-C7-C8	80.1(2)	C3-Co1-C8-K1#1	128.41(17)
C5-C6-C7-Co1	54.8(2)	C6-Co1-C8-K1#1	18.01(12)
K1#1-C6-C7-Co1	136.09(9)	C1-Co1-C8-K1#1	-126.08(12)
C5-C6-C7-K1#1	-81.3(2)	C5-Co1-C8-K1#1	-22.96(13)
Co1-C6-C7-K1#1	-136.09(9)	C4-Co1-C8-K1#1	142.03(12)
C2-Co1-C7-C6	48.6(4)	C2-C3-K1-O2	-25.12(17)
C3-Co1-C7-C6	89.8(2)	C4-C3-K1-O2	92.66(16)
C1-Co1-C7-C6	-120.2(3)	Co1-C3-K1-O2	20.2(3)
C5-Co1-C7-C6	-31.77(18)	C2-C3-K1-O4	-146.66(16)
C8-Co1-C7-C6	-129.7(2)	C4-C3-K1-O4	-28.89(16)
C4-Co1-C7-C6	129.70(17)	Co1-C3-K1-O4	-101.4(2)
C2-Co1-C7-C8	178.3(3)	C2-C3-K1-O3	-85.59(16)
C3-Co1-C7-C8	-140.54(17)	C4-C3-K1-O3	32.19(16)
C6-Co1-C7-C8	129.7(2)	Co1-C3-K1-O3	-40.3(2)

C2-C3-K1-O1	34.16(16)	C1-C2-K1-O6	163.24(17)
C4-C3-K1-O1	151.93(16)	Co1-C2-K1-O6	-112.84(14)
Co1-C3-K1-O1	79.5(2)	C1-C2-K1-C3	-112.3(3)
C2-C3-K1-O5	153.80(17)	Co1-C2-K1-C3	-28.35(14)
C4-C3-K1-O5	-88.43(16)	C3-C2-K1-C7#2	142.5(3)
Co1-C3-K1-O5	-160.9(3)	C1-C2-K1-C7#2	30.2(4)
C2-C3-K1-O6	94.03(16)	Co1-C2-K1-C7#2	114.1(3)
C4-C3-K1-O6	-148.20(16)	C3-C2-K1-C8#2	-87.0(3)
Co1-C3-K1-O6	139.3(3)	C1-C2-K1-C8#2	160.7(2)
C2-C3-K1-C7#2	-156.6(2)	Co1-C2-K1-C8#2	-115.4(2)
C4-C3-K1-C7#2	-38.9(3)	C3-C2-K1-C6#2	164.32(16)
Co1-C3-K1-C7#2	-111.3(3)	C1-C2-K1-C6#2	52.1(2)
C2-C3-K1-C8#2	145.41(16)	Co1-C2-K1-C6#2	135.97(13)
C4-C3-K1-C8#2	-96.8(2)	O2-K1-O1-C20	-148.73(15)
Co1-C3-K1-C8#2	-169.28(19)	O4-K1-O1-C20	99.1(5)
C2-C3-K1-C6#2	-44.8(4)	O3-K1-O1-C20	-166.65(13)
C4-C3-K1-C6#2	73.0(4)	O5-K1-O1-C20	36.85(15)
Co1-C3-K1-C6#2	0.5(5)	O6-K1-O1-C20	19.04(13)
C4-C3-K1-C2	117.8(2)	C3-K1-O1-C20	107.34(15)
Co1-C3-K1-C2	45.3(2)	C7#2-K1-O1-C20	-69.39(15)
C3-C2-K1-O2	154.60(17)	C8#2-K1-O1-C20	-44.87(15)
C1-C2-K1-O2	42.33(17)	C6#2-K1-O1-C20	-84.57(14)
Co1-C2-K1-O2	126.25(15)	C2-K1-O1-C20	121.68(15)
C3-C2-K1-O4	35.76(17)	O2-K1-O1-C9	-17.13(12)
C1-C2-K1-O4	-76.51(17)	O4-K1-O1-C9	-129.3(4)
Co1-C2-K1-O4	7.41(16)	O3-K1-O1-C9	-35.05(14)
C3-C2-K1-O3	93.88(16)	O5-K1-O1-C9	168.45(12)
C1-C2-K1-O3	-18.39(17)	O6-K1-O1-C9	150.64(14)
Co1-C2-K1-O3	65.53(14)	C3-K1-O1-C9	-121.06(14)
C3-C2-K1-O1	-141.89(18)	C7#2-K1-O1-C9	62.21(14)
C1-C2-K1-O1	105.84(18)	C8#2-K1-O1-C9	86.73(14)
Co1-C2-K1-O1	-170.24(16)	C6#2-K1-O1-C9	47.02(14)
C3-C2-K1-O5	-25.52(17)	C2-K1-O1-C9	-106.72(14)
C1-C2-K1-O5	-137.78(17)	O4-K1-O2-C10	155.79(13)
Co1-C2-K1-O5	-53.87(14)	O3-K1-O2-C10	144.19(15)
C3-C2-K1-O6	-84.49(16)	O1-K1-O2-C10	-17.97(13)

O5-K1-O2-C10	48.6(6)	C2-K1-O3-C13	-136.47(14)
O6-K1-O2-C10	-30.09(15)	O2-K1-O4-C15	-158.52(13)
C3-K1-O2-C10	59.77(14)	O3-K1-O4-C15	-146.93(15)
C7#2-K1-O2-C10	-132.42(14)	O1-K1-O4-C15	-49.5(5)
C8#2-K1-O2-C10	-115.41(14)	O5-K1-O4-C15	15.53(13)
C6#2-K1-O2-C10	-124.55(15)	O6-K1-O4-C15	27.35(15)
C2-K1-O2-C10	49.79(14)	C3-K1-O4-C15	-57.66(14)
O4-K1-O2-C11	24.60(15)	C7#2-K1-O4-C15	119.42(15)
O3-K1-O2-C11	13.00(13)	C8#2-K1-O4-C15	95.29(14)
O1-K1-O2-C11	-149.17(14)	C6#2-K1-O4-C15	134.20(14)
O5-K1-O2-C11	-82.6(5)	C2-K1-O4-C15	-71.15(15)
O6-K1-O2-C11	-161.28(13)	O2-K1-O4-C14	-24.96(15)
C3-K1-O2-C11	-71.42(14)	O3-K1-O4-C14	-13.37(13)
C7#2-K1-O2-C11	96.38(14)	O1-K1-O4-C14	84.1(5)
C8#2-K1-O2-C11	113.40(14)	O5-K1-O4-C14	149.09(15)
C6#2-K1-O2-C11	104.25(14)	O6-K1-O4-C14	160.91(13)
C2-K1-O2-C11	-81.40(14)	C3-K1-O4-C14	75.90(14)
O2-K1-O3-C12	21.63(13)	C7#2-K1-O4-C14	-107.02(14)
O4-K1-O3-C12	-147.02(15)	C8#2-K1-O4-C14	-131.15(14)
O1-K1-O3-C12	39.55(15)	C6#2-K1-O4-C14	-92.24(14)
O5-K1-O3-C12	-164.59(13)	C2-K1-O4-C14	62.41(14)
O6-K1-O3-C12	117.8(5)	O2-K1-O5-C16	130.4(5)
C3-K1-O3-C12	122.24(14)	O4-K1-O5-C16	20.19(13)
C7#2-K1-O3-C12	-73.28(14)	O3-K1-O5-C16	37.82(14)
C8#2-K1-O3-C12	-80.96(14)	O1-K1-O5-C16	-165.67(13)
C6#2-K1-O3-C12	-49.78(14)	O6-K1-O5-C16	-147.85(14)
C2-K1-O3-C12	98.79(14)	C3-K1-O5-C16	118.98(14)
O2-K1-O3-C13	146.38(14)	C7#2-K1-O5-C16	-48.60(14)
O4-K1-O3-C13	-22.27(13)	C8#2-K1-O5-C16	-65.18(14)
O1-K1-O3-C13	164.30(13)	C6#2-K1-O5-C16	-56.75(15)
O5-K1-O3-C13	-39.84(14)	C2-K1-O5-C16	129.20(13)
O6-K1-O3-C13	-117.4(5)	O2-K1-O5-C17	-102.0(5)
C3-K1-O3-C13	-113.01(14)	O4-K1-O5-C17	147.87(16)
C7#2-K1-O3-C13	51.47(14)	O3-K1-O5-C17	165.50(14)
C8#2-K1-O3-C13	43.79(14)	O1-K1-O5-C17	-37.99(16)
C6#2-K1-O3-C13	74.97(14)	O6-K1-O5-C17	-20.17(14)

C3-K1-O5-C17	-113.34(15)	K1-O2-C10-C9	50.7(2)
C7#2-K1-O5-C17	79.08(15)	O1-C9-C10-O2	-67.9(2)
C8#2-K1-O5-C17	62.51(15)	C10-O2-C11-C12	-177.01(18)
C6#2-K1-O5-C17	70.93(16)	K1-O2-C11-C12	-45.0(2)
C2-K1-O5-C17	-103.12(15)	C13-O3-C12-C11	-178.22(18)
O2-K1-O6-C18	158.39(13)	K1-O3-C12-C11	-53.7(2)
O4-K1-O6-C18	-27.38(15)	O2-C11-C12-O3	66.7(2)
O3-K1-O6-C18	65.0(6)	C12-O3-C13-C14	-179.57(19)
O1-K1-O6-C18	146.10(15)	K1-O3-C13-C14	55.3(2)
O5-K1-O6-C18	-15.43(13)	C15-O4-C14-C13	-179.15(18)
C3-K1-O6-C18	60.56(14)	K1-O4-C14-C13	46.4(2)
C7#2-K1-O6-C18	-103.78(14)	O3-C13-C14-O4	-69.1(2)
C8#2-K1-O6-C18	-96.67(15)	C14-O4-C15-C16	176.92(18)
C6#2-K1-O6-C18	-127.62(14)	K1-O4-C15-C16	-48.6(2)
C2-K1-O6-C18	84.04(14)	C17-O5-C16-C15	178.55(18)
O2-K1-O6-C19	29.00(16)	K1-O5-C16-C15	-52.94(19)
O4-K1-O6-C19	-156.77(14)	O4-C15-C16-O5	69.2(2)
O3-K1-O6-C19	-64.4(6)	C16-O5-C17-C18	-179.79(18)
O1-K1-O6-C19	16.71(14)	K1-O5-C17-C18	53.1(2)
O5-K1-O6-C19	-144.82(15)	C19-O6-C18-C17	178.15(19)
C3-K1-O6-C19	-68.83(15)	K1-O6-C18-C17	48.4(2)
C7#2-K1-O6-C19	126.83(15)	O5-C17-C18-O6	-68.8(2)
C8#2-K1-O6-C19	133.93(15)	C18-O6-C19-C20	-179.24(18)
C6#2-K1-O6-C19	102.99(15)	K1-O6-C19-C20	-49.3(2)
C2-K1-O6-C19	-45.35(15)	C9-O1-C20-C19	176.51(17)
C20-O1-C9-C10	-178.53(18)	K1-O1-C20-C19	-52.1(2)
K1-O1-C9-C10	49.17(19)	O6-C19-C20-O1	68.4(2)
C11-O2-C10-C9	-176.50(17)		

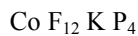
Symmetry transformations used to generate equivalent atoms:

#1 $x+1/2, -y+3/2, z-1/2$ #2 $x-1/2, -y+3/2, z+1/2$

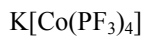
REFERENCE NUMBER: 05247 [3]

[Revised May 29, 2012]

CRYSTAL STRUCTURE REPORT



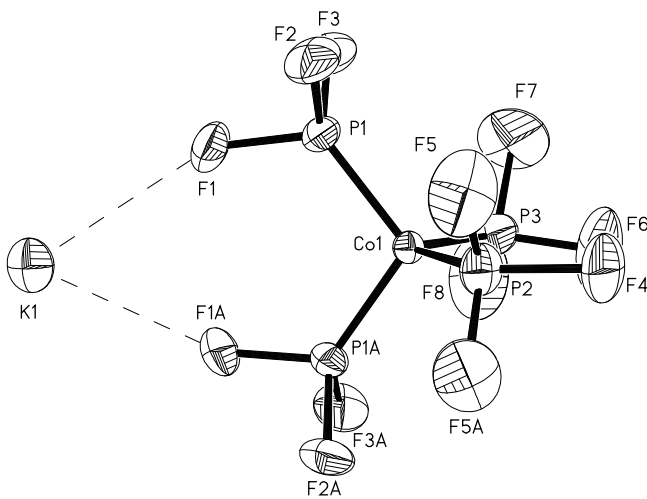
or



Report prepared for:

W. Brennessel, Prof. J. Ellis

August 14, 2005



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Data collection

A crystal ($0.36 \times 0.36 \times 0.32 \text{ mm}^3$) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Siemens SMART CCD Platform diffractometer for a data collection at 223(2) K.¹ The temperature is approximately 20 degrees above that where a phase change occurs, which transforms the crystal from an orthorhombic to a monoclinic setting, the latter which is a non-merohedral twin (180 degree rotation about $[1\ 0\ 0]$). The twinned phase will be examined in a later study. 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 MoK α radiation (graphite monochromator) with a frame time of 10 seconds and a detector distance of 4.92 cm. A randomly oriented region of reciprocal space was surveyed: four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption.² Final cell constants were calculated from the xyz centroids of 3142 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 SHELXS-97⁴ and refined using SHELXL-97.⁵ The space group *Pnma* 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. The final full matrix least squares refinement converged to $R1 = 0.0242$ (F^2 , $I > 2\sigma(I)$) and $wR2 = 0.0555$ (F^2 , all data).

Structure description

The structure is the one suggested. The potassium cation is caged by close contacts to 10 fluorine atoms in a pseudo bicapped octagonal antiprismatic geometry (see diagram). A crystallographic mirror plane coincides with atoms K1, Co1, P2, F4, P3, and F6; thus, one half of the molecule is unique. Atoms of one PF₃ ligand (P3, F6, F7, F8) are disordered slightly over the mirror plane (50:50) and are modeled as such.

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

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

¹ APEX2, version 2011.4-1; Bruker AXS: Madison, WI, 2011.

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

³ *SAINT*, version 7.68A; Bruker AXS: Madison, WI, 2009.

⁴ Altomare, A.; Burla, M. C.; Camalli, M.; Casciarano, 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:

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

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

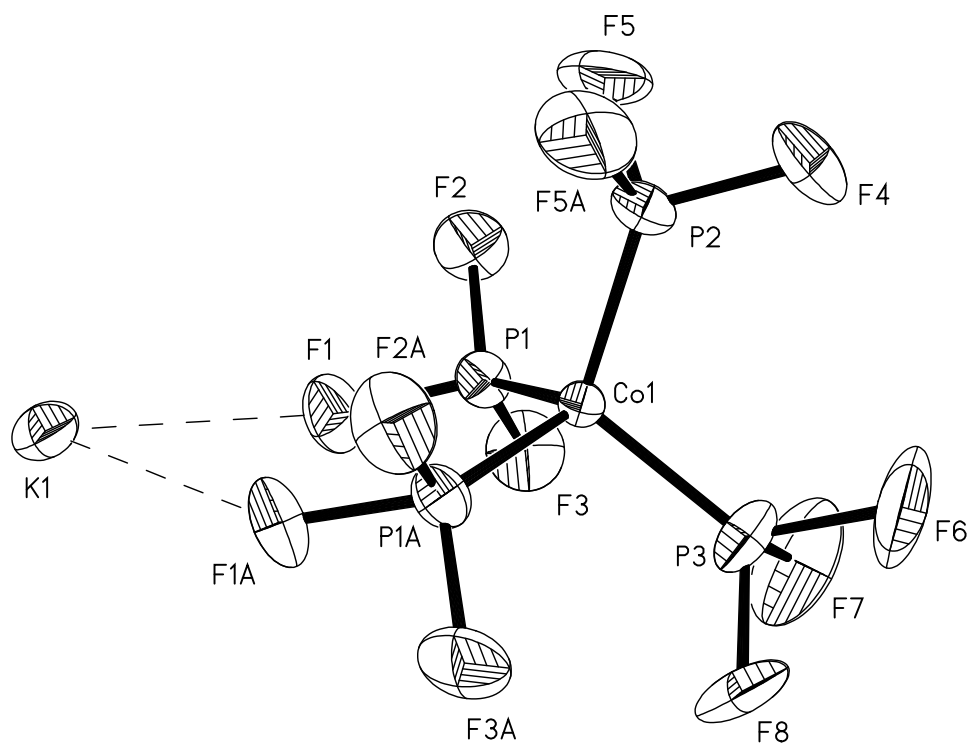
$$wR2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$$

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



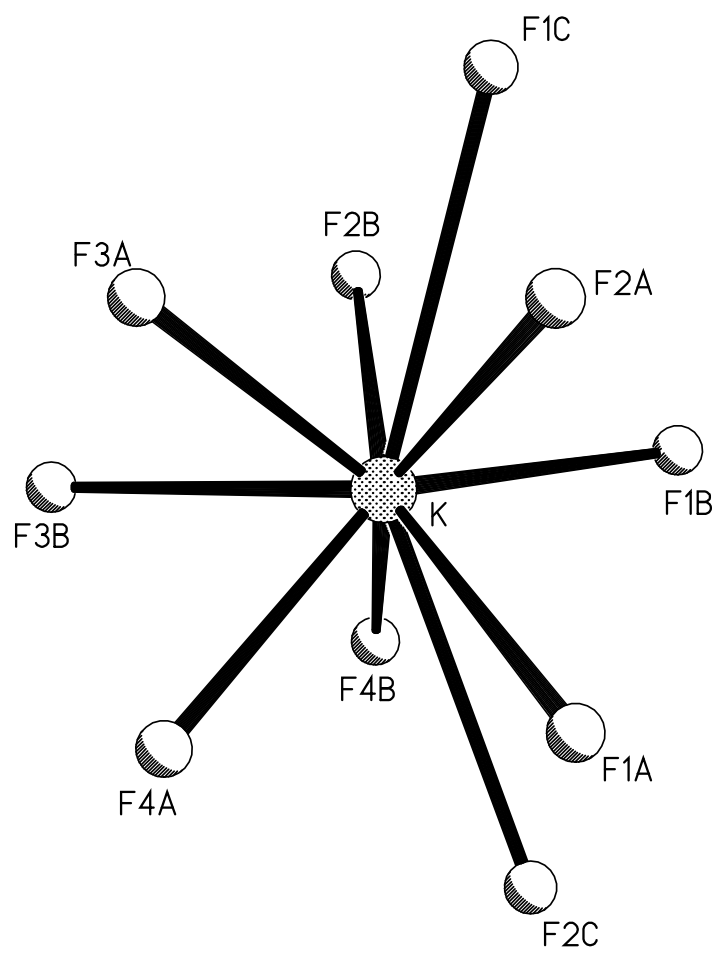
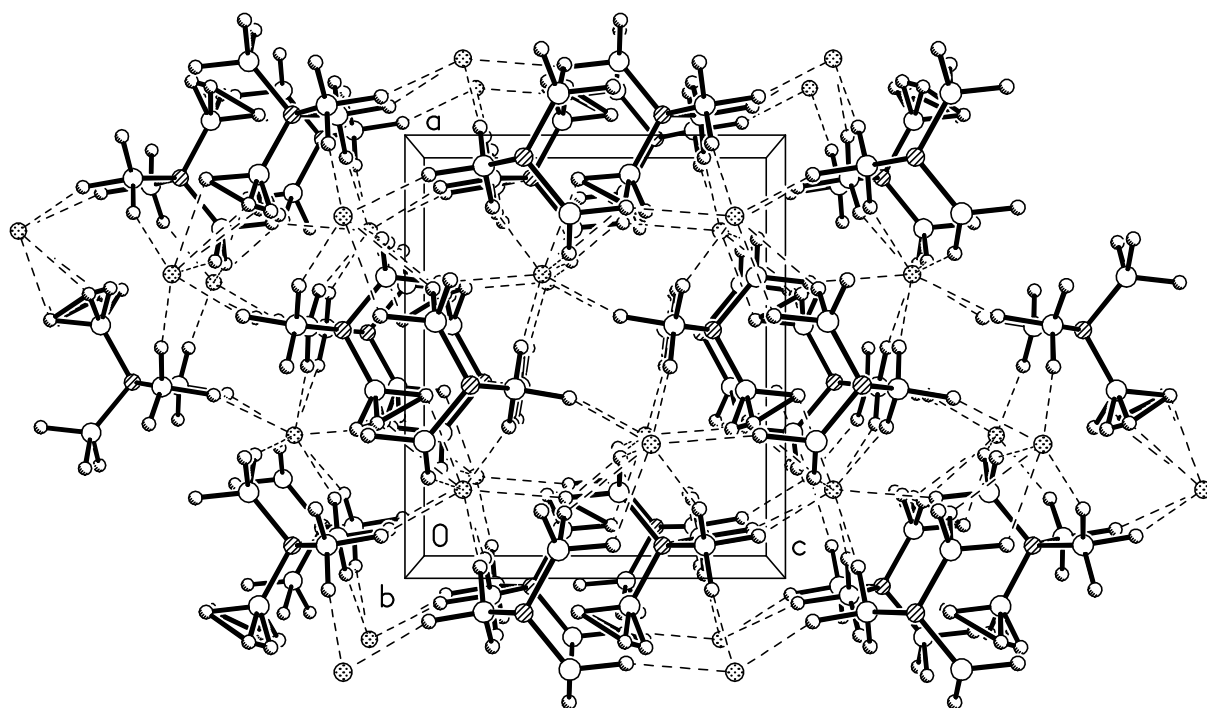


Table 1. Crystal data and structure refinement for 05247.

Identification code	05247	
Empirical formula	Co F ₁₂ K P ₄	
Formula weight	449.91	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	<i>Pnma</i>	
Unit cell dimensions	$a = 12.6253(10)$ Å	$\alpha = 90^\circ$
	$b = 8.5070(7)$ Å	$\beta = 90^\circ$
	$c = 10.8490(9)$ Å	$\gamma = 90^\circ$
Volume	1165.22(16) Å ³	
<i>Z</i>	4	
Density (calculated)	2.565 Mg/m ³	
Absorption coefficient	2.512 mm ⁻¹	
<i>F</i> (000)	856	
Crystal color, morphology	colorless, block	
Crystal size	0.36 x 0.36 x 0.32 mm ³	
Theta range for data collection	2.48 to 27.52°	
Index ranges	$-16 \leq h \leq 16, -11 \leq k \leq 11, -13 \leq l \leq 14$	
Reflections collected	13136	
Independent reflections	1428 [<i>R</i> (int) = 0.0221]	
Observed reflections	1336	
Completeness to theta = 27.52°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.4478 and 0.4161	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	1428 / 3 / 106	
Goodness-of-fit on <i>F</i> ²	1.088	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0242, <i>wR</i> 2 = 0.0543	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0268, <i>wR</i> 2 = 0.0555	
Largest diff. peak and hole	0.518 and -0.391 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05247. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
K1	3083(1)	2500	6431(1)	46(1)
Co1	4380(1)	2500	1820(1)	21(1)
P1	4281(1)	590(1)	2904(1)	31(1)
F1	4078(1)	760(2)	4330(1)	53(1)
F2	3409(1)	-710(2)	2717(1)	56(1)
F3	5218(1)	-620(2)	3043(2)	60(1)
P2	3141(1)	2500	643(1)	37(1)
F4	3276(2)	2500	-793(2)	64(1)
F5	2307(1)	1139(3)	675(2)	79(1)
P3	5775(1)	2574(10)	931(1)	46(1)
F6	5895(3)	2928(11)	-457(3)	106(4)
F7	6510(7)	1109(11)	792(7)	112(3)
F8	6666(6)	3688(13)	1356(6)	104(3)

Table 3. Bond lengths [Å] and angles [°] for 05247.

K(1)-F(3)#1	2.7356(16)	F(3)#2-K(1)-F(2)#3	137.95(6)
K(1)-F(3)#2	2.7356(16)	F(3)#1-K(1)-F(2)#4	137.95(6)
K(1)-F(2)#3	2.7956(16)	F(3)#2-K(1)-F(2)#4	96.06(5)
K(1)-F(2)#4	2.7956(16)	F(2)#3-K(1)-F(2)#4	66.03(7)
K(1)-F(6)#5	2.979(4)	F(3)#1-K(1)-F(6)#5	136.83(18)
K(1)-F(6)#6	2.979(4)	F(3)#2-K(1)-F(6)#5	150.73(18)
K(1)-F(1)	2.9943(16)	F(2)#3-K(1)-F(6)#5	59.05(12)
K(1)-F(1)#7	2.9943(16)	F(2)#4-K(1)-F(6)#5	67.61(14)
K(1)-F(4)#8	3.022(2)	F(3)#1-K(1)-F(6)#6	150.73(18)
K(1)-F(5)#4	3.240(2)	F(3)#2-K(1)-F(6)#6	136.83(18)
K(1)-F(5)#3	3.240(2)	F(2)#3-K(1)-F(6)#6	67.61(14)
K(1)-F(7)#6	3.340(9)	F(2)#4-K(1)-F(6)#6	59.05(12)
Co(1)-P(3)#7	2.0094(10)	F(6)#5-K(1)-F(6)#6	14.1(4)
Co(1)-P(3)	2.0094(10)	F(3)#1-K(1)-F(1)	96.83(5)
Co(1)-P(1)#7	2.0096(6)	F(3)#2-K(1)-F(1)	62.68(5)
Co(1)-P(1)	2.0096(6)	F(2)#3-K(1)-F(1)	158.76(5)
Co(1)-P(2)	2.0183(8)	F(2)#4-K(1)-F(1)	113.17(4)
P(1)-F(2)	1.5729(14)	F(6)#5-K(1)-F(1)	100.34(11)
P(1)-F(1)	1.5740(14)	F(6)#6-K(1)-F(1)	93.35(12)
P(1)-F(3)	1.5765(15)	F(3)#1-K(1)-F(1)#7	62.68(5)
F(2)-K(1)#9	2.7955(16)	F(3)#2-K(1)-F(1)#7	96.83(5)
F(3)-K(1)#2	2.7356(16)	F(2)#3-K(1)-F(1)#7	113.17(4)
P(2)-F(5)	1.5657(18)	F(2)#4-K(1)-F(1)#7	158.75(5)
P(2)-F(5)#7	1.5657(18)	F(6)#5-K(1)-F(1)#7	93.35(12)
P(2)-F(4)	1.568(2)	F(6)#6-K(1)-F(1)#7	100.34(11)
F(4)-K(1)#10	3.022(2)	F(1)-K(1)-F(1)#7	59.25(6)
F(5)-K(1)#9	3.240(2)	F(3)#1-K(1)-F(4)#8	74.24(6)
P(3)-F(8)	1.541(5)	F(3)#2-K(1)-F(4)#8	74.24(5)
P(3)-F(6)	1.543(4)	F(2)#3-K(1)-F(4)#8	63.71(5)
P(3)-F(7)	1.561(6)	F(2)#4-K(1)-F(4)#8	63.71(5)
F(6)-K(1)#11	2.979(4)	F(6)#5-K(1)-F(4)#8	115.38(9)
F(7)-K(1)#11	3.340(9)	F(6)#6-K(1)-F(4)#8	115.38(9)
F(3)#1-K(1)-F(3)#2	71.54(7)	F(1)-K(1)-F(4)#8	136.45(5)
F(3)#1-K(1)-F(2)#3	96.06(5)	F(1)#7-K(1)-F(4)#8	136.45(5)

F(3)#1-K(1)-F(5)#4	136.91(5)	P(3)#7-Co(1)-P(1)	108.1(2)
F(3)#2-K(1)-F(5)#4	67.25(5)	P(3)-Co(1)-P(1)	111.1(2)
F(2)#3-K(1)-F(5)#4	123.00(5)	P(1)#7-Co(1)-P(1)	107.87(4)
F(2)#4-K(1)-F(5)#4	60.23(4)	P(3)#7-Co(1)-P(2)	112.06(5)
F(6)#5-K(1)-F(5)#4	83.48(18)	P(3)-Co(1)-P(2)	112.06(5)
F(6)#6-K(1)-F(5)#4	69.68(18)	P(1)#7-Co(1)-P(2)	108.80(2)
F(1)-K(1)-F(5)#4	53.04(4)	P(1)-Co(1)-P(2)	108.79(2)
F(1)#7-K(1)-F(5)#4	110.08(4)	F(2)-P(1)-F(1)	94.47(8)
F(4)#8-K(1)-F(5)#4	105.34(3)	F(2)-P(1)-F(3)	94.49(9)
F(3)#1-K(1)-F(5)#3	67.25(5)	F(1)-P(1)-F(3)	95.08(9)
F(3)#2-K(1)-F(5)#3	136.91(5)	F(2)-P(1)-Co(1)	122.42(6)
F(2)#3-K(1)-F(5)#3	60.23(4)	F(1)-P(1)-Co(1)	120.73(6)
F(2)#4-K(1)-F(5)#3	123.00(5)	F(3)-P(1)-Co(1)	122.49(7)
F(6)#5-K(1)-F(5)#3	69.68(18)	P(1)-F(1)-K(1)	149.48(9)
F(6)#6-K(1)-F(5)#3	83.48(18)	P(1)-F(2)-K(1)#9	156.75(8)
F(1)-K(1)-F(5)#3	110.08(4)	P(1)-F(3)-K(1)#2	172.15(10)
F(1)#7-K(1)-F(5)#3	53.04(4)	F(5)-P(2)-F(5)#7	95.35(17)
F(4)#8-K(1)-F(5)#3	105.34(3)	F(5)-P(2)-F(4)	95.46(9)
F(5)#4-K(1)-F(5)#3	145.68(7)	F(5)#7-P(2)-F(4)	95.46(9)
F(3)#1-K(1)-F(7)#6	114.19(12)	F(5)-P(2)-Co(1)	120.48(7)
F(3)#2-K(1)-F(7)#6	145.48(17)	F(5)#7-P(2)-Co(1)	120.48(7)
F(2)#3-K(1)-F(7)#6	76.51(17)	F(4)-P(2)-Co(1)	122.99(10)
F(2)#4-K(1)-F(7)#6	98.79(13)	P(2)-F(4)-K(1)#10	169.11(14)
F(6)#5-K(1)-F(7)#6	31.74(16)	P(2)-F(5)-K(1)#9	144.50(10)
F(6)#6-K(1)-F(7)#6	40.20(17)	F(8)-P(3)-F(6)	95.7(4)
F(1)-K(1)-F(7)#6	82.82(17)	F(8)-P(3)-F(7)	94.9(3)
F(1)#7-K(1)-F(7)#6	61.63(13)	F(6)-P(3)-F(7)	90.2(5)
F(4)#8-K(1)-F(7)#6	140.14(17)	F(8)-P(3)-Co(1)	121.0(4)
F(5)#4-K(1)-F(7)#6	93.76(14)	F(6)-P(3)-Co(1)	124.09(18)
F(5)#3-K(1)-F(7)#6	52.31(14)	F(7)-P(3)-Co(1)	122.9(5)
P(3)#7-Co(1)-P(3)	3.6(5)	P(3)-F(6)-K(1)#11	114.4(2)
P(3)#7-Co(1)-P(1)#7	111.1(2)	P(3)-F(7)-K(1)#11	98.1(4)
P(3)-Co(1)-P(1)#7	108.1(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z+1 #2 -x+1,-y,-z+1 #3 -x+1/2,y+1/2,z+1/2

#4 $-x+1/2, -y, z+1/2$ #5 $x-1/2, y, -z+1/2$ #6 $x-1/2, -y+1/2, -z+1/2$

#7 $x, -y+1/2, z$ #8 $x, y, z+1$ #9 $-x+1/2, -y, z-1/2$

#10 $x, y, z-1$ #11 $x+1/2, y, -z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05247. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K1	29(1)	61(1)	48(1)	0	1(1)	0
Co1	20(1)	22(1)	21(1)	0	0(1)	0
P1	39(1)	26(1)	29(1)	5(1)	-2(1)	-2(1)
F1	78(1)	51(1)	29(1)	11(1)	2(1)	-7(1)
F2	72(1)	36(1)	59(1)	6(1)	0(1)	-24(1)
F3	69(1)	43(1)	67(1)	16(1)	-7(1)	21(1)
P2	33(1)	50(1)	30(1)	0	-11(1)	0
F4	77(2)	85(2)	29(1)	0	-18(1)	0
F5	56(1)	112(2)	69(1)	2(1)	-24(1)	-42(1)
P3	31(1)	54(1)	52(1)	16(2)	17(1)	6(2)
F6	91(2)	169(12)	58(2)	30(3)	46(2)	5(3)
F7	86(5)	106(4)	143(8)	16(5)	62(5)	58(4)
F8	39(2)	179(7)	94(5)	-3(4)	8(3)	-55(3)

Table 5. Torsion angles [°] for 05247.

P3#7-Co1-P1-F2	-116.88(15)	P1#7-Co1-P2-F5	-117.72(10)
P3-Co1-P1-F2	-118.83(17)	P1-Co1-P2-F5	-0.44(10)
P1#7-Co1-P1-F2	122.87(8)	P3#7-Co1-P2-F5#7	-122.9(3)
P2-Co1-P1-F2	5.01(8)	P3-Co1-P2-F5#7	-119.0(3)
P3#7-Co1-P1-F1	124.11(14)	P1#7-Co1-P2-F5#7	0.44(10)
P3-Co1-P1-F1	122.16(17)	P1-Co1-P2-F5#7	117.72(10)
P1#7-Co1-P1-F1	3.87(9)	P3#7-Co1-P2-F4	-1.9(3)
P2-Co1-P1-F1	-113.99(8)	P3-Co1-P2-F4	1.9(3)
P3#7-Co1-P1-F3	4.06(15)	P1#7-Co1-P2-F4	121.36(2)
P3-Co1-P1-F3	2.11(17)	P1-Co1-P2-F4	-121.36(2)
P1#7-Co1-P1-F3	-116.18(8)	F5-P2-F4-K1#10	47.96(8)
P2-Co1-P1-F3	125.95(8)	F5#7-P2-F4-K1#10	-47.96(8)
F2-P1-F1-K1	-99.71(17)	Co1-P2-F4-K1#10	180.0
F3-P1-F1-K1	165.37(16)	F5#7-P2-F5-K1#9	-154.72(10)
Co1-P1-F1-K1	32.51(19)	F4-P2-F5-K1#9	109.25(17)
F3#1-K1-F1-P1	-93.29(17)	Co1-P2-F5-K1#9	-24.5(2)
F3#2-K1-F1-P1	-158.41(18)	P3#7-Co1-P3-F8	-134.4(5)
F2#3-K1-F1-P1	33.7(3)	P1#7-Co1-P3-F8	15.1(5)
F2#4-K1-F1-P1	116.86(16)	P1-Co1-P3-F8	-103.1(5)
F6#5-K1-F1-P1	46.9(2)	P2-Co1-P3-F8	134.9(4)
F6#6-K1-F1-P1	59.2(2)	P3#7-Co1-P3-F6	102.4(7)
F1#7-K1-F1-P1	-40.82(18)	P1#7-Co1-P3-F6	-108.2(6)
F4#8-K1-F1-P1	-167.56(15)	P1-Co1-P3-F6	133.7(6)
F5#4-K1-F1-P1	120.56(18)	P2-Co1-P3-F6	11.7(7)
F5#3-K1-F1-P1	-25.07(18)	P3#7-Co1-P3-F7	-13.8(4)
F7#6-K1-F1-P1	20.3(2)	P1#7-Co1-P3-F7	135.6(4)
F1-P1-F2-K1#9	155.9(2)	P1-Co1-P3-F7	17.4(4)
F3-P1-F2-K1#9	-108.6(2)	P2-Co1-P3-F7	-104.5(4)
Co1-P1-F2-K1#9	24.8(3)	F8-P3-F6-K1#11	53.7(6)
F2-P1-F3-K1#2	-129.6(7)	F7-P3-F6-K1#11	-41.3(6)
F1-P1-F3-K1#2	-34.7(7)	Co1-P3-F6-K1#11	-172.4(4)
Co1-P1-F3-K1#2	97.0(7)	F8-P3-F7-K1#11	-63.0(4)
P3#7-Co1-P2-F5	119.0(3)	F6-P3-F7-K1#11	32.8(4)
P3-Co1-P2-F5	122.9(3)	Co1-P3-F7-K1#11	164.78(15)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, y+1/2, -z+1$ #2 $-x+1, -y, -z+1$ #3 $-x+1/2, y+1/2, z+1/2$

#4 $-x+1/2, -y, z+1/2$ #5 $x-1/2, y, -z+1/2$ #6 $x-1/2, -y+1/2, -z+1/2$

#7 $x, -y+1/2, z$ #8 $x, y, z+1$ #9 $-x+1/2, -y, z-1/2$

#10 $x, y, z-1$ #11 $x+1/2, y, -z+1/2$

REFERENCE NUMBER: 01152 [4]

CRYSTAL STRUCTURE REPORT

$C_{30} H_{72} Co K N_2 O_{18} P_4$

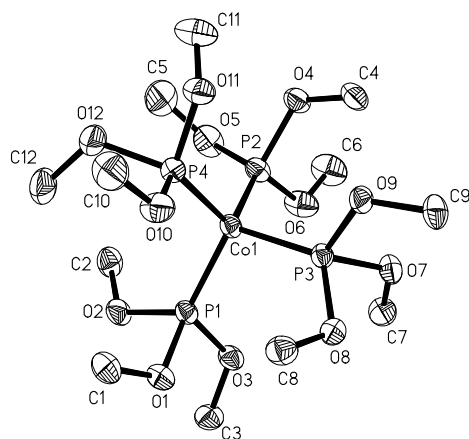
or

$[K(222)][Co(P(OMe)_3)_4]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

May 10, 2001



William W. Brennessel
X-Ray Crystallographic Laboratory
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Data collection

A crystal (approximate dimensions 0.32 x 0.27 x 0.18 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K. A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 326 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 10 seconds and a detector distance of 4.897 cm. A randomly oriented region of reciprocal space was surveyed to the extent of 1.5 hemispheres and to a resolution of 0.84 Å. Three major sections of frames were collected with 0.30° steps in ω at 3 different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).¹ Final cell constants were calculated from the xyz centroids of 3306 strong reflections from the actual data collection after integration (SAINT 6.01, 1999).² Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR³ and refined using SHELXL-97.⁴ The space group P2(1)/c 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 = 0.0368 and wR2 = 0.0991 (F², all data).

Structure description

The structure is the one suggested. It should be noted that it is a polymorph of an earlier structure.⁵ One methyl group is rotationally disordered.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using SGI INDY R4400-SC or Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

¹ An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **1995**, *A51*, 33.

² SAINT V6.1, Bruker Analytical X-Ray Systems, Madison, WI.

³ SIR92, A. Altomare, G. Cascarno, C. Giacovazzo, A. Gualardi, *J. Appl. Cryst.* **1993**, *26*, 343.

⁴ SHELXTL-Plus V5.10, Bruker Analytical X-Ray Systems, Madison, WI.

⁵ Protasiewicz, J. D.; Theopold, K. H.; Schulte, G. *Inorg. Chem* **1988**, 27, 1137..

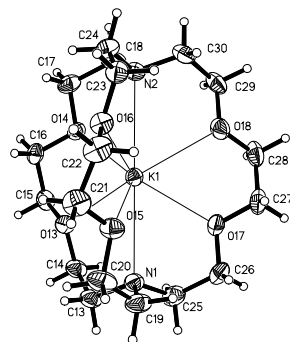
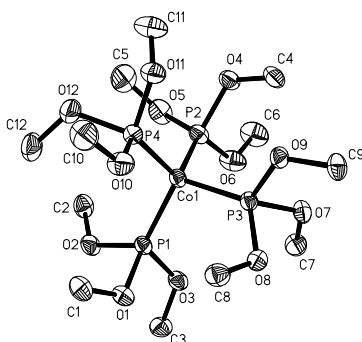
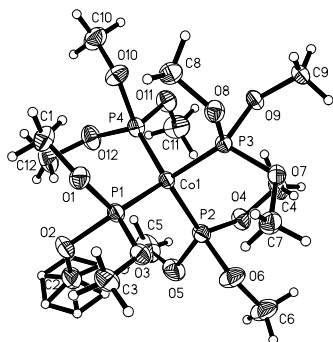
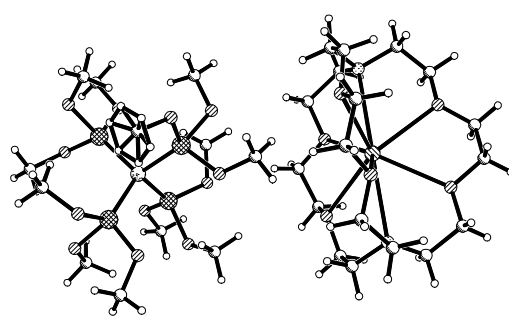
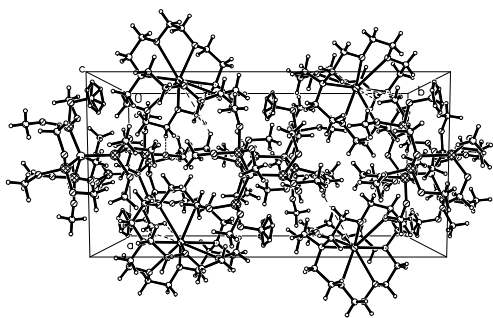
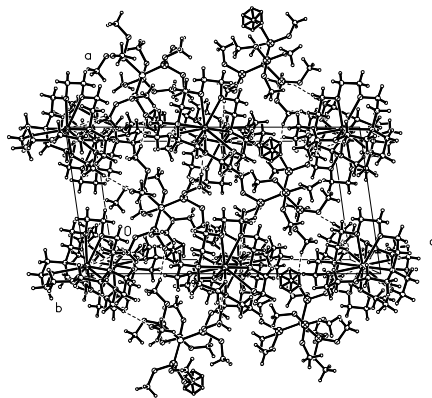
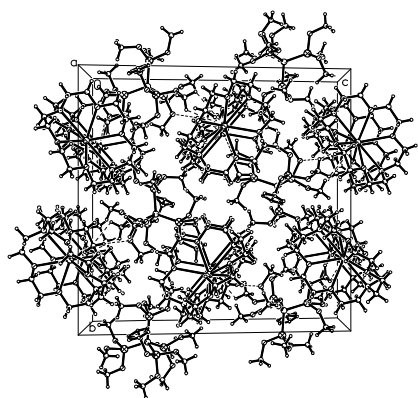


Table 1. Crystal data and structure refinement for 01152.

Identification code	01152	
Empirical formula	C ₃₀ H ₇₂ Co K N ₂ O ₁₈ P ₄	
Formula weight	970.81	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.6444(9) Å	$\alpha = 90^\circ$.
	b = 20.543(2) Å	$\beta = 98.218(2)^\circ$.
	c = 21.227(2) Å	$\gamma = 90^\circ$.
Volume	4593.8(7) Å ³	
Z	4	
Density (calculated)	1.404 Mg/m ³	
Absorption coefficient	0.672 mm ⁻¹	
F(000)	2064	
Crystal habit and color	colorless, block	
Crystal size	0.32 x 0.27 x 0.18 mm ³	
Theta range for data collection	1.39 to 27.52°.	
Index ranges	-13= h = 13, -26= k = 26, -25= l = 27	
Reflections collected	36689	
Independent reflections	10513 [R(int) = 0.0563]	
Observed Reflections	8184	
Completeness to theta = 27.52°	99.3 %	
Absorption correction	Multi-scan	
Max. and min. transmission	1.000000 and 0.823446	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10513 / 0 / 517	
Goodness-of-fit on F ²	0.978	
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.0939	
R indices (all data)	R1 = 0.0497, wR2 = 0.0991	
Largest diff. peak and hole	0.668 and -0.362 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 01152. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co1	5536(1)	4445(1)	-2644(1)	21(1)
P1	7262(1)	4042(1)	-2276(1)	23(1)
P2	5594(1)	5448(1)	-2577(1)	27(1)
P3	4264(1)	4142(1)	-2058(1)	22(1)
P4	4832(1)	4132(1)	-3551(1)	25(1)
O1	7516(1)	3250(1)	-2211(1)	30(1)
O2	8601(1)	4171(1)	-2580(1)	31(1)
O3	7776(1)	4184(1)	-1524(1)	29(1)
O4	4331(1)	5907(1)	-2801(1)	32(1)
O5	6517(2)	5924(1)	-2939(1)	43(1)
O6	6034(2)	5755(1)	-1871(1)	40(1)
O7	4089(1)	4522(1)	-1388(1)	29(1)
O8	4329(1)	3416(1)	-1713(1)	27(1)
O9	2760(1)	4158(1)	-2352(1)	26(1)
O10	4458(1)	3360(1)	-3628(1)	34(1)
O11	3480(1)	4395(1)	-3946(1)	34(1)
O12	5580(1)	4218(1)	-4182(1)	39(1)
C1	7359(2)	2858(1)	-2771(1)	38(1)
C2	8826(2)	4798(1)	-2828(1)	36(1)
C3	8901(2)	3888(1)	-1197(1)	34(1)
C4	3166(2)	5714(1)	-2593(1)	40(1)
C5	6370(3)	5895(1)	-3615(1)	56(1)
C6	5892(3)	6441(1)	-1737(1)	50(1)
C7	5194(2)	4641(1)	-944(1)	34(1)
C8	4440(2)	2858(1)	-2103(1)	32(1)
C9	1784(2)	4025(1)	-1967(1)	30(1)
C10	3984(2)	3080(1)	-4234(1)	44(1)
C11	3417(3)	5030(1)	-4214(1)	49(1)
C12	6856(2)	4018(1)	-4150(1)	48(1)
K1	9808(1)	2794(1)	275(1)	26(1)
N1	9648(2)	3888(1)	1193(1)	32(1)

C13	10792(2)	4299(1)	1242(1)	38(1)
C14	11277(2)	4410(1)	619(1)	36(1)
O13	11655(1)	3802(1)	377(1)	30(1)
C15	12300(2)	3900(1)	-159(1)	32(1)
C16	12643(2)	3254(1)	-409(1)	32(1)
O14	11506(1)	2906(1)	-637(1)	31(1)
C17	11776(2)	2325(1)	-961(1)	38(1)
C18	10566(2)	1956(1)	-1166(1)	39(1)
C19	9525(2)	3602(1)	1812(1)	43(1)
C20	10483(3)	3075(1)	2019(1)	45(1)
O15	10305(2)	2557(1)	1572(1)	35(1)
C21	11196(3)	2048(1)	1742(1)	47(1)
C22	10755(3)	1448(1)	1378(1)	42(1)
O16	10725(1)	1578(1)	715(1)	33(1)
C23	10416(2)	1020(1)	338(1)	35(1)
C24	10705(2)	1149(1)	-325(1)	37(1)
C25	8523(2)	4277(1)	960(1)	45(1)
C26	7331(2)	3885(1)	765(1)	49(1)
O17	7478(1)	3487(1)	234(1)	37(1)
C27	6395(2)	3088(1)	60(1)	45(1)
C28	6495(2)	2761(1)	-558(1)	45(1)
O18	7555(1)	2331(1)	-469(1)	37(1)
C29	7696(2)	1988(1)	-1039(1)	41(1)
C30	8672(2)	1460(1)	-876(1)	40(1)
N2	9960(2)	1695(1)	-639(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for 01152.

Co(1)-P(3)	2.0618(5)	C(2)-H(2D)	0.9800
Co(1)-P(1)	2.0641(6)	C(2)-H(2E)	0.9800
Co(1)-P(4)	2.0652(6)	C(2)-H(2F)	0.9800
Co(1)-P(2)	2.0653(6)	C(3)-H(3A)	0.9800
P(1)-O(3)	1.6391(15)	C(3)-H(3B)	0.9800
P(1)-O(1)	1.6518(14)	C(3)-H(3C)	0.9800
P(1)-O(2)	1.6663(13)	C(4)-H(4A)	0.9800
P(2)-O(6)	1.6315(16)	C(4)-H(4B)	0.9800
P(2)-O(5)	1.6523(15)	C(4)-H(4C)	0.9800
P(2)-O(4)	1.6562(14)	C(5)-H(5A)	0.9800
P(3)-O(9)	1.6332(13)	C(5)-H(5B)	0.9800
P(3)-O(7)	1.6537(13)	C(5)-H(5C)	0.9800
P(3)-O(8)	1.6583(14)	C(6)-H(6A)	0.9800
P(4)-O(10)	1.6379(15)	C(6)-H(6B)	0.9800
P(4)-O(11)	1.6499(15)	C(6)-H(6C)	0.9800
P(4)-O(12)	1.6619(15)	C(7)-H(7A)	0.9800
O(1)-C(1)	1.425(2)	C(7)-H(7B)	0.9800
O(2)-C(2)	1.425(2)	C(7)-H(7C)	0.9800
O(3)-C(3)	1.431(2)	C(8)-H(8A)	0.9800
O(4)-C(4)	1.430(2)	C(8)-H(8B)	0.9800
O(5)-C(5)	1.423(3)	C(8)-H(8C)	0.9800
O(6)-C(6)	1.450(3)	C(9)-H(9A)	0.9800
O(7)-C(7)	1.420(2)	C(9)-H(9B)	0.9800
O(8)-C(8)	1.427(2)	C(9)-H(9C)	0.9800
O(9)-C(9)	1.438(2)	C(10)-H(10A)	0.9800
O(10)-C(10)	1.432(2)	C(10)-H(10B)	0.9800
O(11)-C(11)	1.422(3)	C(10)-H(10C)	0.9800
O(12)-C(12)	1.411(3)	C(11)-H(11A)	0.9800
C(1)-H(1A)	0.9800	C(11)-H(11B)	0.9800
C(1)-H(1B)	0.9800	C(11)-H(11C)	0.9800
C(1)-H(1C)	0.9800	C(12)-H(12A)	0.9800
C(2)-H(2A)	0.9800	C(12)-H(12B)	0.9800
C(2)-H(2B)	0.9800	C(12)-H(12C)	0.9800
C(2)-H(2C)	0.9800	K(1)-O(15)	2.7716(15)

K(1)-O(16)	2.7935(14)	O(15)-C(21)	1.422(3)
K(1)-O(18)	2.8399(15)	C(21)-C(22)	1.495(3)
K(1)-O(14)	2.8407(14)	C(21)-H(21A)	0.9900
K(1)-O(13)	2.8411(14)	C(21)-H(21B)	0.9900
K(1)-O(17)	2.8500(15)	C(22)-O(16)	1.429(2)
K(1)-N(1)	2.9939(17)	C(22)-H(22A)	0.9900
K(1)-N(2)	2.9964(17)	C(22)-H(22B)	0.9900
N(1)-C(19)	1.463(3)	O(16)-C(23)	1.409(2)
N(1)-C(25)	1.466(3)	C(23)-C(24)	1.508(3)
N(1)-C(13)	1.473(3)	C(23)-H(23A)	0.9900
C(13)-C(14)	1.505(3)	C(23)-H(23B)	0.9900
C(13)-H(13A)	0.9900	C(24)-N(2)	1.475(3)
C(13)-H(13B)	0.9900	C(24)-H(24A)	0.9900
C(14)-O(13)	1.431(2)	C(24)-H(24B)	0.9900
C(14)-H(14A)	0.9900	C(25)-C(26)	1.510(3)
C(14)-H(14B)	0.9900	C(25)-H(25A)	0.9900
O(13)-C(15)	1.426(2)	C(25)-H(25B)	0.9900
C(15)-C(16)	1.494(3)	C(26)-O(17)	1.418(3)
C(15)-H(15A)	0.9900	C(26)-H(26A)	0.9900
C(15)-H(15B)	0.9900	C(26)-H(26B)	0.9900
C(16)-O(14)	1.430(2)	O(17)-C(27)	1.420(3)
C(16)-H(16A)	0.9900	C(27)-C(28)	1.490(3)
C(16)-H(16B)	0.9900	C(27)-H(27A)	0.9900
O(14)-C(17)	1.425(2)	C(27)-H(27B)	0.9900
C(17)-C(18)	1.504(3)	C(28)-O(18)	1.424(3)
C(17)-H(17A)	0.9900	C(28)-H(28A)	0.9900
C(17)-H(17B)	0.9900	C(28)-H(28B)	0.9900
C(18)-N(2)	1.472(3)	O(18)-C(29)	1.427(3)
C(18)-H(18A)	0.9900	C(29)-C(30)	1.509(3)
C(18)-H(18B)	0.9900	C(29)-H(29A)	0.9900
C(19)-C(20)	1.508(3)	C(29)-H(29B)	0.9900
C(19)-H(19A)	0.9900	C(30)-N(2)	1.473(3)
C(19)-H(19B)	0.9900	C(30)-H(30A)	0.9900
C(20)-O(15)	1.420(3)	C(30)-H(30B)	0.9900
C(20)-H(20A)	0.9900		
C(20)-H(20B)	0.9900	P(3)-Co(1)-P(1)	106.08(2)

P(3)-Co(1)-P(4)	106.67(2)	C(8)-O(8)-P(3)	117.96(12)
P(1)-Co(1)-P(4)	114.36(2)	C(9)-O(9)-P(3)	121.80(12)
P(3)-Co(1)-P(2)	105.93(2)	C(10)-O(10)-P(4)	121.84(14)
P(1)-Co(1)-P(2)	110.90(2)	C(11)-O(11)-P(4)	119.47(14)
P(4)-Co(1)-P(2)	112.25(2)	C(12)-O(12)-P(4)	119.93(14)
O(3)-P(1)-O(1)	93.79(7)	O(1)-C(1)-H(1A)	109.5
O(3)-P(1)-O(2)	99.45(7)	O(1)-C(1)-H(1B)	109.5
O(1)-P(1)-O(2)	92.85(7)	H(1A)-C(1)-H(1B)	109.5
O(3)-P(1)-Co(1)	116.91(5)	O(1)-C(1)-H(1C)	109.5
O(1)-P(1)-Co(1)	123.51(6)	H(1A)-C(1)-H(1C)	109.5
O(2)-P(1)-Co(1)	123.68(6)	H(1B)-C(1)-H(1C)	109.5
O(6)-P(2)-O(5)	95.00(9)	O(2)-C(2)-H(2A)	109.5
O(6)-P(2)-O(4)	99.05(8)	O(2)-C(2)-H(2B)	109.5
O(5)-P(2)-O(4)	92.34(8)	H(2A)-C(2)-H(2B)	109.5
O(6)-P(2)-Co(1)	116.85(6)	O(2)-C(2)-H(2C)	109.5
O(5)-P(2)-Co(1)	124.91(6)	H(2A)-C(2)-H(2C)	109.5
O(4)-P(2)-Co(1)	122.24(6)	H(2B)-C(2)-H(2C)	109.5
O(9)-P(3)-O(7)	95.45(7)	O(2)-C(2)-H(2D)	109.5
O(9)-P(3)-O(8)	99.40(7)	H(2A)-C(2)-H(2D)	141.1
O(7)-P(3)-O(8)	92.74(7)	H(2B)-C(2)-H(2D)	56.3
O(9)-P(3)-Co(1)	117.08(5)	H(2C)-C(2)-H(2D)	56.3
O(7)-P(3)-Co(1)	122.74(5)	O(2)-C(2)-H(2E)	109.5
O(8)-P(3)-Co(1)	123.21(5)	H(2A)-C(2)-H(2E)	56.3
O(10)-P(4)-O(11)	94.78(8)	H(2B)-C(2)-H(2E)	141.1
O(10)-P(4)-O(12)	99.18(8)	H(2C)-C(2)-H(2E)	56.3
O(11)-P(4)-O(12)	92.21(8)	H(2D)-C(2)-H(2E)	109.5
O(10)-P(4)-Co(1)	116.48(6)	O(2)-C(2)-H(2F)	109.5
O(11)-P(4)-Co(1)	123.08(6)	H(2A)-C(2)-H(2F)	56.3
O(12)-P(4)-Co(1)	124.48(6)	H(2B)-C(2)-H(2F)	56.3
C(1)-O(1)-P(1)	119.31(13)	H(2C)-C(2)-H(2F)	141.1
C(2)-O(2)-P(1)	118.97(12)	H(2D)-C(2)-H(2F)	109.5
C(3)-O(3)-P(1)	122.42(13)	H(2E)-C(2)-H(2F)	109.5
C(4)-O(4)-P(2)	117.22(12)	O(3)-C(3)-H(3A)	109.5
C(5)-O(5)-P(2)	117.25(15)	O(3)-C(3)-H(3B)	109.5
C(6)-O(6)-P(2)	122.17(14)	H(3A)-C(3)-H(3B)	109.5
C(7)-O(7)-P(3)	117.89(12)	O(3)-C(3)-H(3C)	109.5

H(3A)-C(3)-H(3C)	109.5	H(9A)-C(9)-H(9C)	109.5
H(3B)-C(3)-H(3C)	109.5	H(9B)-C(9)-H(9C)	109.5
O(4)-C(4)-H(4A)	109.5	O(10)-C(10)-H(10A)	109.5
O(4)-C(4)-H(4B)	109.5	O(10)-C(10)-H(10B)	109.5
H(4A)-C(4)-H(4B)	109.5	H(10A)-C(10)-H(10B)	109.5
O(4)-C(4)-H(4C)	109.5	O(10)-C(10)-H(10C)	109.5
H(4A)-C(4)-H(4C)	109.5	H(10A)-C(10)-H(10C)	109.5
H(4B)-C(4)-H(4C)	109.5	H(10B)-C(10)-H(10C)	109.5
O(5)-C(5)-H(5A)	109.5	O(11)-C(11)-H(11A)	109.5
O(5)-C(5)-H(5B)	109.5	O(11)-C(11)-H(11B)	109.5
H(5A)-C(5)-H(5B)	109.5	H(11A)-C(11)-H(11B)	109.5
O(5)-C(5)-H(5C)	109.5	O(11)-C(11)-H(11C)	109.5
H(5A)-C(5)-H(5C)	109.5	H(11A)-C(11)-H(11C)	109.5
H(5B)-C(5)-H(5C)	109.5	H(11B)-C(11)-H(11C)	109.5
O(6)-C(6)-H(6A)	109.5	O(12)-C(12)-H(12A)	109.5
O(6)-C(6)-H(6B)	109.5	O(12)-C(12)-H(12B)	109.5
H(6A)-C(6)-H(6B)	109.5	H(12A)-C(12)-H(12B)	109.5
O(6)-C(6)-H(6C)	109.5	O(12)-C(12)-H(12C)	109.5
H(6A)-C(6)-H(6C)	109.5	H(12A)-C(12)-H(12C)	109.5
H(6B)-C(6)-H(6C)	109.5	H(12B)-C(12)-H(12C)	109.5
O(7)-C(7)-H(7A)	109.5	O(15)-K(1)-O(16)	60.18(4)
O(7)-C(7)-H(7B)	109.5	O(15)-K(1)-O(18)	121.28(5)
H(7A)-C(7)-H(7B)	109.5	O(16)-K(1)-O(18)	96.49(4)
O(7)-C(7)-H(7C)	109.5	O(15)-K(1)-O(14)	129.90(5)
H(7A)-C(7)-H(7C)	109.5	O(16)-K(1)-O(14)	94.22(4)
H(7B)-C(7)-H(7C)	109.5	O(18)-K(1)-O(14)	102.55(5)
O(8)-C(8)-H(8A)	109.5	O(15)-K(1)-O(13)	91.18(4)
O(8)-C(8)-H(8B)	109.5	O(16)-K(1)-O(13)	114.88(4)
H(8A)-C(8)-H(8B)	109.5	O(18)-K(1)-O(13)	143.77(4)
O(8)-C(8)-H(8C)	109.5	O(14)-K(1)-O(13)	59.51(4)
H(8A)-C(8)-H(8C)	109.5	O(15)-K(1)-O(17)	99.19(5)
H(8B)-C(8)-H(8C)	109.5	O(16)-K(1)-O(17)	135.86(4)
O(9)-C(9)-H(9A)	109.5	O(18)-K(1)-O(17)	59.23(4)
O(9)-C(9)-H(9B)	109.5	O(14)-K(1)-O(17)	125.10(4)
H(9A)-C(9)-H(9B)	109.5	O(13)-K(1)-O(17)	103.20(4)
O(9)-C(9)-H(9C)	109.5	O(15)-K(1)-N(1)	60.42(5)

O(16)-K(1)-N(1)	120.22(5)	O(13)-C(15)-H(15B)	109.9
O(18)-K(1)-N(1)	119.40(5)	C(16)-C(15)-H(15B)	109.9
O(14)-K(1)-N(1)	118.95(4)	H(15A)-C(15)-H(15B)	108.3
O(13)-K(1)-N(1)	60.46(4)	O(14)-C(16)-C(15)	109.10(16)
O(17)-K(1)-N(1)	60.98(5)	O(14)-C(16)-H(16A)	109.9
O(15)-K(1)-N(2)	119.33(5)	C(15)-C(16)-H(16A)	109.9
O(16)-K(1)-N(2)	59.57(4)	O(14)-C(16)-H(16B)	109.9
O(18)-K(1)-N(2)	60.49(5)	C(15)-C(16)-H(16B)	109.9
O(14)-K(1)-N(2)	61.37(4)	H(16A)-C(16)-H(16B)	108.3
O(13)-K(1)-N(2)	119.83(4)	C(17)-O(14)-C(16)	111.26(15)
O(17)-K(1)-N(2)	118.96(5)	C(17)-O(14)-K(1)	116.93(11)
N(1)-K(1)-N(2)	179.67(5)	C(16)-O(14)-K(1)	113.57(11)
C(19)-N(1)-C(25)	110.35(18)	O(14)-C(17)-C(18)	109.75(17)
C(19)-N(1)-C(13)	110.20(18)	O(14)-C(17)-H(17A)	109.7
C(25)-N(1)-C(13)	109.78(18)	C(18)-C(17)-H(17A)	109.7
C(19)-N(1)-K(1)	107.73(12)	O(14)-C(17)-H(17B)	109.7
C(25)-N(1)-K(1)	108.07(13)	C(18)-C(17)-H(17B)	109.7
C(13)-N(1)-K(1)	110.67(12)	H(17A)-C(17)-H(17B)	108.2
N(1)-C(13)-C(14)	114.15(18)	N(2)-C(18)-C(17)	114.40(18)
N(1)-C(13)-H(13A)	108.7	N(2)-C(18)-H(18A)	108.7
C(14)-C(13)-H(13A)	108.7	C(17)-C(18)-H(18A)	108.7
N(1)-C(13)-H(13B)	108.7	N(2)-C(18)-H(18B)	108.7
C(14)-C(13)-H(13B)	108.7	C(17)-C(18)-H(18B)	108.7
H(13A)-C(13)-H(13B)	107.6	H(18A)-C(18)-H(18B)	107.6
O(13)-C(14)-C(13)	109.34(17)	N(1)-C(19)-C(20)	113.91(18)
O(13)-C(14)-H(14A)	109.8	N(1)-C(19)-H(19A)	108.8
C(13)-C(14)-H(14A)	109.8	C(20)-C(19)-H(19A)	108.8
O(13)-C(14)-H(14B)	109.8	N(1)-C(19)-H(19B)	108.8
C(13)-C(14)-H(14B)	109.8	C(20)-C(19)-H(19B)	108.8
H(14A)-C(14)-H(14B)	108.3	H(19A)-C(19)-H(19B)	107.7
C(15)-O(13)-C(14)	110.75(15)	O(15)-C(20)-C(19)	108.92(19)
C(15)-O(13)-K(1)	116.73(11)	O(15)-C(20)-H(20A)	109.9
C(14)-O(13)-K(1)	115.90(11)	C(19)-C(20)-H(20A)	109.9
O(13)-C(15)-C(16)	109.12(16)	O(15)-C(20)-H(20B)	109.9
O(13)-C(15)-H(15A)	109.9	C(19)-C(20)-H(20B)	109.9
C(16)-C(15)-H(15A)	109.9	H(20A)-C(20)-H(20B)	108.3

C(20)-O(15)-C(21)	111.19(18)	O(17)-C(26)-C(25)	110.01(19)
C(20)-O(15)-K(1)	121.28(12)	O(17)-C(26)-H(26A)	109.7
C(21)-O(15)-K(1)	113.99(12)	C(25)-C(26)-H(26A)	109.7
O(15)-C(21)-C(22)	109.1(2)	O(17)-C(26)-H(26B)	109.7
O(15)-C(21)-H(21A)	109.9	C(25)-C(26)-H(26B)	109.7
C(22)-C(21)-H(21A)	109.9	H(26A)-C(26)-H(26B)	108.2
O(15)-C(21)-H(21B)	109.9	C(26)-O(17)-C(27)	111.28(17)
C(22)-C(21)-H(21B)	109.9	C(26)-O(17)-K(1)	117.26(13)
H(21A)-C(21)-H(21B)	108.3	C(27)-O(17)-K(1)	112.96(12)
O(16)-C(22)-C(21)	108.37(18)	O(17)-C(27)-C(28)	109.39(18)
O(16)-C(22)-H(22A)	110.0	O(17)-C(27)-H(27A)	109.8
C(21)-C(22)-H(22A)	110.0	C(28)-C(27)-H(27A)	109.8
O(16)-C(22)-H(22B)	110.0	O(17)-C(27)-H(27B)	109.8
C(21)-C(22)-H(22B)	110.0	C(28)-C(27)-H(27B)	109.8
H(22A)-C(22)-H(22B)	108.4	H(27A)-C(27)-H(27B)	108.2
C(23)-O(16)-C(22)	112.10(16)	O(18)-C(28)-C(27)	108.5(2)
C(23)-O(16)-K(1)	119.75(12)	O(18)-C(28)-H(28A)	110.0
C(22)-O(16)-K(1)	117.02(12)	C(27)-C(28)-H(28A)	110.0
O(16)-C(23)-C(24)	108.90(17)	O(18)-C(28)-H(28B)	110.0
O(16)-C(23)-H(23A)	109.9	C(27)-C(28)-H(28B)	110.0
C(24)-C(23)-H(23A)	109.9	H(28A)-C(28)-H(28B)	108.4
O(16)-C(23)-H(23B)	109.9	C(28)-O(18)-C(29)	111.76(17)
C(24)-C(23)-H(23B)	109.9	C(28)-O(18)-K(1)	117.12(13)
H(23A)-C(23)-H(23B)	108.3	C(29)-O(18)-K(1)	117.00(12)
N(2)-C(24)-C(23)	112.73(17)	O(18)-C(29)-C(30)	108.25(18)
N(2)-C(24)-H(24A)	109.0	O(18)-C(29)-H(29A)	110.0
C(23)-C(24)-H(24A)	109.0	C(30)-C(29)-H(29A)	110.0
N(2)-C(24)-H(24B)	109.0	O(18)-C(29)-H(29B)	110.0
C(23)-C(24)-H(24B)	109.0	C(30)-C(29)-H(29B)	110.0
H(24A)-C(24)-H(24B)	107.8	H(29A)-C(29)-H(29B)	108.4
N(1)-C(25)-C(26)	114.53(19)	N(2)-C(30)-C(29)	114.82(18)
N(1)-C(25)-H(25A)	108.6	N(2)-C(30)-H(30A)	108.6
C(26)-C(25)-H(25A)	108.6	C(29)-C(30)-H(30A)	108.6
N(1)-C(25)-H(25B)	108.6	N(2)-C(30)-H(30B)	108.6
C(26)-C(25)-H(25B)	108.6	C(29)-C(30)-H(30B)	108.6
H(25A)-C(25)-H(25B)	107.6	H(30A)-C(30)-H(30B)	107.5

C(18)-N(2)-C(30)	110.32(17)	C(18)-N(2)-K(1)	106.74(11)
C(18)-N(2)-C(24)	110.76(17)	C(30)-N(2)-K(1)	109.53(12)
C(30)-N(2)-C(24)	108.59(17)	C(24)-N(2)-K(1)	110.89(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 01152. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	18(1)	21(1)	25(1)	0(1)	5(1)	0(1)
P1	19(1)	24(1)	28(1)	0(1)	5(1)	1(1)
P2	23(1)	22(1)	36(1)	1(1)	5(1)	1(1)
P3	19(1)	24(1)	22(1)	-1(1)	4(1)	0(1)
P4	24(1)	28(1)	24(1)	2(1)	4(1)	3(1)
O1	29(1)	25(1)	35(1)	-1(1)	3(1)	5(1)
O2	21(1)	33(1)	41(1)	5(1)	10(1)	2(1)
O3	21(1)	33(1)	31(1)	-1(1)	0(1)	3(1)
O4	28(1)	28(1)	41(1)	7(1)	7(1)	5(1)
O5	38(1)	28(1)	65(1)	6(1)	17(1)	-6(1)
O6	46(1)	25(1)	45(1)	-6(1)	-7(1)	2(1)
O7	23(1)	36(1)	27(1)	-7(1)	5(1)	1(1)
O8	30(1)	27(1)	26(1)	2(1)	7(1)	2(1)
O9	19(1)	33(1)	26(1)	1(1)	5(1)	-1(1)
O10	42(1)	29(1)	30(1)	-5(1)	-4(1)	2(1)
O11	29(1)	38(1)	34(1)	4(1)	0(1)	5(1)
O12	34(1)	54(1)	30(1)	5(1)	10(1)	5(1)
C1	43(1)	28(1)	42(1)	-5(1)	9(1)	7(1)
C2	31(1)	35(1)	44(1)	-1(1)	14(1)	-3(1)
C3	24(1)	42(1)	34(1)	4(1)	-3(1)	1(1)
C4	28(1)	44(1)	51(1)	13(1)	13(1)	13(1)
C5	57(2)	47(2)	70(2)	20(1)	32(2)	-4(1)
C6	58(2)	29(1)	60(2)	-13(1)	-3(1)	0(1)
C7	33(1)	41(1)	27(1)	-5(1)	0(1)	2(1)
C8	36(1)	25(1)	34(1)	1(1)	4(1)	0(1)
C9	21(1)	37(1)	34(1)	-5(1)	9(1)	-5(1)
C10	45(1)	45(1)	38(1)	-15(1)	-3(1)	3(1)
C11	46(2)	41(1)	55(2)	6(1)	-12(1)	8(1)
C12	37(1)	70(2)	39(1)	1(1)	17(1)	6(1)
K1	26(1)	27(1)	26(1)	1(1)	4(1)	-1(1)
N1	34(1)	28(1)	36(1)	-5(1)	12(1)	-5(1)

C13	42(1)	34(1)	39(1)	-9(1)	13(1)	-12(1)
C14	42(1)	29(1)	38(1)	-5(1)	10(1)	-10(1)
O13	34(1)	30(1)	27(1)	1(1)	10(1)	-6(1)
C15	32(1)	37(1)	30(1)	5(1)	8(1)	-9(1)
C16	26(1)	40(1)	31(1)	6(1)	8(1)	1(1)
O14	29(1)	30(1)	35(1)	-2(1)	10(1)	0(1)
C17	47(1)	35(1)	37(1)	-1(1)	20(1)	3(1)
C18	56(2)	34(1)	26(1)	-4(1)	10(1)	0(1)
C19	56(2)	36(1)	41(1)	-9(1)	25(1)	-11(1)
C20	67(2)	46(1)	23(1)	-2(1)	8(1)	-8(1)
O15	45(1)	35(1)	25(1)	1(1)	2(1)	2(1)
C21	58(2)	52(2)	27(1)	8(1)	-3(1)	12(1)
C22	59(2)	38(1)	31(1)	15(1)	9(1)	11(1)
O16	39(1)	31(1)	28(1)	7(1)	5(1)	2(1)
C23	38(1)	29(1)	39(1)	5(1)	6(1)	1(1)
C24	42(1)	29(1)	40(1)	-1(1)	8(1)	6(1)
C25	46(2)	30(1)	62(2)	-9(1)	15(1)	3(1)
C26	33(1)	50(2)	68(2)	-13(1)	15(1)	8(1)
O17	25(1)	40(1)	48(1)	-3(1)	9(1)	0(1)
C27	23(1)	47(1)	64(2)	3(1)	7(1)	-1(1)
C28	26(1)	47(1)	58(2)	5(1)	-7(1)	-2(1)
O18	31(1)	38(1)	39(1)	0(1)	-6(1)	2(1)
C29	39(1)	40(1)	39(1)	-3(1)	-11(1)	-8(1)
C30	45(1)	30(1)	40(1)	-7(1)	-4(1)	-5(1)
N2	35(1)	27(1)	27(1)	0(1)	3(1)	-1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 01152.

	x	y	z	U(eq)
H1A	7273	2400	-2652	57
H1B	8101	2907	-2992	57
H1C	6595	2995	-3052	57
H2A	9738	4854	-2836	54
H2B	8527	5133	-2557	54
H2C	8370	4837	-3261	54
H2D	8018	5029	-2933	54
H2E	9230	4750	-3212	54
H2F	9387	5046	-2508	54
H3A	9134	4099	-783	51
H3B	9595	3937	-1451	51
H3C	8743	3424	-1133	51
H4A	2544	6066	-2675	60
H4B	3317	5619	-2136	60
H4C	2839	5323	-2826	60
H5A	7166	6023	-3762	84
H5B	5690	6191	-3794	84
H5C	6152	5449	-3756	84
H6A	6401	6549	-1328	75
H6B	4997	6537	-1716	75
H6C	6183	6701	-2075	75
H7A	4976	4919	-601	51
H7B	5833	4859	-1159	51
H7C	5535	4226	-766	51
H8A	5128	2580	-1900	47
H8B	4626	2998	-2521	47
H8C	3640	2614	-2154	47
H9A	954	4028	-2235	46
H9B	1800	4359	-1636	46
H9C	1931	3596	-1767	46

H10A	4059	2605	-4209	65
H10B	4479	3244	-4556	65
H10C	3091	3200	-4353	65
H11A	2543	5122	-4408	74
H11B	3980	5055	-4541	74
H11C	3685	5350	-3880	74
H12A	7308	4319	-4396	71
H12B	6885	3578	-4326	71
H12C	7260	4017	-3705	71
H13A	11472	4092	1542	45
H13B	10600	4726	1422	45
H14A	10602	4610	309	43
H14B	12009	4712	682	43
H15A	13078	4161	-33	39
H15B	11746	4141	-495	39
H16A	13154	3317	-760	38
H16B	13157	3003	-67	38
H17A	12372	2050	-675	46
H17B	12183	2437	-1338	46
H18A	9958	2249	-1425	46
H18B	10751	1590	-1443	46
H19A	8662	3418	1795	51
H19B	9618	3951	2137	51
H20A	11354	3252	2040	54
H20B	10371	2914	2447	54
H21A	11272	1962	2204	56
H21B	12040	2179	1641	56
H22A	11341	1082	1509	51
H22B	9898	1325	1466	51
H23A	9504	916	325	42
H23B	10917	643	525	42
H24A	11620	1247	-305	44
H24B	10523	751	-586	44
H25A	8702	4537	590	54
H25B	8366	4586	1298	54
H26A	7157	3609	1125	59

H26B	6601	4183	653	59
H27A	5616	3357	18	53
H27B	6340	2757	393	53
H28A	5709	2514	-703	54
H28B	6611	3090	-885	54
H29A	7975	2291	-1354	49
H29B	6874	1795	-1225	49
H30A	8388	1174	-549	47
H30B	8710	1192	-1260	47

Table 6. Torsion angles [°] for 01152.

P3-Co1-P1-O3	-54.00(6)	P1-Co1-P4-O12	-58.80(8)
P4-Co1-P1-O3	-171.27(6)	P2-Co1-P4-O12	68.67(8)
P2-Co1-P1-O3	60.57(6)	O3-P1-O1-C1	-172.86(15)
P3-Co1-P1-O1	61.14(7)	O2-P1-O1-C1	-73.19(15)
P4-Co1-P1-O1	-56.13(7)	Co1-P1-O1-C1	61.14(16)
P2-Co1-P1-O1	175.71(6)	O3-P1-O2-C2	-94.58(15)
P3-Co1-P1-O2	-178.00(7)	O1-P1-O2-C2	171.11(15)
P4-Co1-P1-O2	64.73(7)	Co1-P1-O2-C2	36.89(17)
P2-Co1-P1-O2	-63.44(7)	O1-P1-O3-C3	43.52(15)
P3-Co1-P2-O6	59.53(7)	O2-P1-O3-C3	-50.01(15)
P1-Co1-P2-O6	-55.14(7)	Co1-P1-O3-C3	174.37(13)
P4-Co1-P2-O6	175.57(7)	O6-P2-O4-C4	-83.48(16)
P3-Co1-P2-O5	177.72(8)	O5-P2-O4-C4	-178.92(16)
P1-Co1-P2-O5	63.05(9)	Co1-P2-O4-C4	46.41(17)
P4-Co1-P2-O5	-66.24(9)	O6-P2-O5-C5	-172.84(17)
P3-Co1-P2-O4	-62.34(7)	O4-P2-O5-C5	-73.54(17)
P1-Co1-P2-O4	-177.00(6)	Co1-P2-O5-C5	59.28(18)
P4-Co1-P2-O4	53.71(7)	O5-P2-O6-C6	58.15(19)
P1-Co1-P3-O9	-158.78(6)	O4-P2-O6-C6	-35.03(19)
P4-Co1-P3-O9	-36.48(6)	Co1-P2-O6-C6	-168.37(16)
P2-Co1-P3-O9	83.29(6)	O9-P3-O7-C7	-179.32(14)
P1-Co1-P3-O7	84.11(7)	O8-P3-O7-C7	80.96(15)
P4-Co1-P3-O7	-153.58(6)	Co1-P3-O7-C7	-52.09(16)
P2-Co1-P3-O7	-33.81(7)	O9-P3-O8-C8	81.80(14)
P1-Co1-P3-O8	-35.15(7)	O7-P3-O8-C8	177.79(14)
P4-Co1-P3-O8	87.15(7)	Co1-P3-O8-C8	-49.49(15)
P2-Co1-P3-O8	-153.08(6)	O7-P3-O9-C9	-42.06(15)
P3-Co1-P4-O10	-51.78(7)	O8-P3-O9-C9	51.64(15)
P1-Co1-P4-O10	65.15(7)	Co1-P3-O9-C9	-173.28(12)
P2-Co1-P4-O10	-167.38(6)	O11-P4-O10-C10	50.46(17)
P3-Co1-P4-O11	64.05(7)	O12-P4-O10-C10	-42.56(17)
P1-Co1-P4-O11	-179.02(7)	Co1-P4-O10-C10	-178.73(14)
P2-Co1-P4-O11	-51.55(7)	O10-P4-O11-C11	-159.12(17)
P3-Co1-P4-O12	-175.73(7)	O12-P4-O11-C11	-59.71(17)

Co1-P4-O11-C11	74.82(17)	N1-K1-O13-C15	-156.61(14)
O10-P4-O12-C12	-80.74(18)	N2-K1-O13-C15	23.56(14)
O11-P4-O12-C12	-175.95(18)	O15-K1-O13-C14	-77.97(13)
Co1-P4-O12-C12	50.5(2)	O16-K1-O13-C14	-135.37(13)
O15-K1-N1-C19	-18.76(13)	O18-K1-O13-C14	77.09(15)
O16-K1-N1-C19	-25.90(15)	O14-K1-O13-C14	144.94(14)
O18-K1-N1-C19	92.68(14)	O17-K1-O13-C14	21.76(14)
O14-K1-N1-C19	-140.70(13)	N1-K1-O13-C14	-23.35(13)
O13-K1-N1-C19	-129.17(15)	N2-K1-O13-C14	156.82(13)
O17-K1-N1-C19	102.91(14)	C14-O13-C15-C16	-178.27(17)
N2-K1-N1-C19	23(10)	K1-O13-C15-C16	-42.7(2)
O15-K1-N1-C25	-137.99(15)	O13-C15-C16-O14	64.2(2)
O16-K1-N1-C25	-145.13(13)	C15-C16-O14-C17	171.91(16)
O18-K1-N1-C25	-26.55(15)	C15-C16-O14-K1	-53.66(18)
O14-K1-N1-C25	100.07(14)	O15-K1-O14-C17	91.48(15)
O13-K1-N1-C25	111.60(14)	O16-K1-O14-C17	37.51(14)
O17-K1-N1-C25	-16.32(13)	O18-K1-O14-C17	-60.11(15)
N2-K1-N1-C25	-96(10)	O13-K1-O14-C17	154.01(15)
O15-K1-N1-C13	101.77(15)	O17-K1-O14-C17	-121.15(14)
O16-K1-N1-C13	94.63(14)	N1-K1-O14-C17	165.64(14)
O18-K1-N1-C13	-146.79(13)	N2-K1-O14-C17	-14.25(14)
O14-K1-N1-C13	-20.17(16)	O15-K1-O14-C16	-40.24(14)
O13-K1-N1-C13	-8.64(13)	O16-K1-O14-C16	-94.20(12)
O17-K1-N1-C13	-136.56(15)	O18-K1-O14-C16	168.18(12)
N2-K1-N1-C13	144(10)	O13-K1-O14-C16	22.30(12)
C19-N1-C13-C14	158.38(19)	O17-K1-O14-C16	107.14(12)
C25-N1-C13-C14	-79.9(2)	N1-K1-O14-C16	33.93(14)
K1-N1-C13-C14	39.3(2)	N2-K1-O14-C16	-145.96(13)
N1-C13-C14-O13	-63.1(3)	C16-O14-C17-C18	177.35(17)
C13-C14-O13-C15	-170.95(18)	K1-O14-C17-C18	44.6(2)
C13-C14-O13-K1	53.1(2)	O14-C17-C18-N2	-66.5(2)
O15-K1-O13-C15	148.77(13)	C25-N1-C19-C20	166.72(19)
O16-K1-O13-C15	91.37(13)	C13-N1-C19-C20	-71.9(2)
O18-K1-O13-C15	-56.17(16)	K1-N1-C19-C20	48.9(2)
O14-K1-O13-C15	11.68(12)	N1-C19-C20-O15	-61.7(3)
O17-K1-O13-C15	-111.50(13)	C19-C20-O15-C21	179.43(19)

C19-C20-O15-K1	41.2(2)	O16-C23-C24-N2	-61.1(2)
O16-K1-O15-C20	160.50(17)	C19-N1-C25-C26	-70.0(3)
O18-K1-O15-C20	-120.79(16)	C13-N1-C25-C26	168.3(2)
O14-K1-O15-C20	92.14(16)	K1-N1-C25-C26	47.5(2)
O13-K1-O15-C20	42.25(16)	N1-C25-C26-O17	-64.6(3)
O17-K1-O15-C20	-61.32(16)	C25-C26-O17-C27	177.1(2)
N1-K1-O15-C20	-12.39(15)	C25-C26-O17-K1	44.9(2)
N2-K1-O15-C20	167.86(15)	O15-K1-O17-C26	33.32(16)
O16-K1-O15-C21	23.34(15)	O16-K1-O17-C26	89.50(16)
O18-K1-O15-C21	102.05(15)	O18-K1-O17-C26	154.37(16)
O14-K1-O15-C21	-45.03(17)	O14-K1-O17-C26	-121.91(15)
O13-K1-O15-C21	-94.91(15)	O13-K1-O17-C26	-60.09(15)
O17-K1-O15-C21	161.51(15)	N1-K1-O17-C26	-15.26(15)
N1-K1-O15-C21	-149.55(17)	N2-K1-O17-C26	164.37(15)
N2-K1-O15-C21	30.70(17)	O15-K1-O17-C27	-98.11(14)
C20-O15-C21-C22	164.08(18)	O16-K1-O17-C27	-41.93(16)
K1-O15-C21-C22	-54.5(2)	O18-K1-O17-C27	22.94(14)
O15-C21-C22-O16	62.8(2)	O14-K1-O17-C27	106.66(14)
C21-C22-O16-C23	175.25(19)	O13-K1-O17-C27	168.49(14)
C21-C22-O16-K1	-40.8(2)	N1-K1-O17-C27	-146.69(15)
O15-K1-O16-C23	151.56(14)	N2-K1-O17-C27	32.95(15)
O18-K1-O16-C23	29.07(14)	C26-O17-C27-C28	170.8(2)
O14-K1-O16-C23	-74.08(13)	K1-O17-C27-C28	-54.9(2)
O13-K1-O16-C23	-132.31(13)	O17-C27-C28-O18	64.9(2)
O17-K1-O16-C23	80.60(14)	C27-C28-O18-C29	178.71(18)
N1-K1-O16-C23	158.72(13)	C27-C28-O18-K1	-42.4(2)
N2-K1-O16-C23	-20.99(13)	O15-K1-O18-C28	93.01(15)
O15-K1-O16-C22	10.49(14)	O16-K1-O18-C28	151.91(15)
O18-K1-O16-C22	-112.00(15)	O14-K1-O18-C28	-112.28(15)
O14-K1-O16-C22	144.85(15)	O13-K1-O18-C28	-57.43(17)
O13-K1-O16-C22	86.62(15)	O17-K1-O18-C28	11.29(14)
O17-K1-O16-C22	-60.47(17)	N1-K1-O18-C28	21.71(16)
N1-K1-O16-C22	17.65(16)	N2-K1-O18-C28	-158.65(16)
N2-K1-O16-C22	-162.06(16)	O15-K1-O18-C29	-130.24(13)
C22-O16-C23-C24	-166.61(18)	O16-K1-O18-C29	-71.33(14)
K1-O16-C23-C24	50.6(2)	O14-K1-O18-C29	24.47(14)

O13-K1-O18-C29	79.33(15)	O14-K1-N2-C18	-17.62(12)
O17-K1-O18-C29	148.05(15)	O13-K1-N2-C18	-29.28(14)
N1-K1-O18-C29	158.46(13)	O17-K1-N2-C18	98.90(13)
N2-K1-O18-C29	-21.89(13)	N1-K1-N2-C18	178(100)
C28-O18-C29-C30	-169.64(18)	O15-K1-N2-C30	100.83(13)
K1-O18-C29-C30	51.4(2)	O16-K1-N2-C30	108.23(14)
O18-C29-C30-N2	-64.0(2)	O18-K1-N2-C30	-10.66(12)
C17-C18-N2-C30	168.69(18)	O14-K1-N2-C30	-137.06(14)
C17-C18-N2-C24	-71.0(2)	O13-K1-N2-C30	-148.72(12)
C17-C18-N2-K1	49.8(2)	O17-K1-N2-C30	-20.54(14)
C29-C30-N2-C18	-75.0(2)	N1-K1-N2-C30	59(10)
C29-C30-N2-C24	163.43(19)	O15-K1-N2-C24	-19.00(15)
C29-C30-N2-K1	42.2(2)	O16-K1-N2-C24	-11.60(12)
C23-C24-N2-C18	159.64(18)	O18-K1-N2-C24	-130.49(14)
C23-C24-N2-C30	-79.1(2)	O14-K1-N2-C24	103.11(14)
C23-C24-N2-K1	41.3(2)	O13-K1-N2-C24	91.45(13)
O15-K1-N2-C18	-139.73(13)	O17-K1-N2-C24	-140.37(12)
O16-K1-N2-C18	-132.33(14)	N1-K1-N2-C24	-61(10)
O18-K1-N2-C18	108.78(14)		

Symmetry transformations used to generate equivalent atoms:

REFERENCE NUMBER: 04253 [5]

[Revised September 19, 2011]

CRYSTAL STRUCTURE REPORT

$C_{56} H_{124} Co K O_{20} P_4$

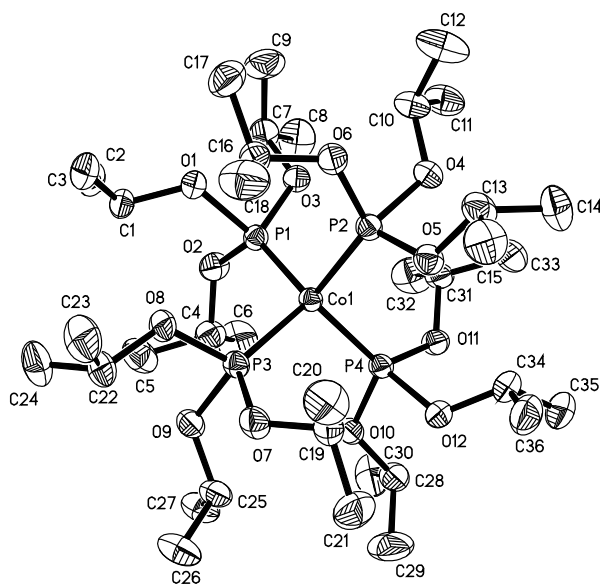
or

$[K(18\text{-crown-6})(THF)_2][Co(P(O^iPr)_3)_4]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

September 27, 2004



William W. Brennessel

X-Ray Crystallographic Laboratory

Department of Chemistry

University of Minnesota

207 Pleasant St. S.E.

Minneapolis, MN 55455

Data collection

A crystal (0.32 x 0.24 x 0.20 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART CCD Platform diffractometer for a data collection at 173(2) 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 MoK α radiation (graphite monochromator) with a frame time of 45 seconds and a detector distance of 4.84 cm. A randomly oriented region of reciprocal space was surveyed: three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption.² Final cell constants were calculated from the xyz centroids of 3895 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 SIR97⁴ and refined using SHELXL-97.⁵ The space group $P2_1/c$ was determined based on systematic absences. 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 $R1 = 0.0493$ (F^2 , $I > 2\sigma(I)$) and $wR2 = 0.1375$ (F^2 , all data).

Structure description

The structure is the one suggested. The atoms of the anion lie on general positions and are well separated from those of the cation. The cation is located on two different crystallographic inversion centers; thus, one half of each is unique. THF solvent molecules occupy the axial positions of the potassium cations. One is modeled as disordered over two positions (77:23) and the other is modeled as disordered over three positions (44:35:21). The geometry about the cobalt center is nearly tetrahedral (twist angle of 82.42(3)°).

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

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

-
- ¹ SMART V5.629, Bruker Analytical X-ray Systems, Madison, WI (2003).
- ² SADABS V2.10, An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
- ³ SAINT V7.06A, Bruker Analytical X-ray Systems, Madison, WI (2003).
- 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:

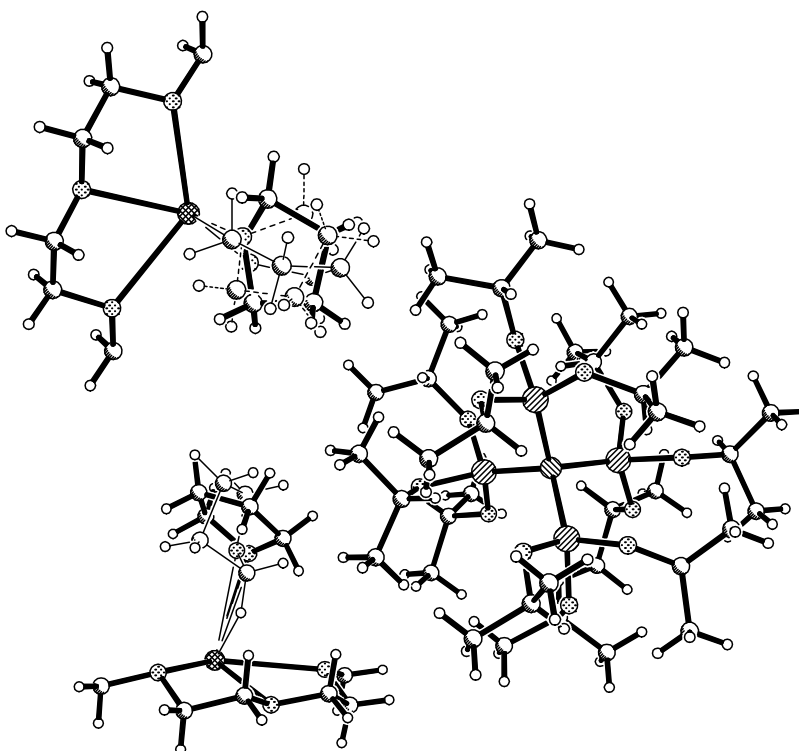
$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = 1 / [\sigma^2(F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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



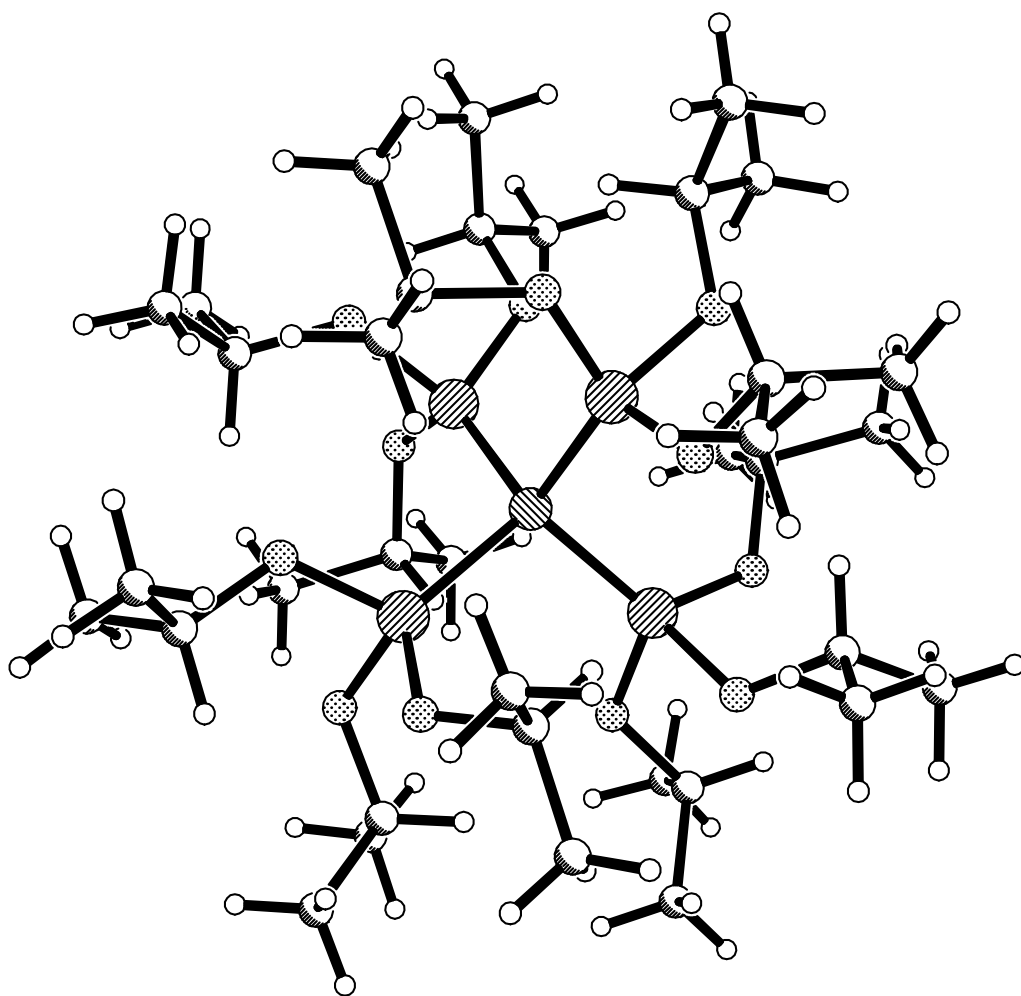
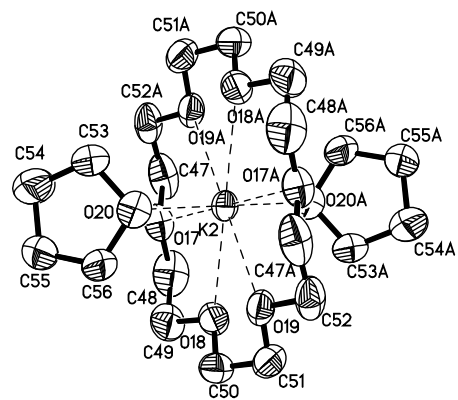


Table 1. Crystal data and structure refinement for 253.

Identification code	04253	
Empirical formula	C ₅₆ H ₁₂₄ Co K O ₂₀ P ₄	
Formula weight	1339.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 24.2720(17) Å	$\alpha = 90^\circ$
	<i>b</i> = 17.8466(12) Å	$\beta = 90.545(1)^\circ$
	<i>c</i> = 17.2666(12) Å	$\gamma = 90^\circ$
Volume	7479.1(9) Å ³	
<i>Z</i>	4	
Density (calculated)	1.190 Mg/m ³	
Absorption coefficient	0.432 mm ⁻¹	
<i>F</i> (000)	2904	
Crystal color, morphology	colorless, block	
Crystal size	0.32 x 0.24 x 0.20 mm ³	
Theta range for data collection	1.42 to 27.53°	
Index ranges	-31 ≤ <i>h</i> ≤ 31, -23 ≤ <i>k</i> ≤ 23, -22 ≤ <i>l</i> ≤ 22	
Reflections collected	66211	
Independent reflections	17158 [<i>R</i> (int) = 0.0660]	
Observed reflections	11159	
Completeness to theta = 27.53°	99.5%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9186 and 0.8742	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	17158 / 76 / 815	
Goodness-of-fit on <i>F</i> ²	1.023	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0493, <i>wR</i> 2 = 0.1133	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0920, <i>wR</i> 2 = 0.1375	
Largest diff. peak and hole	0.933 and -0.487 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 253. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	2517(1)	10000(1)	127(1)	21(1)
P1	2818(1)	9461(1)	1104(1)	25(1)
P2	2681(1)	9259(1)	-769(1)	26(1)
P3	1693(1)	10232(1)	336(1)	25(1)
P4	2873(1)	11014(1)	-166(1)	25(1)
O1	2532(1)	8670(1)	1412(1)	31(1)
O2	2871(1)	9853(1)	1973(1)	35(1)
O3	3442(1)	9104(1)	1072(1)	30(1)
O4	3326(1)	9031(1)	-986(1)	33(1)
O5	2512(1)	9516(1)	-1655(1)	30(1)
O6	2458(1)	8387(1)	-800(1)	38(1)
O7	1259(1)	10559(1)	-329(1)	34(1)
O8	1306(1)	9553(1)	668(1)	31(1)
O9	1502(1)	10838(1)	1016(1)	32(1)
O10	2729(1)	11750(1)	363(1)	31(1)
O11	3546(1)	11162(1)	-222(1)	34(1)
O12	2722(1)	11444(1)	-996(1)	33(1)
C1	2104(1)	8645(2)	1981(2)	33(1)
C2	1692(1)	8048(2)	1745(2)	45(1)
C3	2356(1)	8471(2)	2767(2)	47(1)
C4	2705(1)	10608(2)	2122(2)	38(1)
C5	2240(2)	10599(2)	2697(2)	54(1)
C6	3196(2)	11028(2)	2436(3)	70(1)
C7	3679(1)	8669(2)	1700(2)	39(1)
C8	4223(1)	9013(2)	1923(2)	61(1)
C9	3727(2)	7862(2)	1451(2)	59(1)
C10	3607(1)	8386(2)	-684(2)	40(1)
C11	4193(1)	8615(2)	-483(2)	50(1)
C12	3607(2)	7768(2)	-1287(2)	66(1)
C13	2626(1)	9050(2)	-2324(2)	40(1)
C14	3145(2)	9327(2)	-2724(2)	55(1)

C15	2128(2)	9092(2)	-2854(2)	52(1)
C16	2009(1)	8124(2)	-339(2)	38(1)
C17	2178(2)	7359(2)	-36(2)	49(1)
C18	1494(1)	8089(2)	-830(2)	60(1)
C19	1414(1)	10677(2)	-1116(2)	37(1)
C20	1096(2)	10139(2)	-1623(2)	56(1)
C21	1290(2)	11486(2)	-1319(2)	59(1)
C22	731(1)	9666(2)	850(2)	36(1)
C23	394(1)	9097(2)	403(2)	53(1)
C24	661(1)	9602(2)	1719(2)	54(1)
C25	1444(1)	11626(2)	870(2)	37(1)
C26	840(1)	11824(2)	737(2)	52(1)
C27	1678(1)	12047(2)	1564(2)	48(1)
C28	2956(1)	12482(2)	196(2)	41(1)
C29	2495(2)	12998(2)	-60(3)	78(1)
C30	3253(2)	12744(2)	923(2)	63(1)
C31	3944(1)	10590(2)	-58(2)	36(1)
C32	4236(2)	10773(2)	689(2)	64(1)
C33	4335(2)	10568(2)	-730(2)	67(1)
C34	2994(1)	11262(2)	-1706(2)	38(1)
C35	3440(1)	11842(2)	-1857(2)	52(1)
C36	2566(1)	11250(2)	-2346(2)	50(1)
K1	0	10000	5000	32(1)
C37	-1455(1)	9511(2)	4801(2)	58(1)
O13	-1145(1)	10129(1)	5091(1)	47(1)
C38	-1328(1)	10375(2)	5831(2)	64(1)
C39	-1006(1)	11058(2)	6058(3)	64(1)
O14	-448(1)	10850(1)	6184(1)	43(1)
C40	-120(1)	11473(2)	6417(2)	50(1)
C41	452(1)	11213(2)	6572(2)	49(1)
O15	690(1)	10980(1)	5866(1)	43(1)
C42	1233(1)	10702(2)	5969(2)	56(1)
O16	-116(7)	11150(14)	4022(10)	105(2)
C43	-598(4)	11435(7)	3635(7)	90(3)
C44	-334(5)	11598(11)	2887(7)	122(3)
C45	231(5)	11856(8)	3061(8)	87(3)

C46	270(13)	11749(15)	3907(9)	160(5)
O16'	-160(10)	11190(20)	4050(13)	105(2)
C43'	-356(7)	10996(8)	3288(10)	90(3)
C44'	-345(10)	11676(11)	2801(12)	122(3)
C45'	40(9)	12185(9)	3205(11)	87(3)
C46'	258(16)	11720(20)	3845(16)	160(5)
O16"	160(8)	11126(13)	3940(12)	105(2)
C43"	165(10)	11023(11)	3115(12)	90(3)
C44"	-50(15)	11704(13)	2733(11)	122(3)
C45"	-233(12)	12196(11)	3367(13)	87(3)
C46"	-235(12)	11712(15)	4060(14)	160(5)
K2	5000	10000	5000	42(1)
C47	4668(2)	11489(3)	6291(3)	75(1)
O17	4536(1)	11342(1)	5499(2)	57(1)
C48	4659(2)	11954(2)	5007(3)	84(2)
C49	4531(2)	11772(2)	4193(3)	77(1)
O18	4903(1)	11202(1)	3944(2)	59(1)
C50	4826(2)	10999(3)	3150(2)	72(1)
C51	5238(2)	10418(3)	2952(2)	73(1)
O19	5136(1)	9773(2)	3413(1)	56(1)
C52	5488(2)	9168(3)	3226(2)	71(1)
O20	4059(1)	9202(3)	4623(3)	84(1)
C53	3694(2)	9011(3)	5242(3)	77(2)
C54	3217(3)	9523(4)	5201(3)	111(3)
C55	3223(3)	9820(5)	4405(3)	120(3)
C56	3706(2)	9489(3)	4020(2)	64(1)
O20'	3934(5)	9913(7)	4519(8)	84(1)
C53'	3510(6)	10158(10)	5036(9)	77(2)
C54'	3056(6)	9636(11)	4847(15)	111(3)
C55'	3330(7)	8942(10)	4595(13)	120(3)
C56'	3924(7)	9117(7)	4639(14)	64(1)

Table 3. Bond lengths [Å] and angles [°] for 253.

Co(1)-P(1)	2.0693(7)	C(3)-H(3A)	0.9800
Co(1)-P(4)	2.0712(8)	C(3)-H(3B)	0.9800
Co(1)-P(2)	2.0757(8)	C(3)-H(3C)	0.9800
Co(1)-P(3)	2.0769(7)	C(4)-C(6)	1.503(5)
P(1)-O(3)	1.6427(18)	C(4)-C(5)	1.511(4)
P(1)-O(2)	1.6605(19)	C(4)-H(4A)	1.0000
P(1)-O(1)	1.6633(19)	C(5)-H(5A)	0.9800
P(2)-O(5)	1.6458(19)	C(5)-H(5B)	0.9800
P(2)-O(6)	1.649(2)	C(5)-H(5C)	0.9800
P(2)-O(4)	1.6646(19)	C(6)-H(6A)	0.9800
P(3)-O(8)	1.6401(19)	C(6)-H(6B)	0.9800
P(3)-O(7)	1.6562(19)	C(6)-H(6C)	0.9800
P(3)-O(9)	1.6659(19)	C(7)-C(8)	1.504(4)
P(4)-O(10)	1.6392(19)	C(7)-C(9)	1.509(5)
P(4)-O(11)	1.6587(19)	C(7)-H(7A)	1.0000
P(4)-O(12)	1.6641(19)	C(8)-H(8A)	0.9800
O(1)-C(1)	1.437(3)	C(8)-H(8B)	0.9800
O(2)-C(4)	1.431(3)	C(8)-H(8C)	0.9800
O(3)-C(7)	1.448(3)	C(9)-H(9A)	0.9800
O(4)-C(10)	1.434(3)	C(9)-H(9B)	0.9800
O(5)-C(13)	1.451(3)	C(9)-H(9C)	0.9800
O(6)-C(16)	1.436(3)	C(10)-C(11)	1.516(4)
O(7)-C(19)	1.428(3)	C(10)-C(12)	1.516(4)
O(8)-C(22)	1.449(3)	C(10)-H(10A)	1.0000
O(9)-C(25)	1.435(3)	C(11)-H(11A)	0.9800
O(10)-C(28)	1.447(3)	C(11)-H(11B)	0.9800
O(11)-C(31)	1.431(3)	C(11)-H(11C)	0.9800
O(12)-C(34)	1.435(3)	C(12)-H(12A)	0.9800
C(1)-C(2)	1.515(4)	C(12)-H(12B)	0.9800
C(1)-C(3)	1.515(4)	C(12)-H(12C)	0.9800
C(1)-H(1A)	1.0000	C(13)-C(15)	1.512(4)
C(2)-H(2A)	0.9800	C(13)-C(14)	1.525(4)
C(2)-H(2B)	0.9800	C(13)-H(13A)	1.0000
C(2)-H(2C)	0.9800	C(14)-H(14A)	0.9800

C(14)-H(14B)	0.9800	C(26)-H(26B)	0.9800
C(14)-H(14C)	0.9800	C(26)-H(26C)	0.9800
C(15)-H(15A)	0.9800	C(27)-H(27A)	0.9800
C(15)-H(15B)	0.9800	C(27)-H(27B)	0.9800
C(15)-H(15C)	0.9800	C(27)-H(27C)	0.9800
C(16)-C(18)	1.505(5)	C(28)-C(29)	1.511(5)
C(16)-C(17)	1.517(4)	C(28)-C(30)	1.515(5)
C(16)-H(16A)	1.0000	C(28)-H(28A)	1.0000
C(17)-H(17A)	0.9800	C(29)-H(29A)	0.9800
C(17)-H(17B)	0.9800	C(29)-H(29B)	0.9800
C(17)-H(17C)	0.9800	C(29)-H(29C)	0.9800
C(18)-H(18A)	0.9800	C(30)-H(30A)	0.9800
C(18)-H(18B)	0.9800	C(30)-H(30B)	0.9800
C(18)-H(18C)	0.9800	C(30)-H(30C)	0.9800
C(19)-C(20)	1.508(5)	C(31)-C(32)	1.503(5)
C(19)-C(21)	1.514(4)	C(31)-C(33)	1.507(4)
C(19)-H(19A)	1.0000	C(31)-H(31A)	1.0000
C(20)-H(20A)	0.9800	C(32)-H(32A)	0.9800
C(20)-H(20B)	0.9800	C(32)-H(32B)	0.9800
C(20)-H(20C)	0.9800	C(32)-H(32C)	0.9800
C(21)-H(21A)	0.9800	C(33)-H(33A)	0.9800
C(21)-H(21B)	0.9800	C(33)-H(33B)	0.9800
C(21)-H(21C)	0.9800	C(33)-H(33C)	0.9800
C(22)-C(23)	1.510(4)	C(34)-C(36)	1.509(4)
C(22)-C(24)	1.516(4)	C(34)-C(35)	1.521(4)
C(22)-H(22A)	1.0000	C(34)-H(34A)	1.0000
C(23)-H(23A)	0.9800	C(35)-H(35A)	0.9800
C(23)-H(23B)	0.9800	C(35)-H(35B)	0.9800
C(23)-H(23C)	0.9800	C(35)-H(35C)	0.9800
C(24)-H(24A)	0.9800	C(36)-H(36A)	0.9800
C(24)-H(24B)	0.9800	C(36)-H(36B)	0.9800
C(24)-H(24C)	0.9800	C(36)-H(36C)	0.9800
C(25)-C(27)	1.520(4)	K(1)-O(16)	2.67(2)
C(25)-C(26)	1.524(4)	K(1)-O(16)#1	2.67(2)
C(25)-H(25A)	1.0000	K(1)-O(16')#1	2.71(4)
C(26)-H(26A)	0.9800	K(1)-O(16')	2.71(4)

K(1)-O(16")#1	2.75(2)	C(44)-H(44A)	0.9900
K(1)-O(16")	2.75(2)	C(44)-H(44B)	0.9900
K(1)-O(14)	2.776(2)	C(45)-C(46)	1.4760(10)
K(1)-O(14)#1	2.776(2)	C(45)-H(45A)	0.9900
K(1)-O(13)#1	2.794(2)	C(45)-H(45B)	0.9900
K(1)-O(13)	2.794(2)	C(46)-H(46A)	0.9900
K(1)-O(15)#1	2.839(2)	C(46)-H(46B)	0.9900
K(1)-O(15)	2.839(2)	O(16')-C(43')	1.4360(10)
C(37)-O(13)	1.423(4)	O(16')-C(46')	1.4361(11)
C(37)-C(42)#1	1.489(5)	C(43')-C(44')	1.4760(10)
C(37)-H(37A)	0.9900	C(43')-H(43C)	0.9900
C(37)-H(37B)	0.9900	C(43')-H(43D)	0.9900
O(13)-C(38)	1.426(4)	C(44')-C(45')	1.4742(10)
C(38)-C(39)	1.498(5)	C(44')-H(44C)	0.9900
C(38)-H(38A)	0.9900	C(44')-H(44D)	0.9900
C(38)-H(38B)	0.9900	C(45')-C(46')	1.4760(10)
C(39)-O(14)	1.420(4)	C(45')-H(45C)	0.9900
C(39)-H(39A)	0.9900	C(45')-H(45D)	0.9900
C(39)-H(39B)	0.9900	C(46')-H(46C)	0.9900
O(14)-C(40)	1.425(4)	C(46')-H(46D)	0.9900
C(40)-C(41)	1.484(5)	O(16")-C(43")	1.4359(10)
C(40)-H(40A)	0.9900	O(16")-C(46")	1.4361(10)
C(40)-H(40B)	0.9900	C(43")-C(44")	1.4759(10)
C(41)-O(15)	1.417(4)	C(43")-H(43E)	0.9900
C(41)-H(41A)	0.9900	C(43")-H(43F)	0.9900
C(41)-H(41B)	0.9900	C(44")-C(45")	1.4740(10)
O(15)-C(42)	1.417(4)	C(44")-H(44E)	0.9900
C(42)-C(37)#1	1.489(5)	C(44")-H(44F)	0.9900
C(42)-H(42A)	0.9900	C(45")-C(46")	1.4760(10)
C(42)-H(42B)	0.9900	C(45")-H(45E)	0.9900
O(16)-C(43)	1.4360(10)	C(45")-H(45F)	0.9900
O(16)-C(46)	1.4362(10)	C(46")-H(46E)	0.9900
C(43)-C(44)	1.4762(10)	C(46")-H(46F)	0.9900
C(43)-H(43A)	0.9900	K(2)-O(20')#2	2.715(13)
C(43)-H(43B)	0.9900	K(2)-O(20')	2.715(13)
C(44)-C(45)	1.4743(10)	K(2)-O(20)#2	2.765(4)

K(2)-O(20)	2.765(4)	C(54)-C(55)	1.4734(10)
K(2)-O(17)#2	2.786(2)	C(54)-H(54A)	0.9900
K(2)-O(17)	2.786(2)	C(54)-H(54B)	0.9900
K(2)-O(19)#2	2.792(2)	C(55)-C(56)	1.4761(10)
K(2)-O(19)	2.793(2)	C(55)-H(55A)	0.9900
K(2)-O(18)	2.824(2)	C(55)-H(55B)	0.9900
K(2)-O(18)#2	2.824(2)	C(56)-H(56A)	0.9900
K(2)-C(56')	3.108(16)	C(56)-H(56B)	0.9900
K(2)-C(56')#2	3.108(16)	O(20')-C(53')	1.4360(10)
C(47)-O(17)	1.426(5)	O(20')-C(56')	1.4362(10)
C(47)-C(52)#2	1.489(6)	C(53')-C(54')	1.4760(10)
C(47)-H(47A)	0.9900	C(53')-H(53C)	0.9900
C(47)-H(47B)	0.9900	C(53')-H(53D)	0.9900
O(17)-C(48)	1.418(5)	C(54')-C(55')	1.4740(10)
C(48)-C(49)	1.474(6)	C(54')-H(54C)	0.9900
C(48)-H(48A)	0.9900	C(54')-H(54D)	0.9900
C(48)-H(48B)	0.9900	C(55')-C(56')	1.4761(10)
C(49)-O(18)	1.428(5)	C(55')-H(55C)	0.9900
C(49)-H(49A)	0.9900	C(55')-H(55D)	0.9900
C(49)-H(49B)	0.9900	C(56')-H(56C)	0.9900
O(18)-C(50)	1.428(5)	C(56')-H(56D)	0.9900
C(50)-C(51)	1.482(6)	P(1)-Co(1)-P(4)	117.35(3)
C(50)-H(50A)	0.9900	P(1)-Co(1)-P(2)	104.02(3)
C(50)-H(50B)	0.9900	P(4)-Co(1)-P(2)	106.94(3)
C(51)-O(19)	1.424(5)	P(1)-Co(1)-P(3)	106.55(3)
C(51)-H(51A)	0.9900	P(4)-Co(1)-P(3)	105.84(3)
C(51)-H(51B)	0.9900	P(2)-Co(1)-P(3)	116.66(3)
O(19)-C(52)	1.416(4)	O(3)-P(1)-O(2)	97.49(10)
C(52)-C(47)#2	1.490(6)	O(3)-P(1)-O(1)	93.99(10)
C(52)-H(52A)	0.9900	O(2)-P(1)-O(1)	95.53(10)
C(52)-H(52B)	0.9900	O(3)-P(1)-Co(1)	118.15(7)
O(20)-C(53)	1.4355(10)	O(2)-P(1)-Co(1)	124.38(8)
O(20)-C(56)	1.4355(10)	O(1)-P(1)-Co(1)	120.68(7)
C(53)-C(54)	1.4762(10)	O(5)-P(2)-O(6)	98.80(10)
C(53)-H(53A)	0.9900	O(5)-P(2)-O(4)	94.92(10)
C(53)-H(53B)	0.9900	O(6)-P(2)-O(4)	94.01(10)

O(5)-P(2)-Co(1)	117.89(7)	C(1)-C(2)-H(2C)	109.5
O(6)-P(2)-Co(1)	124.08(8)	H(2A)-C(2)-H(2C)	109.5
O(4)-P(2)-Co(1)	120.77(8)	H(2B)-C(2)-H(2C)	109.5
O(8)-P(3)-O(7)	98.10(10)	C(1)-C(3)-H(3A)	109.5
O(8)-P(3)-O(9)	93.94(10)	C(1)-C(3)-H(3B)	109.5
O(7)-P(3)-O(9)	94.65(10)	H(3A)-C(3)-H(3B)	109.5
O(8)-P(3)-Co(1)	117.91(7)	C(1)-C(3)-H(3C)	109.5
O(7)-P(3)-Co(1)	123.79(7)	H(3A)-C(3)-H(3C)	109.5
O(9)-P(3)-Co(1)	121.83(7)	H(3B)-C(3)-H(3C)	109.5
O(10)-P(4)-O(11)	96.96(10)	O(2)-C(4)-C(6)	108.2(3)
O(10)-P(4)-O(12)	93.71(10)	O(2)-C(4)-C(5)	108.7(3)
O(11)-P(4)-O(12)	94.91(10)	C(6)-C(4)-C(5)	111.3(3)
O(10)-P(4)-Co(1)	118.23(7)	O(2)-C(4)-H(4A)	109.5
O(11)-P(4)-Co(1)	124.55(7)	C(6)-C(4)-H(4A)	109.5
O(12)-P(4)-Co(1)	121.54(8)	C(5)-C(4)-H(4A)	109.5
C(1)-O(1)-P(1)	123.54(17)	C(4)-C(5)-H(5A)	109.5
C(4)-O(2)-P(1)	122.74(17)	C(4)-C(5)-H(5B)	109.5
C(7)-O(3)-P(1)	122.84(17)	H(5A)-C(5)-H(5B)	109.5
C(10)-O(4)-P(2)	124.07(18)	C(4)-C(5)-H(5C)	109.5
C(13)-O(5)-P(2)	122.17(18)	H(5A)-C(5)-H(5C)	109.5
C(16)-O(6)-P(2)	122.78(17)	H(5B)-C(5)-H(5C)	109.5
C(19)-O(7)-P(3)	122.72(16)	C(4)-C(6)-H(6A)	109.5
C(22)-O(8)-P(3)	121.91(18)	C(4)-C(6)-H(6B)	109.5
C(25)-O(9)-P(3)	122.63(18)	H(6A)-C(6)-H(6B)	109.5
C(28)-O(10)-P(4)	121.94(18)	C(4)-C(6)-H(6C)	109.5
C(31)-O(11)-P(4)	122.55(17)	H(6A)-C(6)-H(6C)	109.5
C(34)-O(12)-P(4)	122.20(17)	H(6B)-C(6)-H(6C)	109.5
O(1)-C(1)-C(2)	108.5(2)	O(3)-C(7)-C(8)	108.3(3)
O(1)-C(1)-C(3)	109.3(2)	O(3)-C(7)-C(9)	109.3(2)
C(2)-C(1)-C(3)	110.9(3)	C(8)-C(7)-C(9)	113.1(3)
O(1)-C(1)-H(1A)	109.4	O(3)-C(7)-H(7A)	108.7
C(2)-C(1)-H(1A)	109.4	C(8)-C(7)-H(7A)	108.7
C(3)-C(1)-H(1A)	109.4	C(9)-C(7)-H(7A)	108.7
C(1)-C(2)-H(2A)	109.5	C(7)-C(8)-H(8A)	109.5
C(1)-C(2)-H(2B)	109.5	C(7)-C(8)-H(8B)	109.5
H(2A)-C(2)-H(2B)	109.5	H(8A)-C(8)-H(8B)	109.5

C(7)-C(8)-H(8C)	109.5	C(13)-C(14)-H(14C)	109.5
H(8A)-C(8)-H(8C)	109.5	H(14A)-C(14)-H(14C)	109.5
H(8B)-C(8)-H(8C)	109.5	H(14B)-C(14)-H(14C)	109.5
C(7)-C(9)-H(9A)	109.5	C(13)-C(15)-H(15A)	109.5
C(7)-C(9)-H(9B)	109.5	C(13)-C(15)-H(15B)	109.5
H(9A)-C(9)-H(9B)	109.5	H(15A)-C(15)-H(15B)	109.5
C(7)-C(9)-H(9C)	109.5	C(13)-C(15)-H(15C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(15A)-C(15)-H(15C)	109.5
H(9B)-C(9)-H(9C)	109.5	H(15B)-C(15)-H(15C)	109.5
O(4)-C(10)-C(11)	107.9(2)	O(6)-C(16)-C(18)	109.5(3)
O(4)-C(10)-C(12)	109.7(3)	O(6)-C(16)-C(17)	106.3(2)
C(11)-C(10)-C(12)	110.4(3)	C(18)-C(16)-C(17)	112.3(3)
O(4)-C(10)-H(10A)	109.6	O(6)-C(16)-H(16A)	109.6
C(11)-C(10)-H(10A)	109.6	C(18)-C(16)-H(16A)	109.6
C(12)-C(10)-H(10A)	109.6	C(17)-C(16)-H(16A)	109.6
C(10)-C(11)-H(11A)	109.5	C(16)-C(17)-H(17A)	109.5
C(10)-C(11)-H(11B)	109.5	C(16)-C(17)-H(17B)	109.5
H(11A)-C(11)-H(11B)	109.5	H(17A)-C(17)-H(17B)	109.5
C(10)-C(11)-H(11C)	109.5	C(16)-C(17)-H(17C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(17A)-C(17)-H(17C)	109.5
H(11B)-C(11)-H(11C)	109.5	H(17B)-C(17)-H(17C)	109.5
C(10)-C(12)-H(12A)	109.5	C(16)-C(18)-H(18A)	109.5
C(10)-C(12)-H(12B)	109.5	C(16)-C(18)-H(18B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(18A)-C(18)-H(18B)	109.5
C(10)-C(12)-H(12C)	109.5	C(16)-C(18)-H(18C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(18A)-C(18)-H(18C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(18B)-C(18)-H(18C)	109.5
O(5)-C(13)-C(15)	107.2(2)	O(7)-C(19)-C(20)	108.6(3)
O(5)-C(13)-C(14)	109.8(2)	O(7)-C(19)-C(21)	107.9(3)
C(15)-C(13)-C(14)	111.6(3)	C(20)-C(19)-C(21)	111.9(3)
O(5)-C(13)-H(13A)	109.4	O(7)-C(19)-H(19A)	109.5
C(15)-C(13)-H(13A)	109.4	C(20)-C(19)-H(19A)	109.5
C(14)-C(13)-H(13A)	109.4	C(21)-C(19)-H(19A)	109.5
C(13)-C(14)-H(14A)	109.5	C(19)-C(20)-H(20A)	109.5
C(13)-C(14)-H(14B)	109.5	C(19)-C(20)-H(20B)	109.5
H(14A)-C(14)-H(14B)	109.5	H(20A)-C(20)-H(20B)	109.5

C(19)-C(20)-H(20C)	109.5	C(25)-C(26)-H(26C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(20B)-C(20)-H(20C)	109.5	H(26B)-C(26)-H(26C)	109.5
C(19)-C(21)-H(21A)	109.5	C(25)-C(27)-H(27A)	109.5
C(19)-C(21)-H(21B)	109.5	C(25)-C(27)-H(27B)	109.5
H(21A)-C(21)-H(21B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(19)-C(21)-H(21C)	109.5	C(25)-C(27)-H(27C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(21B)-C(21)-H(21C)	109.5	H(27B)-C(27)-H(27C)	109.5
O(8)-C(22)-C(23)	108.3(2)	O(10)-C(28)-C(29)	109.1(3)
O(8)-C(22)-C(24)	108.7(2)	O(10)-C(28)-C(30)	106.9(3)
C(23)-C(22)-C(24)	112.9(3)	C(29)-C(28)-C(30)	113.6(3)
O(8)-C(22)-H(22A)	108.9	O(10)-C(28)-H(28A)	109.0
C(23)-C(22)-H(22A)	108.9	C(29)-C(28)-H(28A)	109.0
C(24)-C(22)-H(22A)	108.9	C(30)-C(28)-H(28A)	109.0
C(22)-C(23)-H(23A)	109.5	C(28)-C(29)-H(29A)	109.5
C(22)-C(23)-H(23B)	109.5	C(28)-C(29)-H(29B)	109.5
H(23A)-C(23)-H(23B)	109.5	H(29A)-C(29)-H(29B)	109.5
C(22)-C(23)-H(23C)	109.5	C(28)-C(29)-H(29C)	109.5
H(23A)-C(23)-H(23C)	109.5	H(29A)-C(29)-H(29C)	109.5
H(23B)-C(23)-H(23C)	109.5	H(29B)-C(29)-H(29C)	109.5
C(22)-C(24)-H(24A)	109.5	C(28)-C(30)-H(30A)	109.5
C(22)-C(24)-H(24B)	109.5	C(28)-C(30)-H(30B)	109.5
H(24A)-C(24)-H(24B)	109.5	H(30A)-C(30)-H(30B)	109.5
C(22)-C(24)-H(24C)	109.5	C(28)-C(30)-H(30C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(24B)-C(24)-H(24C)	109.5	H(30B)-C(30)-H(30C)	109.5
O(9)-C(25)-C(27)	108.1(2)	O(11)-C(31)-C(32)	109.1(3)
O(9)-C(25)-C(26)	110.2(2)	O(11)-C(31)-C(33)	107.2(2)
C(27)-C(25)-C(26)	110.9(3)	C(32)-C(31)-C(33)	111.8(3)
O(9)-C(25)-H(25A)	109.2	O(11)-C(31)-H(31A)	109.6
C(27)-C(25)-H(25A)	109.2	C(32)-C(31)-H(31A)	109.6
C(26)-C(25)-H(25A)	109.2	C(33)-C(31)-H(31A)	109.6
C(25)-C(26)-H(26A)	109.5	C(31)-C(32)-H(32A)	109.5
C(25)-C(26)-H(26B)	109.5	C(31)-C(32)-H(32B)	109.5
H(26A)-C(26)-H(26B)	109.5	H(32A)-C(32)-H(32B)	109.5

C(31)-C(32)-H(32C)	109.5	O(16')-K(1)-O(16")#1	163.0(7)
H(32A)-C(32)-H(32C)	109.5	O(16)-K(1)-O(16")	14.5(5)
H(32B)-C(32)-H(32C)	109.5	O(16)#1-K(1)-O(16")	165.5(5)
C(31)-C(33)-H(33A)	109.5	O(16')#1-K(1)-O(16")	163.0(7)
C(31)-C(33)-H(33B)	109.5	O(16')-K(1)-O(16")	17.0(7)
H(33A)-C(33)-H(33B)	109.5	O(16")#1-K(1)-O(16")	180.000(2)
C(31)-C(33)-H(33C)	109.5	O(16)-K(1)-O(14)	90.4(4)
H(33A)-C(33)-H(33C)	109.5	O(16)#1-K(1)-O(14)	89.6(4)
H(33B)-C(33)-H(33C)	109.5	O(16')#1-K(1)-O(14)	92.1(5)
O(12)-C(34)-C(36)	108.0(3)	O(16')-K(1)-O(14)	87.9(5)
O(12)-C(34)-C(35)	109.0(3)	O(16")#1-K(1)-O(14)	81.4(5)
C(36)-C(34)-C(35)	111.7(3)	O(16")-K(1)-O(14)	98.6(5)
O(12)-C(34)-H(34A)	109.4	O(16)-K(1)-O(14)#1	89.6(4)
C(36)-C(34)-H(34A)	109.4	O(16)#1-K(1)-O(14)#1	90.4(4)
C(35)-C(34)-H(34A)	109.4	O(16')#1-K(1)-O(14)#1	87.9(5)
C(34)-C(35)-H(35A)	109.5	O(16')-K(1)-O(14)#1	92.1(5)
C(34)-C(35)-H(35B)	109.5	O(16")#1-K(1)-O(14)#1	98.6(5)
H(35A)-C(35)-H(35B)	109.5	O(16")-K(1)-O(14)#1	81.4(5)
C(34)-C(35)-H(35C)	109.5	O(14)-K(1)-O(14)#1	180.0
H(35A)-C(35)-H(35C)	109.5	O(16)-K(1)-O(13)#1	97.3(4)
H(35B)-C(35)-H(35C)	109.5	O(16)#1-K(1)-O(13)#1	82.7(4)
C(34)-C(36)-H(36A)	109.5	O(16')#1-K(1)-O(13)#1	80.4(6)
C(34)-C(36)-H(36B)	109.5	O(16')-K(1)-O(13)#1	99.6(6)
H(36A)-C(36)-H(36B)	109.5	O(16")#1-K(1)-O(13)#1	97.2(4)
C(34)-C(36)-H(36C)	109.5	O(16")-K(1)-O(13)#1	82.8(4)
H(36A)-C(36)-H(36C)	109.5	O(14)-K(1)-O(13)#1	118.89(6)
H(36B)-C(36)-H(36C)	109.5	O(14)#1-K(1)-O(13)#1	61.11(6)
O(16)-K(1)-O(16)#1	179.999(3)	O(16)-K(1)-O(13)	82.7(4)
O(16)-K(1)-O(16')#1	177.2(9)	O(16)#1-K(1)-O(13)	97.3(4)
O(16)#1-K(1)-O(16')#1	2.8(9)	O(16')#1-K(1)-O(13)	99.6(6)
O(16)-K(1)-O(16')	2.8(9)	O(16')-K(1)-O(13)	80.4(6)
O(16)#1-K(1)-O(16')	177.2(9)	O(16")#1-K(1)-O(13)	82.8(4)
O(16')#1-K(1)-O(16')	179.999(2)	O(16")-K(1)-O(13)	97.2(4)
O(16)-K(1)-O(16")#1	165.5(5)	O(14)-K(1)-O(13)	61.11(6)
O(16)#1-K(1)-O(16")#1	14.5(5)	O(14)#1-K(1)-O(13)	118.89(6)
O(16')#1-K(1)-O(16")#1	17.0(7)	O(13)#1-K(1)-O(13)	180.0

O(16)-K(1)-O(15)#1	94.7(4)	O(14)-C(39)-C(38)	108.8(3)
O(16)#1-K(1)-O(15)#1	85.3(4)	O(14)-C(39)-H(39A)	109.9
O(16')#1-K(1)-O(15)#1	85.2(5)	C(38)-C(39)-H(39A)	109.9
O(16')-K(1)-O(15)#1	94.8(5)	O(14)-C(39)-H(39B)	109.9
O(16'')#1-K(1)-O(15)#1	79.3(5)	C(38)-C(39)-H(39B)	109.9
O(16'')-K(1)-O(15)#1	100.7(5)	H(39A)-C(39)-H(39B)	108.3
O(14)-K(1)-O(15)#1	119.44(6)	C(39)-O(14)-C(40)	111.7(3)
O(14)#1-K(1)-O(15)#1	60.56(6)	C(39)-O(14)-K(1)	114.20(19)
O(13)#1-K(1)-O(15)#1	120.13(6)	C(40)-O(14)-K(1)	114.36(18)
O(13)-K(1)-O(15)#1	59.87(6)	O(14)-C(40)-C(41)	109.0(3)
O(16)-K(1)-O(15)	85.3(4)	O(14)-C(40)-H(40A)	109.9
O(16)#1-K(1)-O(15)	94.7(4)	C(41)-C(40)-H(40A)	109.9
O(16')#1-K(1)-O(15)	94.8(5)	O(14)-C(40)-H(40B)	109.9
O(16')-K(1)-O(15)	85.2(5)	C(41)-C(40)-H(40B)	109.9
O(16'')#1-K(1)-O(15)	100.7(5)	H(40A)-C(40)-H(40B)	108.3
O(16'')-K(1)-O(15)	79.3(5)	O(15)-C(41)-C(40)	109.0(3)
O(14)-K(1)-O(15)	60.56(6)	O(15)-C(41)-H(41A)	109.9
O(14)#1-K(1)-O(15)	119.44(6)	C(40)-C(41)-H(41A)	109.9
O(13)#1-K(1)-O(15)	59.87(6)	O(15)-C(41)-H(41B)	109.9
O(13)-K(1)-O(15)	120.13(6)	C(40)-C(41)-H(41B)	109.9
O(15)#1-K(1)-O(15)	180.0	H(41A)-C(41)-H(41B)	108.3
O(13)-C(37)-C(42)#1	108.6(3)	C(41)-O(15)-C(42)	112.5(3)
O(13)-C(37)-H(37A)	110.0	C(41)-O(15)-K(1)	112.95(18)
C(42)#1-C(37)-H(37A)	110.0	C(42)-O(15)-K(1)	113.14(18)
O(13)-C(37)-H(37B)	110.0	O(15)-C(42)-C(37)#1	108.7(3)
C(42)#1-C(37)-H(37B)	110.0	O(15)-C(42)-H(42A)	109.9
H(37A)-C(37)-H(37B)	108.4	C(37)#1-C(42)-H(42A)	109.9
C(37)-O(13)-C(38)	112.7(3)	O(15)-C(42)-H(42B)	109.9
C(37)-O(13)-K(1)	116.06(18)	C(37)#1-C(42)-H(42B)	109.9
C(38)-O(13)-K(1)	113.25(19)	H(42A)-C(42)-H(42B)	108.3
O(13)-C(38)-C(39)	108.6(3)	C(43)-O(16)-C(46)	102(2)
O(13)-C(38)-H(38A)	110.0	C(43)-O(16)-K(1)	130.3(17)
C(39)-C(38)-H(38A)	110.0	C(46)-O(16)-K(1)	126.5(9)
O(13)-C(38)-H(38B)	110.0	O(16)-C(43)-C(44)	96.8(14)
C(39)-C(38)-H(38B)	110.0	O(16)-C(43)-H(43A)	112.4
H(38A)-C(38)-H(38B)	108.4	C(44)-C(43)-H(43A)	112.4

O(16)-C(43)-H(43B)	112.4	C(44')-C(45')-C(46')	103.3(14)
C(44)-C(43)-H(43B)	112.4	C(44')-C(45')-H(45C)	111.1
H(43A)-C(43)-H(43B)	110.0	C(46')-C(45')-H(45C)	111.1
C(45)-C(44)-C(43)	107.1(8)	C(44')-C(45')-H(45D)	111.1
C(45)-C(44)-H(44A)	110.3	C(46')-C(45')-H(45D)	111.1
C(43)-C(44)-H(44A)	110.3	H(45C)-C(45')-H(45D)	109.1
C(45)-C(44)-H(44B)	110.3	O(16')-C(46')-C(45')	108(3)
C(43)-C(44)-H(44B)	110.3	O(16')-C(46')-H(46C)	110.1
H(44A)-C(44)-H(44B)	108.6	C(45')-C(46')-H(46C)	110.1
C(44)-C(45)-C(46)	102.3(11)	O(16')-C(46')-H(46D)	110.1
C(44)-C(45)-H(45A)	111.3	C(45')-C(46')-H(46D)	110.1
C(46)-C(45)-H(45A)	111.3	H(46C)-C(46')-H(46D)	108.5
C(44)-C(45)-H(45B)	111.3	C(43'')-O(16'')-C(46'')	104.4(19)
C(46)-C(45)-H(45B)	111.3	C(43'')-O(16'')-K(1)	124.7(15)
H(45A)-C(45)-H(45B)	109.2	C(46'')-O(16'')-K(1)	109.7(14)
O(16)-C(46)-C(45)	101.4(17)	O(16'')-C(43'')-C(44'')	109.4(16)
O(16)-C(46)-H(46A)	111.5	O(16'')-C(43'')-H(43E)	109.8
C(45)-C(46)-H(46A)	111.5	C(44'')-C(43'')-H(43E)	109.8
O(16)-C(46)-H(46B)	111.5	O(16'')-C(43'')-H(43F)	109.8
C(45)-C(46)-H(46B)	111.5	C(44'')-C(43'')-H(43F)	109.8
H(46A)-C(46)-H(46B)	109.3	H(43E)-C(43'')-H(43F)	108.2
C(43')-O(16')-C(46')	99(3)	C(45'')-C(44'')-C(43'')	105.4(11)
C(43')-O(16')-K(1)	114(2)	C(45'')-C(44'')-H(44E)	110.7
C(46')-O(16')-K(1)	124.7(13)	C(43'')-C(44'')-H(44E)	110.7
O(16')-C(43')-C(44')	109(2)	C(45'')-C(44'')-H(44F)	110.7
O(16')-C(43')-H(43C)	110.0	C(43'')-C(44'')-H(44F)	110.7
C(44')-C(43')-H(43C)	110.0	H(44E)-C(44'')-H(44F)	108.8
O(16')-C(43')-H(43D)	110.0	C(44'')-C(45'')-C(46'')	104.9(12)
C(44')-C(43')-H(43D)	110.0	C(44'')-C(45'')-H(45E)	110.8
H(43C)-C(43')-H(43D)	108.4	C(46'')-C(45'')-H(45E)	110.8
C(45')-C(44')-C(43')	104.5(11)	C(44'')-C(45'')-H(45F)	110.8
C(45')-C(44')-H(44C)	110.9	C(46'')-C(45'')-H(45F)	110.8
C(43')-C(44')-H(44C)	110.9	H(45E)-C(45'')-H(45F)	108.8
C(45')-C(44')-H(44D)	110.9	O(16'')-C(46'')-C(45'')	107.5(17)
C(43')-C(44')-H(44D)	110.9	O(16'')-C(46'')-K(1)	47.6(11)
H(44C)-C(44')-H(44D)	108.9	C(45'')-C(46'')-K(1)	152.1(14)

O(16")-C(46")-H(46E)	110.2	O(20')-K(2)-O(18)	76.9(3)
C(45")-C(46")-H(46E)	110.2	O(20)#2-K(2)-O(18)	79.88(9)
K(1)-C(46")-H(46E)	92.9	O(20)-K(2)-O(18)	100.12(9)
O(16")-C(46")-H(46F)	110.2	O(17)#2-K(2)-O(18)	118.99(8)
C(45")-C(46")-H(46F)	110.2	O(17)-K(2)-O(18)	61.01(8)
K(1)-C(46")-H(46F)	75.1	O(19)#2-K(2)-O(18)	120.87(8)
H(46E)-C(46")-H(46F)	108.5	O(19)-K(2)-O(18)	59.13(8)
O(20')#2-K(2)-O(20')	180.000(1)	O(20')#2-K(2)-O(18)#2	76.9(3)
O(20')#2-K(2)-O(20)#2	27.8(3)	O(20')-K(2)-O(18)#2	103.1(3)
O(20')-K(2)-O(20)#2	152.2(3)	O(20)#2-K(2)-O(18)#2	100.12(9)
O(20')#2-K(2)-O(20)	152.2(3)	O(20)-K(2)-O(18)#2	79.88(9)
O(20')-K(2)-O(20)	27.8(3)	O(17)#2-K(2)-O(18)#2	61.01(8)
O(20)#2-K(2)-O(20)	180.0	O(17)-K(2)-O(18)#2	118.99(8)
O(20')#2-K(2)-O(17)#2	75.9(3)	O(19)#2-K(2)-O(18)#2	59.13(8)
O(20')-K(2)-O(17)#2	104.1(3)	O(19)-K(2)-O(18)#2	120.87(8)
O(20)#2-K(2)-O(17)#2	100.36(11)	O(18)-K(2)-O(18)#2	180.00(8)
O(20)-K(2)-O(17)#2	79.64(11)	O(20')#2-K(2)-C(56')	152.49(17)
O(20')#2-K(2)-O(17)	104.1(3)	O(20')-K(2)-C(56')	27.51(17)
O(20')-K(2)-O(17)	75.9(3)	O(20)#2-K(2)-C(56')	177.8(5)
O(20)#2-K(2)-O(17)	79.64(11)	O(20)-K(2)-C(56')	2.2(5)
O(20)-K(2)-O(17)	100.36(11)	O(17)#2-K(2)-C(56')	81.0(3)
O(17)#2-K(2)-O(17)	180.00(5)	O(17)-K(2)-C(56')	99.0(3)
O(20')#2-K(2)-O(19)#2	79.2(3)	O(19)#2-K(2)-C(56')	99.4(4)
O(20')-K(2)-O(19)#2	100.8(3)	O(19)-K(2)-C(56')	80.6(4)
O(20)#2-K(2)-O(19)#2	78.43(10)	O(18)-K(2)-C(56')	101.0(3)
O(20)-K(2)-O(19)#2	101.57(10)	O(18)#2-K(2)-C(56')	79.0(3)
O(17)#2-K(2)-O(19)#2	118.71(8)	O(20')#2-K(2)-C(56')#2	27.51(17)
O(17)-K(2)-O(19)#2	61.29(8)	O(20')-K(2)-C(56')#2	152.49(17)
O(20')#2-K(2)-O(19)	100.8(3)	O(20)#2-K(2)-C(56')#2	2.2(5)
O(20')-K(2)-O(19)	79.2(3)	O(20)-K(2)-C(56')#2	177.8(5)
O(20)#2-K(2)-O(19)	101.57(10)	O(17)#2-K(2)-C(56')#2	99.0(3)
O(20)-K(2)-O(19)	78.43(10)	O(17)-K(2)-C(56')#2	81.0(3)
O(17)#2-K(2)-O(19)	61.29(8)	O(19)#2-K(2)-C(56')#2	80.6(4)
O(17)-K(2)-O(19)	118.71(8)	O(19)-K(2)-C(56')#2	99.4(4)
O(19)#2-K(2)-O(19)	180.00(9)	O(18)-K(2)-C(56')#2	79.0(3)
O(20')#2-K(2)-O(18)	103.1(3)	O(18)#2-K(2)-C(56')#2	101.0(3)

C(56')-K(2)-C(56')#2	179.999(2)	H(51A)-C(51)-H(51B)	108.4
O(17)-C(47)-C(52)#2	109.6(3)	C(52)-O(19)-C(51)	112.4(3)
O(17)-C(47)-H(47A)	109.7	C(52)-O(19)-K(2)	114.3(2)
C(52)#2-C(47)-H(47A)	109.7	C(51)-O(19)-K(2)	117.0(2)
O(17)-C(47)-H(47B)	109.7	O(19)-C(52)-C(47)#2	108.3(3)
C(52)#2-C(47)-H(47B)	109.7	O(19)-C(52)-H(52A)	110.0
H(47A)-C(47)-H(47B)	108.2	C(47)#2-C(52)-H(52A)	110.0
C(48)-O(17)-C(47)	112.7(3)	O(19)-C(52)-H(52B)	110.0
C(48)-O(17)-K(2)	112.9(2)	C(47)#2-C(52)-H(52B)	110.0
C(47)-O(17)-K(2)	111.5(2)	H(52A)-C(52)-H(52B)	108.4
O(17)-C(48)-C(49)	110.9(3)	C(53)-O(20)-C(56)	104.9(4)
O(17)-C(48)-H(48A)	109.5	C(53)-O(20)-K(2)	117.5(4)
C(49)-C(48)-H(48A)	109.5	C(56)-O(20)-K(2)	118.2(3)
O(17)-C(48)-H(48B)	109.5	O(20)-C(53)-C(54)	107.8(4)
C(49)-C(48)-H(48B)	109.5	O(20)-C(53)-H(53A)	110.1
H(48A)-C(48)-H(48B)	108.0	C(54)-C(53)-H(53A)	110.1
O(18)-C(49)-C(48)	108.4(4)	O(20)-C(53)-H(53B)	110.1
O(18)-C(49)-H(49A)	110.0	C(54)-C(53)-H(53B)	110.1
C(48)-C(49)-H(49A)	110.0	H(53A)-C(53)-H(53B)	108.5
O(18)-C(49)-H(49B)	110.0	C(55)-C(54)-C(53)	104.6(4)
C(48)-C(49)-H(49B)	110.0	C(55)-C(54)-H(54A)	110.8
H(49A)-C(49)-H(49B)	108.4	C(53)-C(54)-H(54A)	110.8
C(50)-O(18)-C(49)	113.1(3)	C(55)-C(54)-H(54B)	110.8
C(50)-O(18)-K(2)	115.8(2)	C(53)-C(54)-H(54B)	110.8
C(49)-O(18)-K(2)	113.3(2)	H(54A)-C(54)-H(54B)	108.9
O(18)-C(50)-C(51)	108.5(3)	C(54)-C(55)-C(56)	106.9(4)
O(18)-C(50)-H(50A)	110.0	C(54)-C(55)-H(55A)	110.3
C(51)-C(50)-H(50A)	110.0	C(56)-C(55)-H(55A)	110.3
O(18)-C(50)-H(50B)	110.0	C(54)-C(55)-H(55B)	110.3
C(51)-C(50)-H(50B)	110.0	C(56)-C(55)-H(55B)	110.3
H(50A)-C(50)-H(50B)	108.4	H(55A)-C(55)-H(55B)	108.6
O(19)-C(51)-C(50)	108.4(3)	O(20)-C(56)-C(55)	106.7(4)
O(19)-C(51)-H(51A)	110.0	O(20)-C(56)-H(56A)	110.4
C(50)-C(51)-H(51A)	110.0	C(55)-C(56)-H(56A)	110.4
O(19)-C(51)-H(51B)	110.0	O(20)-C(56)-H(56B)	110.4
C(50)-C(51)-H(51B)	110.0	C(55)-C(56)-H(56B)	110.4

H(56A)-C(56)-H(56B)	108.6	C(54')-C(55')-C(56')	104.6(11)
C(53')-O(20')-C(56')	101.5(12)	C(54')-C(55')-H(55C)	110.8
C(53')-O(20')-K(2)	118.7(10)	C(56')-C(55')-H(55C)	110.8
C(56')-O(20')-K(2)	91.7(9)	C(54')-C(55')-H(55D)	110.8
O(20')-C(53')-C(54')	102.1(11)	C(56')-C(55')-H(55D)	110.8
O(20')-C(53')-H(53C)	111.3	H(55C)-C(55')-H(55D)	108.9
C(54')-C(53')-H(53C)	111.3	O(20')-C(56')-C(55')	102.6(12)
O(20')-C(53')-H(53D)	111.3	O(20')-C(56')-K(2)	60.8(8)
C(54')-C(53')-H(53D)	111.3	C(55')-C(56')-K(2)	159.3(11)
H(53C)-C(53')-H(53D)	109.2	O(20')-C(56')-H(56C)	111.2
C(55')-C(54')-C(53')	104.8(10)	C(55')-C(56')-H(56C)	111.2
C(55')-C(54')-H(54C)	110.8	K(2)-C(56')-H(56C)	68.1
C(53')-C(54')-H(54C)	110.8	O(20')-C(56')-H(56D)	111.2
C(55')-C(54')-H(54D)	110.8	C(55')-C(56')-H(56D)	111.2
C(53')-C(54')-H(54D)	110.8	K(2)-C(56')-H(56D)	87.5
H(54C)-C(54')-H(54D)	108.9	H(56C)-C(56')-H(56D)	109.2

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 -x+1,-y+2,-z+1

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 253. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	18(1)	22(1)	24(1)	0(1)	0(1)	0(1)
P1	24(1)	26(1)	26(1)	1(1)	0(1)	0(1)
P2	25(1)	25(1)	28(1)	-1(1)	2(1)	0(1)
P3	20(1)	28(1)	28(1)	0(1)	0(1)	0(1)
P4	20(1)	24(1)	32(1)	1(1)	3(1)	1(1)
O1	32(1)	30(1)	31(1)	2(1)	5(1)	-2(1)
O2	44(1)	33(1)	27(1)	-1(1)	-4(1)	2(1)
O3	26(1)	34(1)	31(1)	5(1)	-1(1)	5(1)
O4	29(1)	33(1)	37(1)	0(1)	5(1)	6(1)
O5	33(1)	32(1)	25(1)	-2(1)	-1(1)	2(1)
O6	44(1)	28(1)	41(1)	-5(1)	13(1)	-6(1)
O7	23(1)	47(1)	33(1)	5(1)	-2(1)	6(1)
O8	20(1)	36(1)	38(1)	4(1)	3(1)	-3(1)
O9	28(1)	33(1)	35(1)	-2(1)	4(1)	3(1)
O10	29(1)	23(1)	40(1)	-3(1)	10(1)	-3(1)
O11	21(1)	29(1)	52(1)	8(1)	6(1)	1(1)
O12	33(1)	32(1)	35(1)	8(1)	5(1)	4(1)
C1	32(2)	34(2)	33(2)	8(1)	6(1)	-1(1)
C2	42(2)	43(2)	50(2)	6(2)	10(2)	-10(1)
C3	46(2)	58(2)	38(2)	15(2)	5(1)	3(2)
C4	49(2)	33(2)	31(2)	-6(1)	1(1)	3(1)
C5	56(2)	66(2)	40(2)	-7(2)	4(2)	16(2)
C6	74(3)	58(2)	78(3)	-25(2)	1(2)	-24(2)
C7	33(2)	49(2)	34(2)	9(1)	-5(1)	8(1)
C8	39(2)	86(3)	56(2)	13(2)	-16(2)	2(2)
C9	74(3)	46(2)	57(2)	14(2)	-7(2)	21(2)
C10	37(2)	34(2)	48(2)	-4(1)	-1(1)	10(1)
C11	34(2)	50(2)	65(2)	-4(2)	-5(2)	14(2)
C12	64(2)	53(2)	82(3)	-28(2)	-12(2)	21(2)
C13	47(2)	42(2)	30(2)	-8(1)	2(1)	4(1)
C14	55(2)	72(3)	37(2)	-5(2)	14(2)	2(2)

C15	60(2)	57(2)	37(2)	-10(2)	-10(2)	-3(2)
C16	42(2)	28(2)	43(2)	-6(1)	11(1)	-8(1)
C17	67(2)	36(2)	45(2)	1(2)	4(2)	-9(2)
C18	46(2)	46(2)	89(3)	-8(2)	-8(2)	-4(2)
C19	26(1)	52(2)	32(2)	10(1)	0(1)	8(1)
C20	57(2)	68(3)	44(2)	-3(2)	-10(2)	6(2)
C21	59(2)	60(2)	59(2)	21(2)	-4(2)	10(2)
C22	20(1)	44(2)	45(2)	1(1)	4(1)	-5(1)
C23	29(2)	65(2)	64(2)	-6(2)	2(2)	-14(2)
C24	31(2)	83(3)	48(2)	5(2)	9(2)	1(2)
C25	30(2)	32(2)	49(2)	-4(1)	3(1)	6(1)
C26	36(2)	50(2)	70(2)	-14(2)	-3(2)	14(2)
C27	41(2)	39(2)	63(2)	-15(2)	-1(2)	6(1)
C28	38(2)	26(2)	61(2)	-3(1)	13(2)	-6(1)
C29	59(2)	31(2)	144(4)	19(2)	15(3)	4(2)
C30	72(3)	50(2)	67(2)	-23(2)	15(2)	-29(2)
C31	20(1)	32(2)	56(2)	6(1)	6(1)	3(1)
C32	41(2)	69(3)	83(3)	4(2)	-16(2)	6(2)
C33	45(2)	65(3)	93(3)	21(2)	35(2)	21(2)
C34	43(2)	34(2)	38(2)	9(1)	8(1)	0(1)
C35	55(2)	47(2)	55(2)	16(2)	16(2)	-5(2)
C36	58(2)	55(2)	37(2)	12(2)	4(2)	-1(2)
K1	30(1)	32(1)	35(1)	-1(1)	2(1)	0(1)
C37	33(2)	56(2)	84(3)	-12(2)	6(2)	-11(2)
O13	32(1)	48(1)	60(2)	-9(1)	8(1)	-6(1)
C38	35(2)	83(3)	73(3)	-18(2)	19(2)	-2(2)
C39	40(2)	68(3)	86(3)	-31(2)	8(2)	10(2)
O14	38(1)	42(1)	48(1)	-8(1)	8(1)	2(1)
C40	60(2)	43(2)	48(2)	-13(2)	3(2)	-1(2)
C41	57(2)	49(2)	42(2)	-6(2)	-4(2)	-5(2)
O15	39(1)	48(1)	41(1)	-3(1)	-2(1)	-1(1)
C42	37(2)	62(2)	67(2)	-10(2)	-12(2)	-6(2)
O16	84(4)	105(4)	125(4)	79(3)	-30(3)	-26(4)
C43	71(6)	74(6)	125(8)	46(6)	-10(5)	-1(4)
C44	140(8)	123(6)	103(6)	32(5)	-60(6)	-53(6)
C45	86(9)	97(9)	77(7)	19(6)	17(6)	-12(6)

C46	172(9)	166(8)	142(8)	97(6)	-86(7)	-107(7)
O16'	84(4)	105(4)	125(4)	79(3)	-30(3)	-26(4)
C43'	71(6)	74(6)	125(8)	46(6)	-10(5)	-1(4)
C44'	140(8)	123(6)	103(6)	32(5)	-60(6)	-53(6)
C45'	86(9)	97(9)	77(7)	19(6)	17(6)	-12(6)
C46'	172(9)	166(8)	142(8)	97(6)	-86(7)	-107(7)
O16"	84(4)	105(4)	125(4)	79(3)	-30(3)	-26(4)
C43"	71(6)	74(6)	125(8)	46(6)	-10(5)	-1(4)
C44"	140(8)	123(6)	103(6)	32(5)	-60(6)	-53(6)
C45"	86(9)	97(9)	77(7)	19(6)	17(6)	-12(6)
C46"	172(9)	166(8)	142(8)	97(6)	-86(7)	-107(7)
K2	39(1)	42(1)	46(1)	-6(1)	4(1)	4(1)
C47	56(2)	77(3)	93(3)	-49(3)	-12(2)	16(2)
O17	51(1)	44(1)	74(2)	-17(1)	-2(1)	5(1)
C48	82(3)	40(2)	129(5)	-18(3)	14(3)	4(2)
C49	71(3)	51(2)	109(4)	22(3)	7(3)	12(2)
O18	50(2)	58(2)	69(2)	8(1)	-2(1)	2(1)
C50	60(3)	91(3)	64(3)	27(2)	-4(2)	-5(2)
C51	55(2)	115(4)	50(2)	5(2)	5(2)	-9(2)
O19	40(1)	79(2)	50(1)	-12(1)	4(1)	4(1)
C52	48(2)	104(4)	60(3)	-35(2)	-1(2)	11(2)
O20	50(2)	102(3)	99(3)	29(3)	5(2)	-6(2)
C53	54(3)	107(5)	70(4)	38(3)	6(3)	4(3)
C54	91(5)	179(7)	62(5)	34(5)	21(4)	35(5)
C55	117(6)	181(8)	63(4)	14(5)	-5(4)	80(6)
C56	56(3)	94(4)	43(3)	6(3)	-5(2)	-6(3)
O20'	50(2)	102(3)	99(3)	29(3)	5(2)	-6(2)
C53'	54(3)	107(5)	70(4)	38(3)	6(3)	4(3)
C54'	91(5)	179(7)	62(5)	34(5)	21(4)	35(5)
C55'	117(6)	181(8)	63(4)	14(5)	-5(4)	80(6)
C56'	56(3)	94(4)	43(3)	6(3)	-5(2)	-6(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 253.

	x	y	z	U(eq)
H1A	1915	9142	2002	39
H2A	1517	8189	1252	68
H2B	1411	8001	2144	68
H2C	1883	7568	1684	68
H3A	2623	8861	2905	71
H3B	2542	7984	2747	71
H3C	2065	8454	3156	71
H4A	2577	10847	1629	45
H5A	1907	10399	2447	81
H5B	2169	11110	2878	81
H5C	2342	10281	3139	81
H6A	3494	11014	2058	105
H6B	3321	10794	2920	105
H6C	3092	11550	2535	105
H7A	3427	8697	2155	47
H8A	4167	9535	2079	91
H8B	4472	8996	1480	91
H8C	4386	8732	2356	91
H9A	3361	7666	1320	88
H9B	3888	7566	1874	88
H9C	3964	7829	996	88
H10A	3418	8207	-207	47
H11A	4187	8998	-76	75
H11B	4371	8819	-944	75
H11C	4399	8177	-297	75
H12A	3227	7611	-1394	100
H12B	3819	7340	-1091	100
H12C	3774	7954	-1764	100
H13A	2682	8520	-2151	47
H14A	3450	9345	-2349	82

H14B	3079	9830	-2934	82
H14C	3238	8985	-3146	82
H15A	1807	8884	-2589	77
H15B	2197	8803	-3325	77
H15C	2055	9616	-2991	77
H16A	1951	8473	106	45
H17A	2501	7412	305	74
H17B	2270	7032	-472	74
H17C	1874	7140	256	74
H18A	1403	8592	-1020	91
H18B	1188	7899	-518	91
H18C	1553	7754	-1270	91
H19A	1818	10582	-1172	44
H20A	1166	9625	-1450	84
H20B	1213	10195	-2161	84
H20C	701	10248	-1587	84
H21A	1512	11817	-990	89
H21B	898	11587	-1235	89
H21C	1378	11576	-1864	89
H22A	619	10181	681	44
H23A	448	9170	-153	79
H23B	3	9161	524	79
H23C	512	8591	549	79
H24A	900	9968	1980	80
H24B	761	9095	1888	80
H24C	276	9702	1852	80
H25A	1658	11761	399	44
H26A	699	11554	282	78
H26B	804	12365	651	78
H26C	626	11680	1193	78
H27A	2071	11930	1623	71
H27B	1483	11895	2033	71
H27C	1632	12587	1484	71
H28A	3228	12435	-232	50
H29A	2321	12798	-531	116
H29B	2646	13497	-167	116

H29C	2221	13034	351	116
H30A	3552	12394	1049	94
H30B	2993	12762	1354	94
H30C	3406	13244	837	94
H31A	3754	10095	-11	43
H32A	3970	10778	1113	97
H32B	4410	11267	648	97
H32C	4519	10394	794	97
H33A	4132	10433	-1204	101
H33B	4623	10195	-629	101
H33C	4504	11062	-796	101
H34A	3167	10755	-1660	46
H35A	3722	11813	-1448	78
H35B	3276	12344	-1859	78
H35C	3609	11744	-2360	78
H36A	2290	10866	-2234	75
H36B	2744	11136	-2839	75
H36C	2387	11741	-2379	75
H37A	-1848	9652	4750	69
H37B	-1426	9083	5162	69
H38A	-1271	9974	6220	76
H38B	-1726	10495	5807	76
H39A	-1031	11438	5642	77
H39B	-1160	11277	6537	77
H40A	-274	11702	6890	60
H40B	-119	11856	6002	60
H41A	672	11625	6803	59
H41B	448	10790	6943	59
H42A	1229	10259	6315	67
H42B	1470	11091	6210	67
H43A	-744	11892	3886	108
H43B	-893	11054	3587	108
H44A	-325	11142	2561	147
H44B	-542	11992	2605	147
H45A	280	12389	2918	104
H45B	507	11549	2787	104

H46A	647	11603	4070	193
H46B	159	12207	4190	193
H43C	-736	10799	3316	108
H43D	-118	10604	3061	108
H44C	-212	11557	2274	147
H44D	-716	11902	2759	147
H45C	-154	12631	3405	104
H45D	339	12349	2858	104
H46C	596	11455	3680	193
H46D	352	12039	4297	193
H43E	-66	10587	2972	108
H43F	546	10925	2942	108
H44E	241	11951	2428	147
H44F	-362	11579	2383	147
H45E	-607	12395	3258	104
H45F	24	12621	3438	104
H46E	-134	12008	4526	193
H46F	-606	11496	4137	193
H47A	4467	11939	6468	90
H47B	5068	11586	6347	90
H48A	5055	12082	5059	100
H48B	4442	12397	5167	100
H49A	4146	11592	4144	93
H49B	4572	12224	3866	93
H50A	4874	11444	2815	86
H50B	4449	10801	3067	86
H51A	5207	10289	2395	88
H51B	5614	10609	3054	88
H52A	5877	9307	3330	85
H52B	5449	9042	2669	85
H53A	3886	9065	5747	92
H53B	3569	8485	5187	92
H54A	2869	9251	5300	133
H54B	3256	9933	5584	133
H55A	3253	10373	4412	145
H55B	2880	9681	4125	145

H56A	3589	9080	3668	77
H56B	3902	9873	3715	77
H53C	3403	10684	4932	92
H53D	3628	10109	5584	92
H54C	2826	9542	5308	133
H54D	2819	9841	4428	133
H55C	3219	8810	4060	145
H55D	3238	8520	4943	145
H56C	4082	8982	5151	77
H56D	4130	8851	4230	77

Table 6. Torsion angles [°] for 253.

P4-Co1-P1-O3	-69.57(9)	P2-Co1-P4-O12	55.72(9)
P2-Co1-P1-O3	48.28(9)	P3-Co1-P4-O12	-69.31(9)
P3-Co1-P1-O3	172.11(8)	O3-P1-O1-C1	140.8(2)
P4-Co1-P1-O2	53.47(10)	O2-P1-O1-C1	42.8(2)
P2-Co1-P1-O2	171.32(9)	Co1-P1-O1-C1	-92.97(19)
P3-Co1-P1-O2	-64.85(10)	O3-P1-O2-C4	132.2(2)
P4-Co1-P1-O1	176.26(8)	O1-P1-O2-C4	-133.0(2)
P2-Co1-P1-O1	-65.88(9)	Co1-P1-O2-C4	0.4(2)
P3-Co1-P1-O1	57.94(9)	O2-P1-O3-C7	48.8(2)
P1-Co1-P2-O5	-178.18(8)	O1-P1-O3-C7	-47.3(2)
P4-Co1-P2-O5	-53.36(9)	Co1-P1-O3-C7	-175.41(18)
P3-Co1-P2-O5	64.82(9)	O5-P2-O4-C10	-139.4(2)
P1-Co1-P2-O6	57.26(10)	O6-P2-O4-C10	-40.2(2)
P4-Co1-P2-O6	-177.92(10)	Co1-P2-O4-C10	93.9(2)
P3-Co1-P2-O6	-59.74(10)	O6-P2-O5-C13	-45.7(2)
P1-Co1-P2-O4	-62.83(9)	O4-P2-O5-C13	49.1(2)
P4-Co1-P2-O4	61.99(9)	Co1-P2-O5-C13	177.90(17)
P3-Co1-P2-O4	-179.82(8)	O5-P2-O6-C16	-114.1(2)
P1-Co1-P3-O8	-48.35(9)	O4-P2-O6-C16	150.3(2)
P4-Co1-P3-O8	-173.98(8)	Co1-P2-O6-C16	18.4(3)
P2-Co1-P3-O8	67.24(9)	O8-P3-O7-C19	-128.8(2)
P1-Co1-P3-O7	-171.46(9)	O9-P3-O7-C19	136.5(2)
P4-Co1-P3-O7	62.91(10)	Co1-P3-O7-C19	2.8(3)
P2-Co1-P3-O7	-55.87(10)	O7-P3-O8-C22	-46.3(2)
P1-Co1-P3-O9	66.51(9)	O9-P3-O8-C22	49.0(2)
P4-Co1-P3-O9	-59.13(9)	Co1-P3-O8-C22	178.41(17)
P2-Co1-P3-O9	-177.90(8)	O8-P3-O9-C25	-145.64(19)
P1-Co1-P4-O10	-73.45(9)	O7-P3-O9-C25	-47.2(2)
P2-Co1-P4-O10	170.28(8)	Co1-P3-O9-C25	87.8(2)
P3-Co1-P4-O10	45.25(9)	O11-P4-O10-C28	45.0(2)
P1-Co1-P4-O11	49.01(10)	O12-P4-O10-C28	-50.4(2)
P2-Co1-P4-O11	-67.26(10)	Co1-P4-O10-C28	-179.39(18)
P3-Co1-P4-O11	167.71(10)	O10-P4-O11-C31	130.5(2)
P1-Co1-P4-O12	171.99(8)	O12-P4-O11-C31	-135.1(2)

Co1-P4-O11-C31	-1.0(3)	O14-K1-O13-C37	-150.6(3)
O10-P4-O12-C34	149.1(2)	O14#1-K1-O13-C37	29.4(3)
O11-P4-O12-C34	51.7(2)	O13#1-K1-O13-C37	8(11)
Co1-P4-O12-C34	-84.4(2)	O15#1-K1-O13-C37	15.1(2)
P1-O1-C1-C2	140.8(2)	O15-K1-O13-C37	-164.9(2)
P1-O1-C1-C3	-98.3(3)	O16-K1-O13-C38	-112.4(4)
P1-O2-C4-C6	-121.8(3)	O16#1-K1-O13-C38	67.6(4)
P1-O2-C4-C5	117.2(2)	O16'1-K1-O13-C38	69.1(5)
P1-O3-C7-C8	-126.1(2)	O16'-K1-O13-C38	-110.9(5)
P1-O3-C7-C9	110.3(3)	O16"#1-K1-O13-C38	66.1(5)
P2-O4-C10-C11	-138.6(2)	O16"-K1-O13-C38	-113.9(5)
P2-O4-C10-C12	101.0(3)	O14-K1-O13-C38	-18.0(2)
P2-O5-C13-C15	139.1(2)	O14#1-K1-O13-C38	162.0(2)
P2-O5-C13-C14	-99.5(3)	O13#1-K1-O13-C38	141(11)
P2-O6-C16-C18	100.7(3)	O15#1-K1-O13-C38	147.8(2)
P2-O6-C16-C17	-137.8(2)	O15-K1-O13-C38	-32.2(2)
P3-O7-C19-C20	114.0(2)	C37-O13-C38-C39	-175.8(3)
P3-O7-C19-C21	-124.5(2)	K1-O13-C38-C39	49.9(4)
P3-O8-C22-C23	124.9(2)	O13-C38-C39-O14	-67.0(4)
P3-O8-C22-C24	-112.0(3)	C38-C39-O14-C40	-178.9(3)
P3-O9-C25-C27	-139.0(2)	C38-C39-O14-K1	49.4(4)
P3-O9-C25-C26	99.6(3)	O16-K1-O14-C39	64.3(5)
P4-O10-C28-C29	113.0(3)	O16#1-K1-O14-C39	-115.7(5)
P4-O10-C28-C30	-123.8(2)	O16'1-K1-O14-C39	-117.0(6)
P4-O11-C31-C32	-109.5(3)	O16'-K1-O14-C39	63.0(6)
P4-O11-C31-C33	129.3(3)	O16"#1-K1-O14-C39	-103.7(5)
P4-O12-C34-C36	138.7(2)	O16"-K1-O14-C39	76.3(5)
P4-O12-C34-C35	-99.7(3)	O14#1-K1-O14-C39	-5(16)
C42#1-C37-O13-C38	180.0(3)	O13#1-K1-O14-C39	162.8(2)
C42#1-C37-O13-K1	-47.1(4)	O13-K1-O14-C39	-17.2(2)
O16-K1-O13-C37	114.9(4)	O15#1-K1-O14-C39	-31.3(3)
O16#1-K1-O13-C37	-65.1(4)	O15-K1-O14-C39	148.7(3)
O16'1-K1-O13-C37	-63.6(5)	O16-K1-O14-C40	-66.1(5)
O16'-K1-O13-C37	116.4(5)	O16#1-K1-O14-C40	113.9(5)
O16"#1-K1-O13-C37	-66.6(5)	O16'1-K1-O14-C40	112.6(6)
O16"-K1-O13-C37	113.4(5)	O16'-K1-O14-C40	-67.4(6)

O16"#1-K1-O14-C40	125.9(5)	O16#1-K1-O16-C43	-142(7)
O16"-K1-O14-C40	-54.1(5)	O16#1-K1-O16-C43	132(19)
O14#1-K1-O14-C40	-136(16)	O16'-K1-O16-C43	-48(19)
O13#1-K1-O14-C40	32.4(2)	O16"#1-K1-O16-C43	-22(3)
O13-K1-O14-C40	-147.6(2)	O16"-K1-O16-C43	158(3)
O15#1-K1-O14-C40	-161.70(19)	O14-K1-O16-C43	-76.5(14)
O15-K1-O14-C40	18.30(19)	O14#1-K1-O16-C43	103.5(14)
C39-O14-C40-C41	177.5(3)	O13#1-K1-O16-C43	164.3(14)
K1-O14-C40-C41	-50.8(3)	O13-K1-O16-C43	-15.7(14)
O14-C40-C41-O15	67.3(4)	O15#1-K1-O16-C43	43.1(14)
C40-C41-O15-C42	-178.2(3)	O15-K1-O16-C43	-136.9(14)
C40-C41-O15-K1	-48.7(3)	O16#1-K1-O16-C46	21(8)
O16-K1-O15-C41	109.7(4)	O16#1-K1-O16-C46	-64(20)
O16#1-K1-O15-C41	-70.3(4)	O16'-K1-O16-C46	116(20)
O16"#1-K1-O15-C41	-73.1(6)	O16"#1-K1-O16-C46	141(2)
O16'-K1-O15-C41	106.9(6)	O16"-K1-O16-C46	-39(2)
O16"#1-K1-O15-C41	-57.0(5)	O14-K1-O16-C46	86.5(16)
O16"-K1-O15-C41	123.0(5)	O14#1-K1-O16-C46	-93.5(16)
O14-K1-O15-C41	16.59(19)	O13#1-K1-O16-C46	-32.7(16)
O14#1-K1-O15-C41	-163.41(19)	O13-K1-O16-C46	147.3(16)
O13#1-K1-O15-C41	-149.1(2)	O15#1-K1-O16-C46	-153.9(16)
O13-K1-O15-C41	30.9(2)	O15-K1-O16-C46	26.1(16)
O15#1-K1-O15-C41	-154(12)	C46-O16-C43-C44	53.4(15)
O16-K1-O15-C42	-121.1(4)	K1-O16-C43-C44	-140.5(12)
O16#1-K1-O15-C42	58.9(4)	O16-C43-C44-C45	-35.6(16)
O16#1-K1-O15-C42	56.1(6)	C43-C44-C45-C46	5.4(18)
O16'-K1-O15-C42	-123.9(6)	C43-O16-C46-C45	-52.0(18)
O16"#1-K1-O15-C42	72.2(5)	K1-O16-C46-C45	141.1(12)
O16"-K1-O15-C42	-107.8(5)	C44-C45-C46-O16	27(2)
O14-K1-O15-C42	145.8(2)	O16-K1-O16'-C43'	70(18)
O14#1-K1-O15-C42	-34.2(2)	O16#1-K1-O16'-C43'	-110(18)
O13#1-K1-O15-C42	-19.9(2)	O16#1-K1-O16'-C43'	-87(10)
O13-K1-O15-C42	160.1(2)	O16"#1-K1-O16'-C43'	-89(3)
O15#1-K1-O15-C42	-25(14)	O16"-K1-O16'-C43'	91(3)
C41-O15-C42-C37#1	-178.7(3)	O14-K1-O16'-C43'	-139.4(16)
K1-O15-C42-C37#1	51.9(3)	O14#1-K1-O16'-C43'	40.5(16)

O13#1-K1-O16'-C43'	101.6(16)	O16'-K1-O16"-C46"	24(2)
O13-K1-O16'-C43'	-78.4(16)	O16"#1-K1-O16"-C46"	3(40)
O15#1-K1-O16'-C43'	-20.1(16)	O14-K1-O16"-C46"	-27.9(19)
O15-K1-O16'-C43'	159.9(16)	O14#1-K1-O16"-C46"	152.1(19)
O16-K1-O16'-C46'	-52(19)	O13#1-K1-O16"-C46"	-146.2(19)
O16#1-K1-O16'-C46'	128(19)	O13-K1-O16"-C46"	33.8(19)
O16"#1-K1-O16'-C46'	151(13)	O15#1-K1-O16"-C46"	94.4(19)
O16"#1-K1-O16'-C46'	149(3)	O15-K1-O16"-C46"	-85.6(19)
O16"-K1-O16'-C46'	-31(3)	C46"-O16"-C43"-C44"	21(3)
O14-K1-O16'-C46'	99(2)	K1-O16"-C43"-C44"	148(2)
O14#1-K1-O16'-C46'	-81(2)	O16"-C43"-C44"-C45"	-5(4)
O13#1-K1-O16'-C46'	-20(2)	C43"-C44"-C45"-C46"	-13(4)
O13-K1-O16'-C46'	160(2)	C43"-O16"-C46"-C45"	-29(3)
O15#1-K1-O16'-C46'	-142(2)	K1-O16"-C46"-C45"	-165.1(19)
O15-K1-O16'-C46'	38(2)	C43"-O16"-C46"-K1	136(2)
C46'-O16'-C43'-C44'	-37(3)	C44"-C45"-C46"-O16"	26(4)
K1-O16'-C43'-C44'	-171.6(16)	C44"-C45"-C46"-K1	2(6)
O16'-C43'-C44'-C45'	20(3)	O16-K1-C46"-O16"	-35(3)
C43'-C44'-C45'-C46'	6(3)	O16#1-K1-C46"-O16"	145(3)
C43'-O16'-C46'-C45'	41(3)	O16"#1-K1-C46"-O16"	136(4)
K1-O16'-C46'-C45'	168.9(16)	O16'-K1-C46"-O16"	-44(4)
C44'-C45'-C46'-O16'	-29(3)	O16"#1-K1-C46"-O16"	180.000(14)
O16-K1-O16"-C43"	-97(3)	O14-K1-C46"-O16"	151.8(19)
O16#1-K1-O16"-C43"	83(3)	O14#1-K1-C46"-O16"	-28.2(19)
O16"#1-K1-O16"-C43"	79(3)	O13#1-K1-C46"-O16"	34.3(19)
O16'-K1-O16"-C43"	-101(3)	O13-K1-C46"-O16"	-145.7(19)
O16"#1-K1-O16"-C43"	-122(36)	O15#1-K1-C46"-O16"	-90.1(19)
O14-K1-O16"-C43"	-152.6(17)	O15-K1-C46"-O16"	89.9(19)
O14#1-K1-O16"-C43"	27.4(17)	O16-K1-C46"-C45"	-3(4)
O13#1-K1-O16"-C43"	89.1(17)	O16#1-K1-C46"-C45"	177(4)
O13-K1-O16"-C43"	-90.9(17)	O16"#1-K1-C46"-C45"	167(4)
O15#1-K1-O16"-C43"	-30.3(17)	O16'-K1-C46"-C45"	-13(4)
O15-K1-O16"-C43"	149.7(17)	O16"#1-K1-C46"-C45"	-148(4)
O16-K1-O16"-C46"	28(2)	O16"-K1-C46"-C45"	32(4)
O16#1-K1-O16"-C46"	-152(2)	O14-K1-C46"-C45"	-177(5)
O16"#1-K1-O16"-C46"	-156(2)	O14#1-K1-C46"-C45"	3(5)

O13#1-K1-C46"-C45"	66(5)	O20-K2-O18-C50	-53.0(3)
O13-K1-C46"-C45"	-114(5)	O17#2-K2-O18-C50	30.7(3)
O15#1-K1-C46"-C45"	-59(5)	O17-K2-O18-C50	-149.3(3)
O15-K1-C46"-C45"	121(5)	O19#2-K2-O18-C50	-163.1(2)
C52#2-C47-O17-C48	178.2(3)	O19-K2-O18-C50	16.9(2)
C52#2-C47-O17-K2	-53.6(3)	O18#2-K2-O18-C50	95(11)
O20#2-K2-O17-C48	79.6(4)	C56'-K2-O18-C50	-55.0(5)
O20'-K2-O17-C48	-100.4(4)	C56'#2-K2-O18-C50	125.0(5)
O20#2-K2-O17-C48	66.3(3)	O20#2-K2-O18-C49	-115.2(4)
O20-K2-O17-C48	-113.7(3)	O20'-K2-O18-C49	64.8(4)
O17#2-K2-O17-C48	-169(26)	O20#2-K2-O18-C49	-99.9(3)
O19#2-K2-O17-C48	148.7(3)	O20-K2-O18-C49	80.1(3)
O19-K2-O17-C48	-31.3(3)	O17#2-K2-O18-C49	163.8(3)
O18-K2-O17-C48	-17.8(3)	O17-K2-O18-C49	-16.2(3)
O18#2-K2-O17-C48	162.2(3)	O19#2-K2-O18-C49	-30.0(3)
C56'-K2-O17-C48	-115.5(5)	O19-K2-O18-C49	150.0(3)
C56'#2-K2-O17-C48	64.5(5)	O18#2-K2-O18-C49	-132(11)
O20#2-K2-O17-C47	-48.5(4)	C56'-K2-O18-C49	78.1(5)
O20'-K2-O17-C47	131.5(4)	C56'#2-K2-O18-C49	-101.9(5)
O20#2-K2-O17-C47	-61.8(3)	C49-O18-C50-C51	178.9(3)
O20-K2-O17-C47	118.2(3)	K2-O18-C50-C51	-47.9(4)
O17#2-K2-O17-C47	63(26)	O18-C50-C51-O19	62.9(4)
O19#2-K2-O17-C47	20.6(2)	C50-C51-O19-C52	176.1(3)
O19-K2-O17-C47	-159.4(2)	C50-C51-O19-K2	-48.7(4)
O18-K2-O17-C47	-145.9(3)	O20#2-K2-O19-C52	52.9(4)
O18#2-K2-O17-C47	34.1(3)	O20'-K2-O19-C52	-127.1(4)
C56'-K2-O17-C47	116.5(5)	O20#2-K2-O19-C52	81.3(3)
C56'#2-K2-O17-C47	-63.5(5)	O20-K2-O19-C52	-98.7(3)
C47-O17-C48-C49	178.4(3)	O17#2-K2-O19-C52	-14.3(2)
K2-O17-C48-C49	51.0(4)	O17-K2-O19-C52	165.7(2)
O17-C48-C49-O18	-67.2(5)	O19#2-K2-O19-C52	172(100)
C48-C49-O18-C50	-178.1(3)	O18-K2-O19-C52	151.9(3)
C48-C49-O18-K2	47.5(4)	O18#2-K2-O19-C52	-28.1(3)
O20#2-K2-O18-C50	111.7(4)	C56'-K2-O19-C52	-99.1(4)
O20'-K2-O18-C50	-68.3(4)	C56'#2-K2-O19-C52	80.9(4)
O20#2-K2-O18-C50	127.0(3)	O20#2-K2-O19-C51	-81.5(4)

O20'-K2-O19-C51	98.5(4)	O20-C53-C54-C55	19.3(9)
O20#2-K2-O19-C51	-53.1(2)	C53-C54-C55-C56	-1.4(10)
O20-K2-O19-C51	126.9(2)	C53-O20-C56-C55	28.8(7)
O17#2-K2-O19-C51	-148.7(3)	K2-O20-C56-C55	-104.4(5)
O17-K2-O19-C51	31.3(3)	C54-C55-C56-O20	-16.9(9)
O19#2-K2-O19-C51	38(45)	O20#2-K2-O20'-C53'	-169(84)
O18-K2-O19-C51	17.5(2)	O20#2-K2-O20'-C53'	-71.3(13)
O18#2-K2-O19-C51	-162.5(2)	O20-K2-O20'-C53'	108.7(13)
C56'-K2-O19-C51	126.4(3)	O17#2-K2-O20'-C53'	137.8(10)
C56#2-K2-O19-C51	-53.6(3)	O17-K2-O20'-C53'	-42.2(10)
C51-O19-C52-C47#2	-177.2(3)	O19#2-K2-O20'-C53'	14.3(11)
K2-O19-C52-C47#2	46.3(4)	O19-K2-O20'-C53'	-165.7(11)
O20#2-K2-O20-C53	86.0(7)	O18-K2-O20'-C53'	-105.1(11)
O20'-K2-O20-C53	-94.0(7)	O18#2-K2-O20'-C53'	74.9(11)
O20#2-K2-O20-C53	66(24)	C56'-K2-O20'-C53'	104.1(15)
O17#2-K2-O20-C53	114.6(3)	C56#2-K2-O20'-C53'	-75.9(15)
O17-K2-O20-C53	-65.4(3)	O20#2-K2-O20'-C56'	87(86)
O19#2-K2-O20-C53	-2.8(3)	O20#2-K2-O20'-C56'	-175.3(11)
O19-K2-O20-C53	177.2(3)	O20-K2-O20'-C56'	4.7(11)
O18-K2-O20-C53	-127.5(3)	O17#2-K2-O20'-C56'	33.8(11)
O18#2-K2-O20-C53	52.5(3)	O17-K2-O20'-C56'	-146.2(11)
C56'-K2-O20-C53	-14(8)	O19#2-K2-O20'-C56'	-89.7(11)
C56#2-K2-O20-C53	166(8)	O19-K2-O20'-C56'	90.3(11)
O20#2-K2-O20-C56	-146.6(6)	O18-K2-O20'-C56'	150.8(11)
O20'-K2-O20-C56	33.4(6)	O18#2-K2-O20'-C56'	-29.2(11)
O20#2-K2-O20-C56	-166(24)	C56#2-K2-O20'-C56'	179.999(2)
O17#2-K2-O20-C56	-118.0(4)	C56'-O20'-C53'-C54'	-47.6(18)
O17-K2-O20-C56	62.0(4)	K2-O20'-C53'-C54'	-145.9(13)
O19#2-K2-O20-C56	124.5(3)	O20'-C53'-C54'-C55'	30(2)
O19-K2-O20-C56	-55.5(3)	C53'-C54'-C55'-C56'	-1(3)
O18-K2-O20-C56	-0.1(4)	C53'-O20'-C56'-C55'	46.9(19)
O18#2-K2-O20-C56	179.9(4)	K2-O20'-C56'-C55'	166.6(15)
C56'-K2-O20-C56	114(8)	C53'-O20'-C56'-K2	-119.7(12)
C56#2-K2-O20-C56	-66(8)	C54'-C55'-C56'-O20'	-28(2)
C56-O20-C53-C54	-30.1(7)	C54'-C55'-C56'-K2	7(5)
K2-O20-C53-C54	103.4(5)	O20#2-K2-C56'-O20'	180.001(2)

O20#2-K2-C56'-O20'	85(8)	O20'-K2-C56'-C55'	-40(4)
O20-K2-C56'-O20'	-95(8)	O20#2-K2-C56'-C55'	45(11)
O17#2-K2-C56'-O20'	-146.9(11)	O20-K2-C56'-C55'	-135(11)
O17-K2-C56'-O20'	33.1(11)	O17#2-K2-C56'-C55'	173(4)
O19#2-K2-C56'-O20'	95.3(10)	O17-K2-C56'-C55'	-7(4)
O19-K2-C56'-O20'	-84.7(10)	O19#2-K2-C56'-C55'	56(4)
O18-K2-C56'-O20'	-28.9(11)	O19-K2-C56'-C55'	-124(4)
O18#2-K2-C56'-O20'	151.1(11)	O18-K2-C56'-C55'	-69(4)
C56'#2-K2-C56'-O20'	-139(24)	O18#2-K2-C56'-C55'	111(4)
O20'#2-K2-C56'-C55'	140(4)	C56'#2-K2-C56'-C55'	-179(26)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 -x+1,-y+2,-z+1

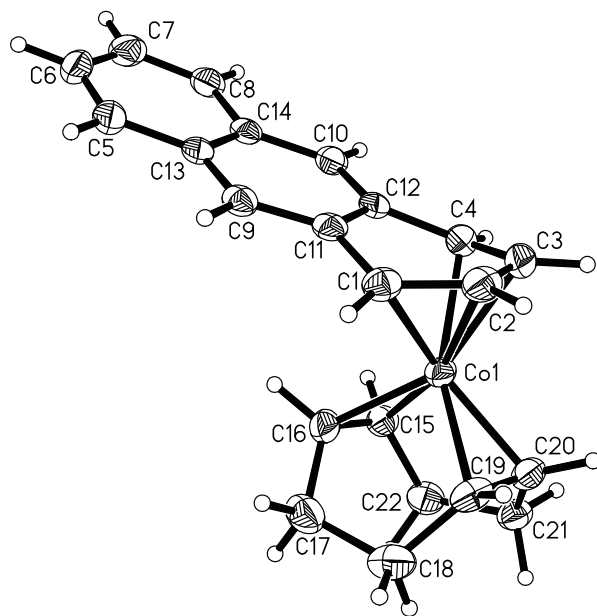
REFERENCE NUMBER: 04060m [8]

CRYSTAL STRUCTURE REPORT

$C_{40} H_{58} Co K N_2 O_6$

Report prepared for:
William Brennessel

April 8, 2004



Ben Kucera

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Data collection

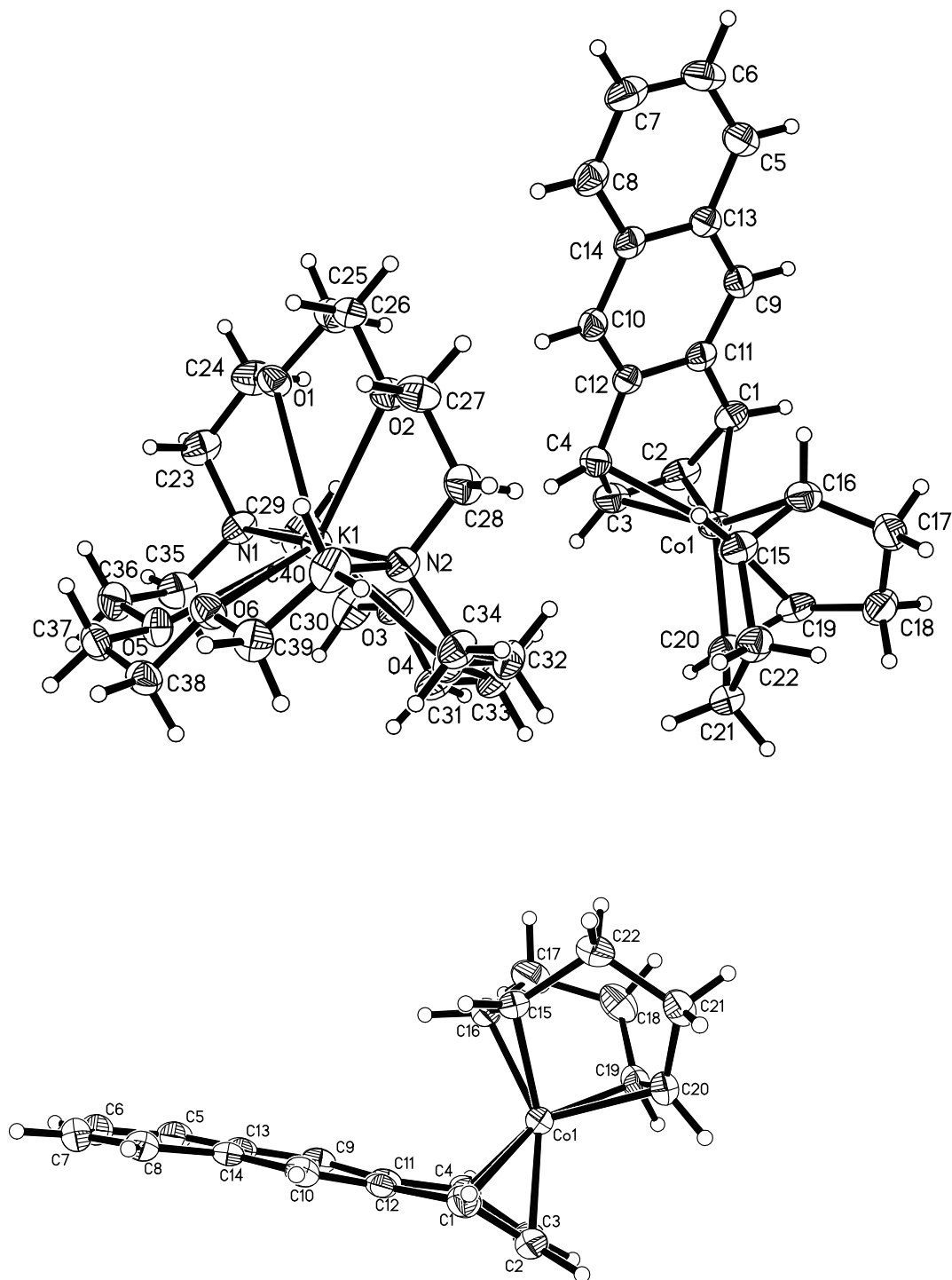
A crystal (approximate dimensions 0.50 x 0.35 x 0.10 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K. A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 48 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 30 seconds and a detector distance of 4.926 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).¹ Final cell constants were calculated from the xyz centroids of 3592 strong reflections from the actual data collection after integration (SAINT).² Please refer to Table 1 for additional crystal and refinement information.

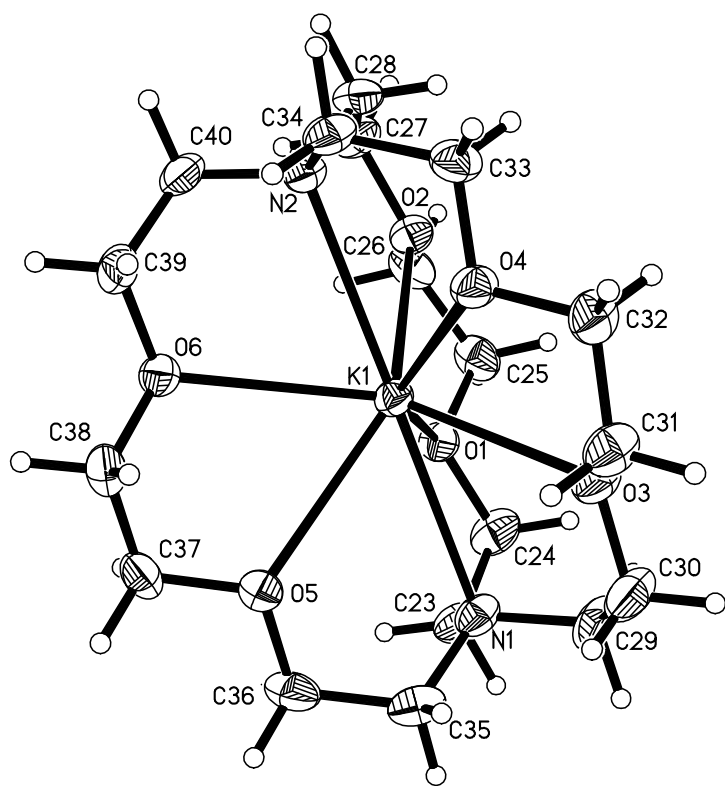
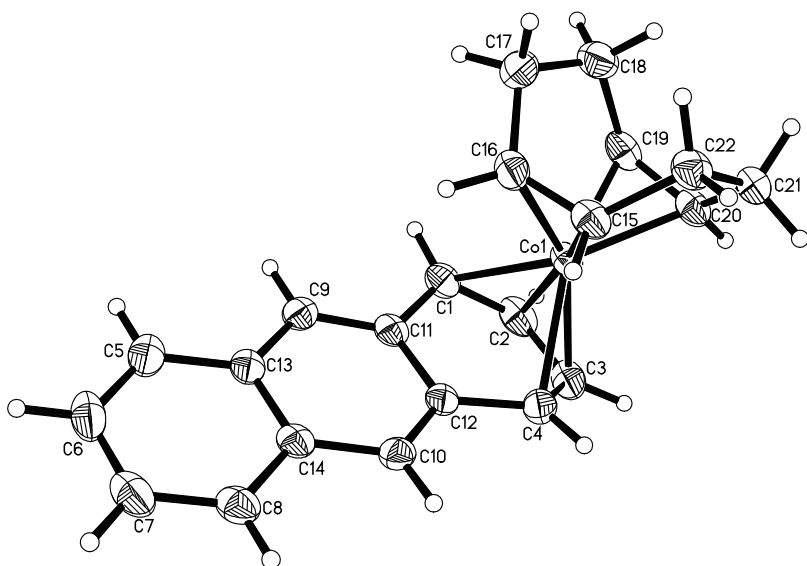
Structure solution and refinement

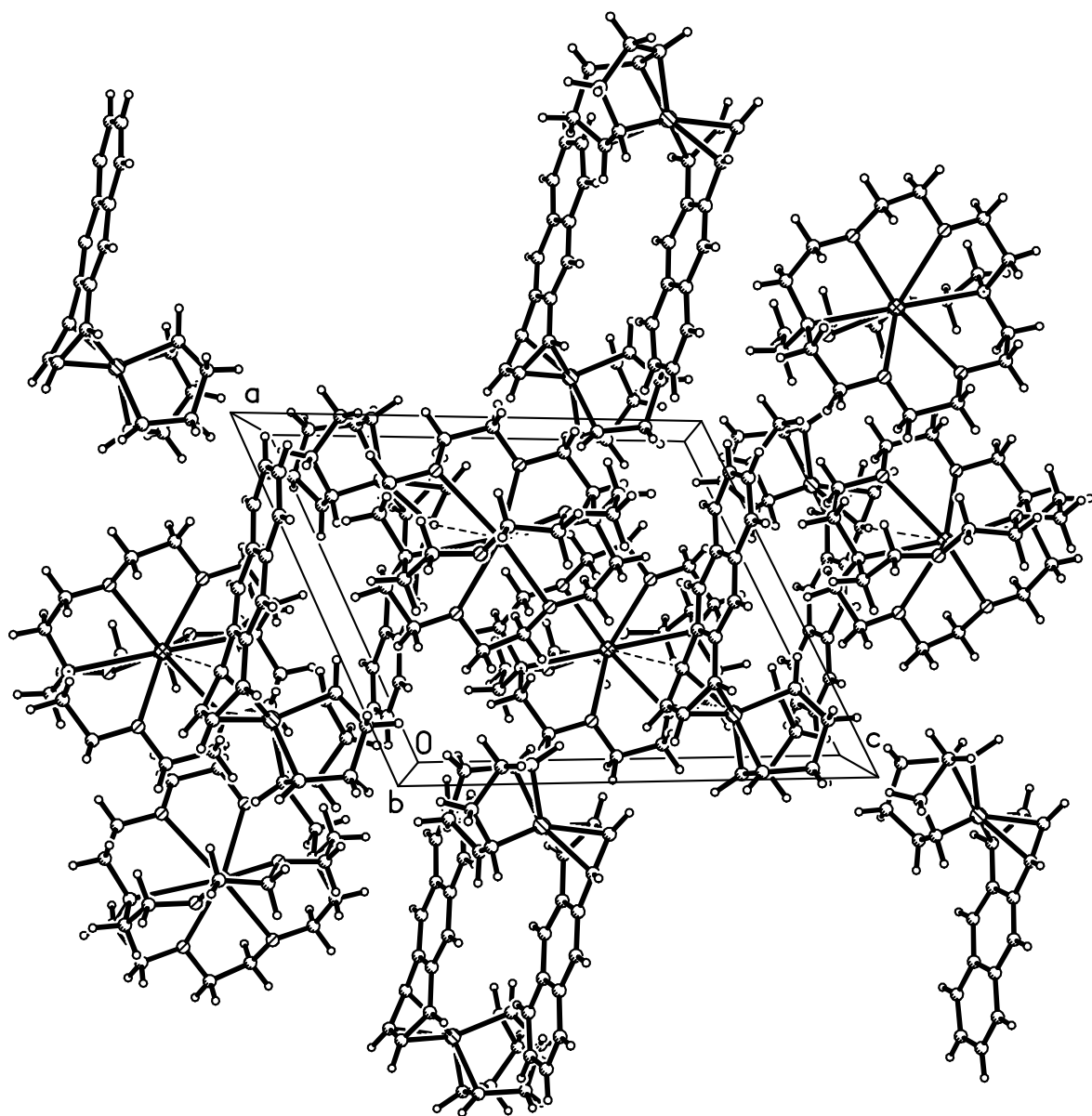
The structure was solved using SHELXS-97³ and refined using SHELXL-97.³ The space group P-1 was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms (except those on carbons attached to the Cobalt center) were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The remaining hydrogens were found from the difference map and refined with individual isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0359$ and $wR2 = 0.0994$ (F^2 , all data).

Structure description

The structure is the one suggested.







Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include Ben Kucera as a coauthor or 2)acknowledge Ben Kucera, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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- ¹ An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
² SAINT V6.2, Bruker Analytical X-Ray Systems, Madison, WI (2001).
³ SHELXTL V6.10, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

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

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2 (F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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

Table 1. Crystal data and structure refinement for 04060m.

Identification code	04060m	
Empirical formula	C40 H58 Co K N2 O6	
Formula weight	760.91	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	$a = 12.1042(10)$ Å	$\alpha = 108.664(2)^\circ$
	$b = 13.1580(11)$ Å	$\beta = 107.142(2)^\circ$
	$c = 14.4109(13)$ Å	$\gamma = 106.915(2)^\circ$
Volume	1880.3(3) Å ³	
<i>Z</i>	2	
Density (calculated)	1.344 Mg/m ³	
Absorption coefficient	0.616 mm ⁻¹	
<i>F</i> (000)	812	
Crystal color, morphology	Metallic red-violet, Plate	
Crystal size	0.50 x 0.35 x 0.10 mm ³	
Theta range for data collection	1.65 to 27.50°	
Index ranges	$-15 \leq h \leq 15$, $-17 \leq k \leq 17$, $-18 \leq l \leq 18$	
Reflections collected	20765	
Independent reflections	8487 [<i>R</i> (int) = 0.0355]	
Observed reflections	6724	
Completeness to theta = 27.50°	98.2%	
Absorption correction	Multi-scan	
Max. and min. transmission	1.000000 and 0.883859	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	8487 / 0 / 451	
Goodness-of-fit on <i>F</i> ²	1.015	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0359, <i>wR</i> 2 = 0.0890	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0518, <i>wR</i> 2 = 0.0994	
Largest diff. peak and hole	0.390 and -0.218 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04060m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	8429(1)	4229(1)	2293(1)	25(1)
K1	6626(1)	8292(1)	4386(1)	23(1)
O1	4685(1)	6894(1)	4743(1)	28(1)
O2	4499(1)	6283(1)	2639(1)	28(1)
O3	8751(1)	7999(1)	5550(1)	34(1)
O4	8542(1)	8335(1)	3679(1)	29(1)
O5	7287(1)	10554(1)	6025(1)	31(1)
O6	6154(1)	10064(1)	3828(1)	28(1)
N1	7182(2)	8615(1)	6611(1)	29(1)
N2	6095(1)	8006(1)	2174(1)	25(1)
C1	7480(2)	2666(2)	2431(2)	29(1)
C2	8383(2)	3657(2)	3435(2)	33(1)
C3	8193(2)	4703(2)	3693(2)	34(1)
C4	7120(2)	4677(2)	2941(2)	29(1)
C5	2834(2)	271(2)	-40(2)	33(1)
C6	1622(2)	203(2)	-433(2)	39(1)
C7	1426(2)	1233(2)	-146(2)	39(1)
C8	2453(2)	2323(2)	529(2)	32(1)
C9	5157(2)	1446(2)	1166(1)	26(1)
C10	4784(2)	3521(2)	1721(1)	26(1)
C11	6174(2)	2509(2)	1930(1)	24(1)
C12	5980(2)	3580(2)	2202(1)	23(1)
C13	3907(2)	1367(2)	682(1)	25(1)
C14	3709(2)	2422(2)	966(1)	25(1)
C15	7915(2)	4616(2)	1027(1)	28(1)
C16	7690(2)	3424(2)	662(1)	31(1)
C17	8567(2)	2951(2)	291(2)	40(1)
C18	9966(2)	3622(2)	1140(2)	40(1)
C19	10093(2)	4249(2)	2284(2)	32(1)
C20	10209(2)	5423(2)	2725(2)	30(1)
C21	10215(2)	6148(2)	2090(2)	31(1)

C22	9015(2)	5525(2)	1009(2)	32(1)
C23	5947(2)	8107(2)	6654(2)	36(1)
C24	5049(2)	6886(2)	5775(2)	39(1)
C25	3906(2)	5722(2)	3889(2)	36(1)
C26	3437(2)	5764(2)	2831(2)	32(1)
C27	4096(2)	6225(2)	1581(2)	34(1)
C28	5254(2)	6752(2)	1408(2)	32(1)
C29	7964(2)	7992(2)	6886(2)	43(1)
C30	9129(2)	8307(2)	6671(2)	44(1)
C31	9832(2)	8462(2)	5360(2)	36(1)
C32	9469(2)	7978(2)	4174(2)	34(1)
C33	8191(2)	7884(2)	2547(2)	32(1)
C34	7297(2)	8354(2)	2055(2)	31(1)
C35	7856(2)	9884(2)	7376(2)	38(1)
C36	7266(2)	10639(2)	7030(2)	37(1)
C37	6762(2)	11280(2)	5683(2)	32(1)
C38	6883(2)	11241(2)	4677(2)	31(1)
C39	6143(2)	10028(2)	2824(2)	34(1)
C40	5465(2)	8764(2)	1957(2)	32(1)

Table 3. Bond lengths [Å] and angles [°] for 04060m.

Co(1)-C(19)	2.0105(19)	C(1)-C(2)	1.421(3)
Co(1)-C(16)	2.0156(18)	C(1)-C(11)	1.451(3)
Co(1)-C(2)	2.0235(19)	C(1)-H(1)	1.0000
Co(1)-C(15)	2.0219(18)	C(2)-C(3)	1.411(3)
Co(1)-C(20)	2.0282(18)	C(2)-H(2)	1.0000
Co(1)-C(3)	2.0439(19)	C(3)-C(4)	1.409(3)
Co(1)-C(1)	2.1470(19)	C(3)-H(3)	1.0000
Co(1)-C(4)	2.1894(19)	C(4)-C(12)	1.454(2)
K(1)-O(4)	2.7879(13)	C(4)-H(4)	1.0000
K(1)-O(2)	2.8126(13)	C(5)-C(6)	1.372(3)
K(1)-O(1)	2.8233(13)	C(5)-C(13)	1.414(3)
K(1)-O(3)	2.8328(13)	C(5)-H(5)	0.9500
K(1)-O(5)	2.8427(13)	C(6)-C(7)	1.397(3)
K(1)-O(6)	2.8488(13)	C(6)-H(6)	0.9500
K(1)-N(2)	2.9327(15)	C(7)-C(8)	1.380(3)
K(1)-N(1)	2.9330(15)	C(7)-H(7)	0.9500
O(1)-C(25)	1.427(2)	C(8)-C(14)	1.411(3)
O(1)-C(24)	1.426(2)	C(8)-H(8)	0.9500
O(2)-C(26)	1.420(2)	C(9)-C(11)	1.378(3)
O(2)-C(27)	1.427(2)	C(9)-C(13)	1.423(3)
O(3)-C(31)	1.418(2)	C(9)-H(9)	0.9500
O(3)-C(30)	1.422(2)	C(10)-C(12)	1.375(3)
O(4)-C(33)	1.421(2)	C(10)-C(14)	1.426(2)
O(4)-C(32)	1.427(2)	C(10)-H(10)	0.9500
O(5)-C(37)	1.423(2)	C(11)-C(12)	1.445(3)
O(5)-C(36)	1.426(2)	C(13)-C(14)	1.428(3)
O(6)-C(38)	1.425(2)	C(15)-C(16)	1.397(3)
O(6)-C(39)	1.427(2)	C(15)-C(22)	1.523(3)
N(1)-C(29)	1.471(3)	C(15)-H(15)	1.0000
N(1)-C(35)	1.472(3)	C(16)-C(17)	1.520(3)
N(1)-C(23)	1.479(2)	C(16)-H(16)	1.0000
N(2)-C(34)	1.472(2)	C(17)-C(18)	1.536(3)
N(2)-C(40)	1.475(2)	C(17)-H(17A)	0.9900
N(2)-C(28)	1.473(2)	C(17)-H(17B)	0.9900

C(18)-C(19)	1.526(3)	C(32)-H(32B)	0.9900
C(18)-H(18A)	0.9900	C(33)-C(34)	1.507(3)
C(18)-H(18B)	0.9900	C(33)-H(33A)	0.9900
C(19)-C(20)	1.415(3)	C(33)-H(33B)	0.9900
C(19)-H(19)	1.0000	C(34)-H(34A)	0.9900
C(20)-C(21)	1.519(3)	C(34)-H(34B)	0.9900
C(20)-H(20)	1.0000	C(35)-C(36)	1.505(3)
C(21)-C(22)	1.537(3)	C(35)-H(35A)	0.9900
C(21)-H(21A)	0.9900	C(35)-H(35B)	0.9900
C(21)-H(21B)	0.9900	C(36)-H(36A)	0.9900
C(22)-H(22A)	0.9900	C(36)-H(36B)	0.9900
C(22)-H(22B)	0.9900	C(37)-C(38)	1.486(3)
C(23)-C(24)	1.495(3)	C(37)-H(37A)	0.9900
C(23)-H(23A)	0.9900	C(37)-H(37B)	0.9900
C(23)-H(23B)	0.9900	C(38)-H(38A)	0.9900
C(24)-H(24A)	0.9900	C(38)-H(38B)	0.9900
C(24)-H(24B)	0.9900	C(39)-C(40)	1.507(3)
C(25)-C(26)	1.488(3)	C(39)-H(39A)	0.9900
C(25)-H(25A)	0.9900	C(39)-H(39B)	0.9900
C(25)-H(25B)	0.9900	C(40)-H(40A)	0.9900
C(26)-H(26A)	0.9900	C(40)-H(40B)	0.9900
C(26)-H(26B)	0.9900		
C(27)-C(28)	1.503(3)	C(19)-Co(1)-C(16)	86.67(8)
C(27)-H(27A)	0.9900	C(19)-Co(1)-C(2)	100.01(8)
C(27)-H(27B)	0.9900	C(16)-Co(1)-C(2)	134.24(8)
C(28)-H(28A)	0.9900	C(19)-Co(1)-C(15)	95.79(8)
C(28)-H(28B)	0.9900	C(16)-Co(1)-C(15)	40.47(8)
C(29)-C(30)	1.502(3)	C(2)-Co(1)-C(15)	163.06(8)
C(29)-H(29A)	0.9900	C(19)-Co(1)-C(20)	41.02(8)
C(29)-H(29B)	0.9900	C(16)-Co(1)-C(20)	103.19(8)
C(30)-H(30A)	0.9900	C(2)-Co(1)-C(20)	111.32(8)
C(30)-H(30B)	0.9900	C(15)-Co(1)-C(20)	84.71(8)
C(31)-C(32)	1.490(3)	C(19)-Co(1)-C(3)	121.73(8)
C(31)-H(31A)	0.9900	C(16)-Co(1)-C(3)	150.49(8)
C(31)-H(31B)	0.9900	C(2)-Co(1)-C(3)	40.60(8)
C(32)-H(32A)	0.9900	C(15)-Co(1)-C(3)	132.25(8)

C(20)-Co(1)-C(3)	104.05(8)	O(2)-K(1)-N(1)	119.84(4)
C(19)-Co(1)-C(1)	107.38(8)	O(1)-K(1)-N(1)	62.12(4)
C(16)-Co(1)-C(1)	94.94(8)	O(3)-K(1)-N(1)	60.39(4)
C(2)-Co(1)-C(1)	39.71(8)	O(5)-K(1)-N(1)	60.59(4)
C(15)-Co(1)-C(1)	128.68(7)	O(6)-K(1)-N(1)	118.15(4)
C(20)-Co(1)-C(1)	140.79(7)	N(2)-K(1)-N(1)	179.14(5)
C(3)-Co(1)-C(1)	70.44(8)	C(25)-O(1)-C(24)	111.08(15)
C(19)-Co(1)-C(4)	158.20(8)	C(25)-O(1)-K(1)	114.61(10)
C(16)-Co(1)-C(4)	114.46(7)	C(24)-O(1)-K(1)	116.81(11)
C(2)-Co(1)-C(4)	69.66(8)	C(26)-O(2)-C(27)	111.16(14)
C(15)-Co(1)-C(4)	97.32(7)	C(26)-O(2)-K(1)	117.75(10)
C(20)-Co(1)-C(4)	123.33(8)	C(27)-O(2)-K(1)	119.80(10)
C(3)-Co(1)-C(4)	38.68(7)	C(31)-O(3)-C(30)	110.21(15)
C(1)-Co(1)-C(4)	77.41(7)	C(31)-O(3)-K(1)	112.90(11)
O(4)-K(1)-O(2)	101.76(4)	C(30)-O(3)-K(1)	119.94(11)
O(4)-K(1)-O(1)	145.22(4)	C(33)-O(4)-C(32)	110.36(14)
O(2)-K(1)-O(1)	59.50(4)	C(33)-O(4)-K(1)	118.25(10)
O(4)-K(1)-O(3)	60.23(4)	C(32)-O(4)-K(1)	117.39(11)
O(2)-K(1)-O(3)	118.86(4)	C(37)-O(5)-C(36)	110.77(15)
O(1)-K(1)-O(3)	101.09(4)	C(37)-O(5)-K(1)	116.49(10)
O(4)-K(1)-O(5)	111.06(4)	C(36)-O(5)-K(1)	118.62(11)
O(2)-K(1)-O(5)	141.39(4)	C(38)-O(6)-C(39)	110.78(14)
O(1)-K(1)-O(5)	99.06(4)	C(38)-O(6)-K(1)	114.49(10)
O(3)-K(1)-O(5)	95.40(4)	C(39)-O(6)-K(1)	117.57(10)
O(4)-K(1)-O(6)	95.65(4)	C(29)-N(1)-C(35)	110.25(17)
O(2)-K(1)-O(6)	98.59(4)	C(29)-N(1)-C(23)	110.31(16)
O(1)-K(1)-O(6)	115.01(4)	C(35)-N(1)-C(23)	109.03(15)
O(3)-K(1)-O(6)	137.86(4)	C(29)-N(1)-K(1)	109.20(11)
O(5)-K(1)-O(6)	59.35(4)	C(35)-N(1)-K(1)	110.51(11)
O(4)-K(1)-N(2)	61.33(4)	C(23)-N(1)-K(1)	107.50(11)
O(2)-K(1)-N(2)	60.99(4)	C(34)-N(2)-C(40)	109.54(15)
O(1)-K(1)-N(2)	118.61(4)	C(34)-N(2)-C(28)	109.38(14)
O(3)-K(1)-N(2)	119.58(4)	C(40)-N(2)-C(28)	110.16(14)
O(5)-K(1)-N(2)	118.65(4)	C(34)-N(2)-K(1)	109.85(10)
O(6)-K(1)-N(2)	61.23(4)	C(40)-N(2)-K(1)	109.11(10)
O(4)-K(1)-N(1)	118.40(4)	C(28)-N(2)-K(1)	108.78(11)

C(2)-C(1)-C(11)	121.32(17)	C(11)-C(9)-C(13)	121.70(16)
C(2)-C(1)-Co(1)	65.46(11)	C(11)-C(9)-H(9)	119.1
C(11)-C(1)-Co(1)	98.62(12)	C(13)-C(9)-H(9)	119.1
C(2)-C(1)-H(1)	118.4	C(12)-C(10)-C(14)	121.78(17)
C(11)-C(1)-H(1)	118.4	C(12)-C(10)-H(10)	119.1
Co(1)-C(1)-H(1)	118.4	C(14)-C(10)-H(10)	119.1
C(3)-C(2)-C(1)	117.27(17)	C(9)-C(11)-C(12)	119.02(16)
C(3)-C(2)-Co(1)	70.48(11)	C(9)-C(11)-C(1)	124.85(17)
C(1)-C(2)-Co(1)	74.83(11)	C(12)-C(11)-C(1)	115.92(16)
C(3)-C(2)-H(2)	121.3	C(10)-C(12)-C(11)	119.89(16)
C(1)-C(2)-H(2)	121.3	C(10)-C(12)-C(4)	124.22(17)
Co(1)-C(2)-H(2)	121.3	C(11)-C(12)-C(4)	115.79(16)
C(4)-C(3)-C(2)	117.45(17)	C(5)-C(13)-C(9)	122.40(17)
C(4)-C(3)-Co(1)	76.25(11)	C(5)-C(13)-C(14)	118.29(17)
C(2)-C(3)-Co(1)	68.92(11)	C(9)-C(13)-C(14)	119.26(16)
C(4)-C(3)-H(3)	121.2	C(8)-C(14)-C(10)	123.01(17)
C(2)-C(3)-H(3)	121.2	C(8)-C(14)-C(13)	118.66(17)
Co(1)-C(3)-H(3)	121.2	C(10)-C(14)-C(13)	118.26(16)
C(3)-C(4)-C(12)	121.66(17)	C(16)-C(15)-C(22)	122.13(17)
C(3)-C(4)-Co(1)	65.07(11)	C(16)-C(15)-Co(1)	69.52(11)
C(12)-C(4)-Co(1)	97.69(11)	C(22)-C(15)-Co(1)	114.20(12)
C(3)-C(4)-H(4)	118.5	C(16)-C(15)-H(15)	114.4
C(12)-C(4)-H(4)	118.5	C(22)-C(15)-H(15)	114.4
Co(1)-C(4)-H(4)	118.5	Co(1)-C(15)-H(15)	114.4
C(6)-C(5)-C(13)	121.60(19)	C(15)-C(16)-C(17)	122.87(17)
C(6)-C(5)-H(5)	119.2	C(15)-C(16)-Co(1)	70.01(10)
C(13)-C(5)-H(5)	119.2	C(17)-C(16)-Co(1)	110.59(13)
C(5)-C(6)-C(7)	120.12(19)	C(15)-C(16)-H(16)	115.0
C(5)-C(6)-H(6)	119.9	C(17)-C(16)-H(16)	115.0
C(7)-C(6)-H(6)	119.9	Co(1)-C(16)-H(16)	115.0
C(8)-C(7)-C(6)	119.98(19)	C(16)-C(17)-C(18)	112.83(16)
C(8)-C(7)-H(7)	120.0	C(16)-C(17)-H(17A)	109.0
C(6)-C(7)-H(7)	120.0	C(18)-C(17)-H(17A)	109.0
C(7)-C(8)-C(14)	121.30(19)	C(16)-C(17)-H(17B)	109.0
C(7)-C(8)-H(8)	119.3	C(18)-C(17)-H(17B)	109.0
C(14)-C(8)-H(8)	119.3	H(17A)-C(17)-H(17B)	107.8

C(19)-C(18)-C(17)	112.41(16)	O(1)-C(24)-C(23)	110.42(16)
C(19)-C(18)-H(18A)	109.1	O(1)-C(24)-H(24A)	109.6
C(17)-C(18)-H(18A)	109.1	C(23)-C(24)-H(24A)	109.6
C(19)-C(18)-H(18B)	109.1	O(1)-C(24)-H(24B)	109.6
C(17)-C(18)-H(18B)	109.1	C(23)-C(24)-H(24B)	109.6
H(18A)-C(18)-H(18B)	107.9	H(24A)-C(24)-H(24B)	108.1
C(20)-C(19)-C(18)	122.53(18)	O(1)-C(25)-C(26)	110.00(15)
C(20)-C(19)-Co(1)	70.16(11)	O(1)-C(25)-H(25A)	109.7
C(18)-C(19)-Co(1)	112.28(14)	C(26)-C(25)-H(25A)	109.7
C(20)-C(19)-H(19)	114.7	O(1)-C(25)-H(25B)	109.7
C(18)-C(19)-H(19)	114.7	C(26)-C(25)-H(25B)	109.7
Co(1)-C(19)-H(19)	114.7	H(25A)-C(25)-H(25B)	108.2
C(19)-C(20)-C(21)	122.18(17)	O(2)-C(26)-C(25)	109.06(16)
C(19)-C(20)-Co(1)	68.82(11)	O(2)-C(26)-H(26A)	109.9
C(21)-C(20)-Co(1)	112.78(12)	C(25)-C(26)-H(26A)	109.9
C(19)-C(20)-H(20)	114.9	O(2)-C(26)-H(26B)	109.9
C(21)-C(20)-H(20)	114.9	C(25)-C(26)-H(26B)	109.9
Co(1)-C(20)-H(20)	114.9	H(26A)-C(26)-H(26B)	108.3
C(20)-C(21)-C(22)	112.31(15)	O(2)-C(27)-C(28)	109.00(15)
C(20)-C(21)-H(21A)	109.1	O(2)-C(27)-H(27A)	109.9
C(22)-C(21)-H(21A)	109.1	C(28)-C(27)-H(27A)	109.9
C(20)-C(21)-H(21B)	109.1	O(2)-C(27)-H(27B)	109.9
C(22)-C(21)-H(21B)	109.1	C(28)-C(27)-H(27B)	109.9
H(21A)-C(21)-H(21B)	107.9	H(27A)-C(27)-H(27B)	108.3
C(15)-C(22)-C(21)	111.58(15)	N(2)-C(28)-C(27)	114.65(16)
C(15)-C(22)-H(22A)	109.3	N(2)-C(28)-H(28A)	108.6
C(21)-C(22)-H(22A)	109.3	C(27)-C(28)-H(28A)	108.6
C(15)-C(22)-H(22B)	109.3	N(2)-C(28)-H(28B)	108.6
C(21)-C(22)-H(22B)	109.3	C(27)-C(28)-H(28B)	108.6
H(22A)-C(22)-H(22B)	108.0	H(28A)-C(28)-H(28B)	107.6
N(1)-C(23)-C(24)	114.92(17)	N(1)-C(29)-C(30)	113.51(18)
N(1)-C(23)-H(23A)	108.5	N(1)-C(29)-H(29A)	108.9
C(24)-C(23)-H(23A)	108.5	C(30)-C(29)-H(29A)	108.9
N(1)-C(23)-H(23B)	108.5	N(1)-C(29)-H(29B)	108.9
C(24)-C(23)-H(23B)	108.5	C(30)-C(29)-H(29B)	108.9
H(23A)-C(23)-H(23B)	107.5	H(29A)-C(29)-H(29B)	107.7

O(3)-C(30)-C(29)	109.52(17)	N(1)-C(35)-H(35B)	108.7
O(3)-C(30)-H(30A)	109.8	C(36)-C(35)-H(35B)	108.7
C(29)-C(30)-H(30A)	109.8	H(35A)-C(35)-H(35B)	107.6
O(3)-C(30)-H(30B)	109.8	O(5)-C(36)-C(35)	109.13(16)
C(29)-C(30)-H(30B)	109.8	O(5)-C(36)-H(36A)	109.9
H(30A)-C(30)-H(30B)	108.2	C(35)-C(36)-H(36A)	109.9
O(3)-C(31)-C(32)	110.11(16)	O(5)-C(36)-H(36B)	109.9
O(3)-C(31)-H(31A)	109.6	C(35)-C(36)-H(36B)	109.9
C(32)-C(31)-H(31A)	109.6	H(36A)-C(36)-H(36B)	108.3
O(3)-C(31)-H(31B)	109.6	O(5)-C(37)-C(38)	109.52(15)
C(32)-C(31)-H(31B)	109.6	O(5)-C(37)-H(37A)	109.8
H(31A)-C(31)-H(31B)	108.2	C(38)-C(37)-H(37A)	109.8
O(4)-C(32)-C(31)	109.75(16)	O(5)-C(37)-H(37B)	109.8
O(4)-C(32)-H(32A)	109.7	C(38)-C(37)-H(37B)	109.8
C(31)-C(32)-H(32A)	109.7	H(37A)-C(37)-H(37B)	108.2
O(4)-C(32)-H(32B)	109.7	O(6)-C(38)-C(37)	109.74(15)
C(31)-C(32)-H(32B)	109.7	O(6)-C(38)-H(38A)	109.7
H(32A)-C(32)-H(32B)	108.2	C(37)-C(38)-H(38A)	109.7
O(4)-C(33)-C(34)	109.56(15)	O(6)-C(38)-H(38B)	109.7
O(4)-C(33)-H(33A)	109.8	C(37)-C(38)-H(38B)	109.7
C(34)-C(33)-H(33A)	109.8	H(38A)-C(38)-H(38B)	108.2
O(4)-C(33)-H(33B)	109.8	O(6)-C(39)-C(40)	109.99(15)
C(34)-C(33)-H(33B)	109.8	O(6)-C(39)-H(39A)	109.7
H(33A)-C(33)-H(33B)	108.2	C(40)-C(39)-H(39A)	109.7
N(2)-C(34)-C(33)	113.96(16)	O(6)-C(39)-H(39B)	109.7
N(2)-C(34)-H(34A)	108.8	C(40)-C(39)-H(39B)	109.7
C(33)-C(34)-H(34A)	108.8	H(39A)-C(39)-H(39B)	108.2
N(2)-C(34)-H(34B)	108.8	N(2)-C(40)-C(39)	113.81(15)
C(33)-C(34)-H(34B)	108.8	N(2)-C(40)-H(40A)	108.8
H(34A)-C(34)-H(34B)	107.7	C(39)-C(40)-H(40A)	108.8
N(1)-C(35)-C(36)	114.12(16)	N(2)-C(40)-H(40B)	108.8
N(1)-C(35)-H(35A)	108.7	C(39)-C(40)-H(40B)	108.8
C(36)-C(35)-H(35A)	108.7	H(40A)-C(40)-H(40B)	107.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04060m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	21(1)	29(1)	22(1)	13(1)	9(1)	7(1)
K1	25(1)	26(1)	21(1)	12(1)	11(1)	11(1)
O1	35(1)	23(1)	28(1)	14(1)	15(1)	9(1)
O2	26(1)	29(1)	25(1)	12(1)	9(1)	9(1)
O3	28(1)	48(1)	32(1)	22(1)	14(1)	19(1)
O4	28(1)	39(1)	24(1)	14(1)	12(1)	18(1)
O5	37(1)	33(1)	26(1)	12(1)	15(1)	19(1)
O6	35(1)	24(1)	26(1)	13(1)	13(1)	11(1)
N1	29(1)	39(1)	26(1)	19(1)	14(1)	15(1)
N2	26(1)	29(1)	22(1)	12(1)	11(1)	12(1)
C1	29(1)	33(1)	31(1)	19(1)	16(1)	13(1)
C2	28(1)	47(1)	28(1)	24(1)	11(1)	12(1)
C3	30(1)	37(1)	22(1)	10(1)	10(1)	3(1)
C4	30(1)	26(1)	26(1)	9(1)	14(1)	8(1)
C5	37(1)	30(1)	25(1)	11(1)	14(1)	5(1)
C6	31(1)	40(1)	25(1)	10(1)	9(1)	-2(1)
C7	24(1)	57(1)	29(1)	17(1)	11(1)	11(1)
C8	29(1)	43(1)	25(1)	15(1)	14(1)	16(1)
C9	34(1)	25(1)	26(1)	14(1)	17(1)	13(1)
C10	30(1)	26(1)	25(1)	12(1)	16(1)	12(1)
C11	28(1)	29(1)	23(1)	16(1)	15(1)	11(1)
C12	27(1)	26(1)	19(1)	11(1)	14(1)	8(1)
C13	29(1)	27(1)	19(1)	12(1)	14(1)	8(1)
C14	26(1)	33(1)	19(1)	13(1)	13(1)	11(1)
C15	25(1)	37(1)	21(1)	15(1)	9(1)	10(1)
C16	27(1)	33(1)	21(1)	10(1)	9(1)	3(1)
C17	52(1)	28(1)	38(1)	12(1)	27(1)	12(1)
C18	43(1)	37(1)	56(1)	24(1)	33(1)	21(1)
C19	23(1)	39(1)	42(1)	24(1)	15(1)	13(1)
C20	21(1)	36(1)	29(1)	15(1)	10(1)	8(1)
C21	27(1)	29(1)	36(1)	14(1)	17(1)	9(1)

C22	37(1)	35(1)	33(1)	20(1)	19(1)	16(1)
C23	38(1)	49(1)	26(1)	22(1)	19(1)	15(1)
C24	42(1)	43(1)	37(1)	28(1)	19(1)	12(1)
C25	45(1)	23(1)	42(1)	15(1)	24(1)	10(1)
C26	26(1)	24(1)	36(1)	6(1)	15(1)	5(1)
C27	31(1)	34(1)	25(1)	12(1)	4(1)	6(1)
C28	36(1)	34(1)	19(1)	8(1)	9(1)	11(1)
C29	51(1)	66(2)	40(1)	39(1)	25(1)	36(1)
C30	42(1)	71(2)	36(1)	33(1)	17(1)	35(1)
C31	25(1)	50(1)	35(1)	21(1)	12(1)	15(1)
C32	26(1)	44(1)	38(1)	20(1)	15(1)	19(1)
C33	31(1)	39(1)	27(1)	11(1)	16(1)	17(1)
C34	32(1)	41(1)	24(1)	17(1)	15(1)	15(1)
C35	37(1)	46(1)	23(1)	14(1)	11(1)	12(1)
C36	47(1)	34(1)	26(1)	7(1)	20(1)	14(1)
C37	28(1)	22(1)	35(1)	5(1)	8(1)	12(1)
C38	25(1)	24(1)	38(1)	14(1)	9(1)	11(1)
C39	44(1)	36(1)	35(1)	24(1)	21(1)	22(1)
C40	36(1)	43(1)	24(1)	21(1)	13(1)	21(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04060m.

	x	y	z	U(eq)
H1	7683	1973	2166	35
H2	9154	3633	3913	40
H3	8832	5451	4357	41
H4	7067	5445	3029	34
H5	2956	-434	-257	40
H6	915	-546	-901	46
H7	585	1184	-416	47
H8	2312	3020	703	38
H9	5293	747	958	31
H10	4671	4233	1896	31
H15	7125	4755	880	34
H16	6768	2850	291	37
H17A	8518	3010	-387	48
H17B	8266	2102	128	48
H18A	10357	3056	1122	48
H18B	10441	4215	952	48
H19	10566	4025	2823	39
H20	10747	5893	3524	36
H21A	10982	6292	1944	37
H21B	10268	6926	2533	37
H22A	8753	6124	862	38
H22B	9218	5125	415	38
H23A	5520	8640	6618	43
H23B	6118	8087	7362	43
H24A	5469	6345	5791	46
H24B	4280	6591	5897	46
H25A	3171	5335	4018	43
H25B	4410	5248	3874	43
H26A	2875	4952	2242	39
H26B	2934	6239	2843	39

H27A	3567	6670	1506	41
H27B	3572	5390	1029	41
H28A	5757	6283	1466	39
H28B	4969	6680	662	39
H29A	7432	7127	6462	51
H29B	8236	8183	7663	51
H30A	9681	9167	7105	53
H30B	9624	7874	6885	53
H31A	10506	8247	5708	44
H31B	10177	9337	5685	44
H32A	10235	8274	4047	41
H32B	9112	7102	3846	41
H33A	7766	7007	2202	38
H33B	8965	8128	2418	38
H34A	7741	9230	2399	37
H34B	7094	8065	1274	37
H35A	8751	10179	7466	45
H35B	7875	9976	8090	45
H36A	6374	10365	6947	45
H36B	7750	11475	7588	45
H37A	7221	12106	6260	38
H37B	5851	10992	5546	38
H38A	6571	11786	4464	37
H38B	7791	11502	4807	37
H39A	7030	10381	2910	40
H39B	5702	10497	2608	40
H40A	4582	8419	1885	38
H40B	5409	8761	1257	38

Table 6. Torsion angles [°] for 04060m.

O4-K1-O1-C25	-44.31(15)	N1-K1-O3-C31	-140.93(14)
O2-K1-O1-C25	20.01(12)	O4-K1-O3-C30	154.41(16)
O3-K1-O1-C25	-97.08(12)	O2-K1-O3-C30	-118.30(15)
O5-K1-O1-C25	165.54(12)	O1-K1-O3-C30	-57.15(15)
O6-K1-O1-C25	105.23(12)	O5-K1-O3-C30	43.20(15)
N2-K1-O1-C25	35.75(13)	O6-K1-O3-C30	92.00(16)
N1-K1-O1-C25	-144.77(13)	N2-K1-O3-C30	170.60(15)
O4-K1-O1-C24	88.13(14)	N1-K1-O3-C30	-8.40(15)
O2-K1-O1-C24	152.45(14)	O2-K1-O4-C33	30.43(13)
O3-K1-O1-C24	35.35(13)	O1-K1-O4-C33	82.91(14)
O5-K1-O1-C24	-62.02(13)	O3-K1-O4-C33	147.10(14)
O6-K1-O1-C24	-122.34(13)	O5-K1-O4-C33	-128.87(12)
N2-K1-O1-C24	168.19(12)	O6-K1-O4-C33	-69.59(13)
N1-K1-O1-C24	-12.33(13)	N2-K1-O4-C33	-16.85(12)
O4-K1-O2-C26	161.27(12)	N1-K1-O4-C33	164.09(12)
O1-K1-O2-C26	12.94(11)	O2-K1-O4-C32	-105.89(12)
O3-K1-O2-C26	98.94(12)	O1-K1-O4-C32	-53.41(15)
O5-K1-O2-C26	-50.65(14)	O3-K1-O4-C32	10.78(12)
O6-K1-O2-C26	-101.09(12)	O5-K1-O4-C32	94.81(13)
N2-K1-O2-C26	-151.26(13)	O6-K1-O4-C32	154.09(12)
N1-K1-O2-C26	28.46(13)	N2-K1-O4-C32	-153.16(14)
O4-K1-O2-C27	-58.26(13)	N1-K1-O4-C32	27.77(14)
O1-K1-O2-C27	153.41(14)	O4-K1-O5-C37	97.79(12)
O3-K1-O2-C27	-120.59(13)	O2-K1-O5-C37	-48.52(14)
O5-K1-O2-C27	89.82(14)	O1-K1-O5-C37	-99.92(12)
O6-K1-O2-C27	39.38(13)	O3-K1-O5-C37	157.92(12)
N2-K1-O2-C27	-10.79(12)	O6-K1-O5-C37	13.85(11)
N1-K1-O2-C27	168.93(12)	N2-K1-O5-C37	29.85(13)
O4-K1-O3-C31	21.87(12)	N1-K1-O5-C37	-150.62(13)
O2-K1-O3-C31	109.17(13)	O4-K1-O5-C36	-125.89(13)
O1-K1-O3-C31	170.32(12)	O2-K1-O5-C36	87.80(14)
O5-K1-O3-C31	-89.33(13)	O1-K1-O5-C36	36.40(13)
O6-K1-O3-C31	-40.53(15)	O3-K1-O5-C36	-65.76(13)
N2-K1-O3-C31	38.07(14)	O6-K1-O5-C36	150.17(14)

N2-K1-O5-C36	166.17(12)	N2-K1-N1-C23	130(3)
N1-K1-O5-C36	-14.30(12)	O4-K1-N2-C34	-14.33(11)
O4-K1-O6-C38	-91.59(11)	O2-K1-N2-C34	-139.00(13)
O2-K1-O6-C38	165.58(11)	O1-K1-N2-C34	-154.51(11)
O1-K1-O6-C38	105.30(11)	O3-K1-N2-C34	-30.35(13)
O3-K1-O6-C38	-40.97(13)	O5-K1-N2-C34	85.34(12)
O5-K1-O6-C38	19.58(11)	O6-K1-N2-C34	101.03(12)
N2-K1-O6-C38	-144.41(12)	N1-K1-N2-C34	57(3)
N1-K1-O6-C38	34.91(12)	O4-K1-N2-C40	-134.43(12)
O4-K1-O6-C39	41.06(13)	O2-K1-N2-C40	100.90(12)
O2-K1-O6-C39	-61.77(13)	O1-K1-N2-C40	85.40(12)
O1-K1-O6-C39	-122.05(12)	O3-K1-N2-C40	-150.45(11)
O3-K1-O6-C39	91.68(13)	O5-K1-N2-C40	-34.76(12)
O5-K1-O6-C39	152.23(13)	O6-K1-N2-C40	-19.07(11)
N2-K1-O6-C39	-11.76(12)	N1-K1-N2-C40	-63(3)
N1-K1-O6-C39	167.56(12)	O4-K1-N2-C28	105.37(12)
O4-K1-N1-C29	-38.65(14)	O2-K1-N2-C28	-19.30(10)
O2-K1-N1-C29	86.61(14)	O1-K1-N2-C28	-34.81(12)
O1-K1-N1-C29	101.72(14)	O3-K1-N2-C28	89.35(12)
O3-K1-N1-C29	-21.70(13)	O5-K1-N2-C28	-154.96(11)
O5-K1-N1-C29	-138.10(14)	O6-K1-N2-C28	-139.27(12)
O6-K1-N1-C29	-153.24(13)	N1-K1-N2-C28	177(100)
N2-K1-N1-C29	-110(3)	C19-Co1-C1-C2	84.73(13)
O4-K1-N1-C35	82.79(12)	C16-Co1-C1-C2	172.78(12)
O2-K1-N1-C35	-151.95(11)	C15-Co1-C1-C2	-162.57(12)
O1-K1-N1-C35	-136.84(13)	C20-Co1-C1-C2	54.86(17)
O3-K1-N1-C35	99.74(13)	C3-Co1-C1-C2	-33.54(12)
O5-K1-N1-C35	-16.66(11)	C4-Co1-C1-C2	-73.24(12)
O6-K1-N1-C35	-31.80(13)	C19-Co1-C1-C11	-154.69(12)
N2-K1-N1-C35	11(3)	C16-Co1-C1-C11	-66.64(12)
O4-K1-N1-C23	-158.33(11)	C2-Co1-C1-C11	120.58(17)
O2-K1-N1-C23	-33.07(13)	C15-Co1-C1-C11	-41.99(15)
O1-K1-N1-C23	-17.96(11)	C20-Co1-C1-C11	175.43(11)
O3-K1-N1-C23	-141.38(13)	C3-Co1-C1-C11	87.03(13)
O5-K1-N1-C23	102.22(13)	C4-Co1-C1-C11	47.34(11)
O6-K1-N1-C23	87.08(12)	C11-C1-C2-C3	-27.1(3)

Co1-C1-C2-C3	58.04(15)	C20-Co1-C4-C3	-69.11(14)
C11-C1-C2-Co1	-85.13(16)	C1-Co1-C4-C3	74.34(12)
C19-Co1-C2-C3	127.94(12)	C19-Co1-C4-C12	-152.47(18)
C16-Co1-C2-C3	-136.92(13)	C16-Co1-C4-C12	42.66(14)
C15-Co1-C2-C3	-73.5(3)	C2-Co1-C4-C12	-87.79(13)
C20-Co1-C2-C3	86.85(12)	C15-Co1-C4-C12	81.02(12)
C1-Co1-C2-C3	-126.86(16)	C20-Co1-C4-C12	169.48(11)
C4-Co1-C2-C3	-32.13(11)	C3-Co1-C4-C12	-121.41(17)
C19-Co1-C2-C1	-105.20(12)	C1-Co1-C4-C12	-47.07(11)
C16-Co1-C2-C1	-10.07(17)	C13-C5-C6-C7	1.7(3)
C15-Co1-C2-C1	53.4(3)	C5-C6-C7-C8	0.4(3)
C20-Co1-C2-C1	-146.30(11)	C6-C7-C8-C14	-1.7(3)
C3-Co1-C2-C1	126.86(16)	C13-C9-C11-C12	-3.3(3)
C4-Co1-C2-C1	94.73(12)	C13-C9-C11-C1	-177.81(16)
C1-C2-C3-C4	0.5(3)	C2-C1-C11-C9	-159.12(18)
Co1-C2-C3-C4	60.84(16)	Co1-C1-C11-C9	134.43(16)
C1-C2-C3-Co1	-60.32(15)	C2-C1-C11-C12	26.3(2)
C19-Co1-C3-C4	166.98(11)	Co1-C1-C11-C12	-40.20(16)
C16-Co1-C3-C4	-30.5(2)	C14-C10-C12-C11	1.2(3)
C2-Co1-C3-C4	-127.08(17)	C14-C10-C12-C4	177.25(16)
C15-Co1-C3-C4	30.75(16)	C9-C11-C12-C10	1.7(2)
C20-Co1-C3-C4	126.42(12)	C1-C11-C12-C10	176.64(16)
C1-Co1-C3-C4	-94.22(12)	C9-C11-C12-C4	-174.73(16)
C19-Co1-C3-C2	-65.94(14)	C1-C11-C12-C4	0.2(2)
C16-Co1-C3-C2	96.61(19)	C3-C4-C12-C10	157.22(18)
C15-Co1-C3-C2	157.83(11)	Co1-C4-C12-C10	-137.39(15)
C20-Co1-C3-C2	-106.50(12)	C3-C4-C12-C11	-26.5(2)
C1-Co1-C3-C2	32.85(11)	Co1-C4-C12-C11	38.84(16)
C4-Co1-C3-C2	127.08(17)	C6-C5-C13-C9	174.81(17)
C2-C3-C4-C12	26.5(3)	C6-C5-C13-C14	-2.4(3)
Co1-C3-C4-C12	83.50(16)	C11-C9-C13-C5	-174.99(17)
C2-C3-C4-Co1	-57.03(15)	C11-C9-C13-C14	2.1(3)
C19-Co1-C4-C3	-31.1(3)	C7-C8-C14-C10	-175.79(17)
C16-Co1-C4-C3	164.08(12)	C7-C8-C14-C13	1.0(3)
C2-Co1-C4-C3	33.62(12)	C12-C10-C14-C8	174.53(17)
C15-Co1-C4-C3	-157.57(12)	C12-C10-C14-C13	-2.3(3)

C5-C13-C14-C8	1.0(2)	C17-C18-C19-C20	-89.5(2)
C9-C13-C14-C8	-176.29(16)	C17-C18-C19-Co1	-9.5(2)
C5-C13-C14-C10	177.95(15)	C16-Co1-C19-C20	114.54(12)
C9-C13-C14-C10	0.7(2)	C2-Co1-C19-C20	-111.09(12)
C19-Co1-C15-C16	77.95(12)	C15-Co1-C19-C20	75.05(12)
C2-Co1-C15-C16	-80.9(3)	C3-Co1-C19-C20	-73.97(14)
C20-Co1-C15-C16	117.50(12)	C1-Co1-C19-C20	-151.33(11)
C3-Co1-C15-C16	-138.31(12)	C4-Co1-C19-C20	-51.7(2)
C1-Co1-C15-C16	-39.81(15)	C16-Co1-C19-C18	-3.50(14)
C4-Co1-C15-C16	-119.51(11)	C2-Co1-C19-C18	130.88(14)
C19-Co1-C15-C22	-39.09(15)	C15-Co1-C19-C18	-42.99(15)
C16-Co1-C15-C22	-117.04(19)	C20-Co1-C19-C18	-118.04(19)
C2-Co1-C15-C22	162.1(2)	C3-Co1-C19-C18	167.99(13)
C20-Co1-C15-C22	0.46(14)	C1-Co1-C19-C18	90.64(15)
C3-Co1-C15-C22	104.65(15)	C4-Co1-C19-C18	-169.73(17)
C1-Co1-C15-C22	-156.85(13)	C18-C19-C20-C21	0.1(3)
C4-Co1-C15-C22	123.45(14)	Co1-C19-C20-C21	-104.29(16)
C22-C15-C16-C17	4.2(3)	C18-C19-C20-Co1	104.35(18)
Co1-C15-C16-C17	-102.15(18)	C16-Co1-C20-C19	-68.87(13)
C22-C15-C16-Co1	106.39(17)	C2-Co1-C20-C19	80.53(13)
C19-Co1-C16-C15	-102.94(12)	C15-Co1-C20-C19	-105.13(12)
C2-Co1-C16-C15	156.33(12)	C3-Co1-C20-C19	122.58(12)
C20-Co1-C16-C15	-65.12(12)	C1-Co1-C20-C19	46.42(17)
C3-Co1-C16-C15	91.86(19)	C4-Co1-C20-C19	159.59(11)
C1-Co1-C16-C15	149.89(11)	C19-Co1-C20-C21	117.18(19)
C4-Co1-C16-C15	71.49(12)	C16-Co1-C20-C21	48.30(15)
C19-Co1-C16-C17	15.76(14)	C2-Co1-C20-C21	-162.30(13)
C2-Co1-C16-C17	-84.98(16)	C15-Co1-C20-C21	12.05(14)
C15-Co1-C16-C17	118.70(18)	C3-Co1-C20-C21	-120.24(14)
C20-Co1-C16-C17	53.58(15)	C1-Co1-C20-C21	163.59(12)
C3-Co1-C16-C17	-149.44(16)	C4-Co1-C20-C21	-83.24(15)
C1-Co1-C16-C17	-91.41(14)	C19-C20-C21-C22	56.5(2)
C4-Co1-C16-C17	-169.81(13)	Co1-C20-C21-C22	-22.1(2)
C15-C16-C17-C18	54.0(3)	C16-C15-C22-C21	-92.8(2)
Co1-C16-C17-C18	-24.9(2)	Co1-C15-C22-C21	-12.6(2)
C16-C17-C18-C19	22.5(2)	C20-C21-C22-C15	22.2(2)

C29-N1-C23-C24	-69.9(2)	K1-O4-C32-C31	-40.72(19)
C35-N1-C23-C24	168.87(17)	O3-C31-C32-O4	62.1(2)
K1-N1-C23-C24	49.04(19)	C32-O4-C33-C34	-175.29(16)
C25-O1-C24-C23	175.52(17)	K1-O4-C33-C34	45.56(19)
K1-O1-C24-C23	41.5(2)	C40-N2-C34-C33	164.06(15)
N1-C23-C24-O1	-63.6(2)	C28-N2-C34-C33	-75.11(19)
C24-O1-C25-C26	174.58(16)	K1-N2-C34-C33	44.22(18)
K1-O1-C25-C26	-50.32(18)	O4-C33-C34-N2	-61.2(2)
C27-O2-C26-C25	173.61(15)	C29-N1-C35-C36	167.87(16)
K1-O2-C26-C25	-42.70(18)	C23-N1-C35-C36	-70.9(2)
O1-C25-C26-O2	61.3(2)	K1-N1-C35-C36	47.06(19)
C26-O2-C27-C28	-178.34(15)	C37-O5-C36-C35	-178.67(16)
K1-O2-C27-C28	38.8(2)	K1-O5-C36-C35	42.7(2)
C34-N2-C28-C27	169.66(16)	N1-C35-C36-O5	-61.1(2)
C40-N2-C28-C27	-69.9(2)	C36-O5-C37-C38	175.95(15)
K1-N2-C28-C27	49.67(18)	K1-O5-C37-C38	-44.47(18)
O2-C27-C28-N2	-60.6(2)	C39-O6-C38-C37	173.76(15)
C35-N1-C29-C30	-69.8(2)	K1-O6-C38-C37	-50.45(16)
C23-N1-C29-C30	169.77(18)	O5-C37-C38-O6	63.15(19)
K1-N1-C29-C30	51.8(2)	C38-O6-C39-C40	175.16(15)
C31-O3-C30-C29	170.51(18)	K1-O6-C39-C40	40.87(19)
K1-O3-C30-C29	36.8(2)	C34-N2-C40-C39	-70.43(19)
N1-C29-C30-O3	-60.6(3)	C28-N2-C40-C39	169.21(16)
C30-O3-C31-C32	170.82(18)	K1-N2-C40-C39	49.86(17)
K1-O3-C31-C32	-52.06(19)	O6-C39-C40-N2	-62.8(2)
C33-O4-C32-C31	179.74(16)		

Symmetry transformations used to generate equivalent atoms:

REFERENCE NUMBER: 04051 [9]

CRYSTAL STRUCTURE REPORT

$C_{34} H_{60} Co K N_2 O_6$

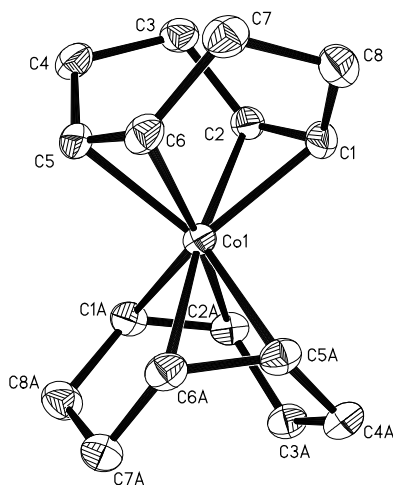
or

$[K(222\text{-cryptand})][Co(1,5\text{-COD})_2]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

April 06, 2004



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University of Minnesota
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Minneapolis, MN 55455

Data collection

A crystal (approximate dimensions 0.45 x 0.24 x 0.19 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Siemens SMART Platform CCD diffractometer for a data collection at 173(2) K. A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 221 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 10 seconds and a detector distance of 4.89 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).¹ Final cell constants were calculated from the xyz centroids of 3578 strong reflections from the actual data collection after integration (SAINT).² Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97³ and refined using SHELXL-97.⁴ The space group *Pccn* 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. Hydrogen atoms on the coordinated carbon atoms were found from the difference map and refined with individual isotropic displacement parameters. The remaining 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 $R1 = 0.0424$ and $wR2 = 0.0815$ (F^2 , all data).

Structure description

The structure is the one suggested. The cobalt and potassium atoms are located on different two-fold axes (both parallel to the *c* axis); thus, one half of each molecule is unique. With a twist angle is 67.3°, the geometry is closer to tetrahedral than square planar.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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- ¹ An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
- ² SAINT V6.2, Bruker Analytical X-Ray Systems, Madison, WI (2001).
- ³ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
- ⁴ SHELXTL V6.10, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

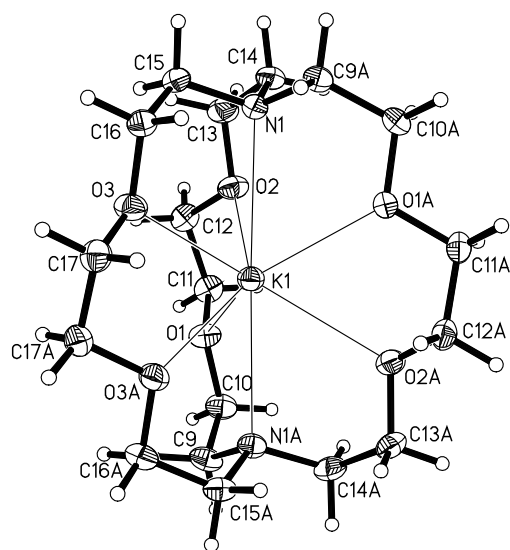
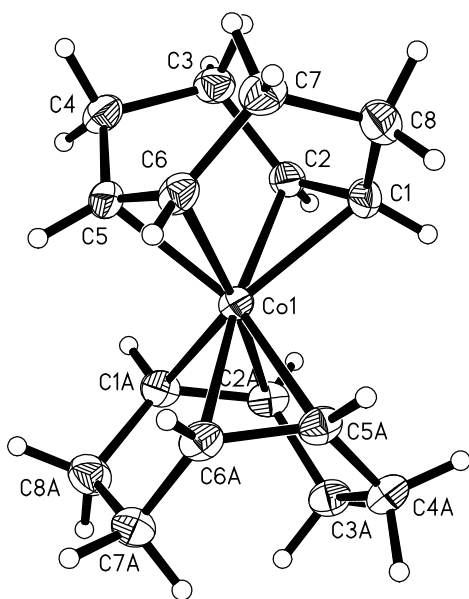
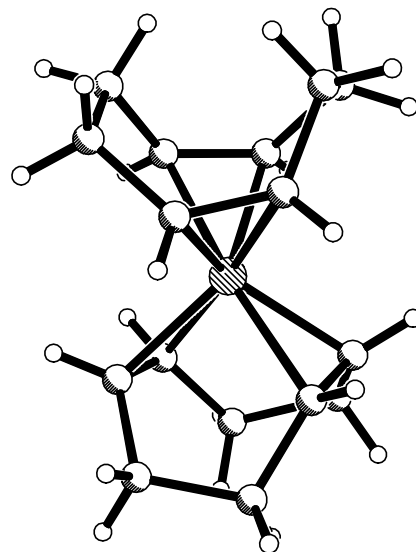
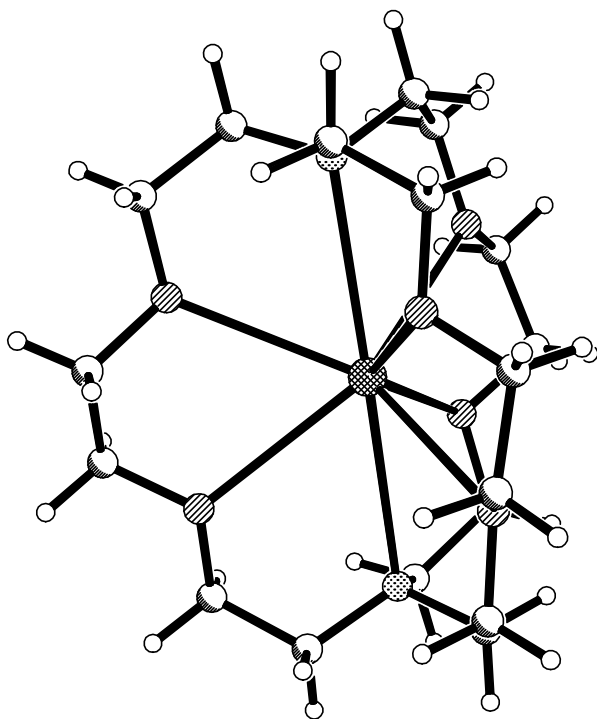
$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2 (F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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



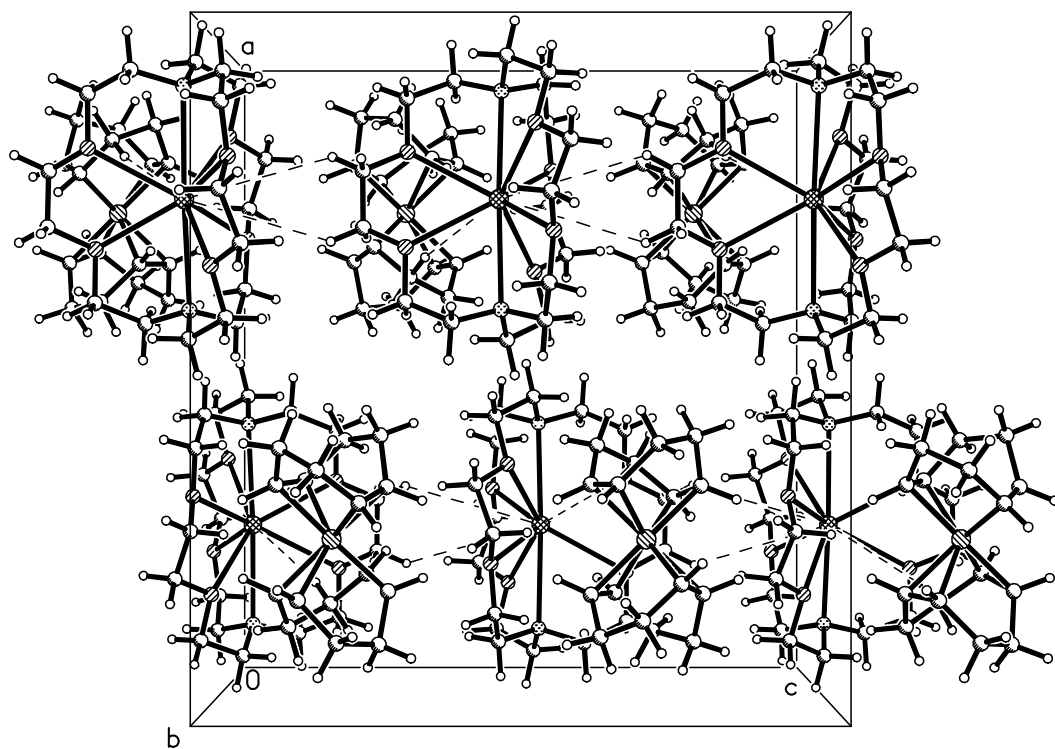


Table 1. Crystal data and structure refinement for 04051.

Identification code	04051	
Empirical formula	C ₃₄ H ₆₀ Co K N ₂ O ₆	
Formula weight	690.87	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	<i>Pccn</i>	
Unit cell dimensions	$a = 17.889(2)$ Å	$\alpha = 90^\circ$
	$b = 11.8653(13)$ Å	$\beta = 90^\circ$
	$c = 16.562(2)$ Å	$\gamma = 90^\circ$
Volume	3515.4(7) Å ³	
<i>Z</i>	4	
Density (calculated)	1.305 Mg/m ³	
Absorption coefficient	0.651 mm ⁻¹	
<i>F</i> (000)	1488	
Crystal color, morphology	yellow, block	
Crystal size	0.45 x 0.24 x 0.19 mm ³	
Theta range for data collection	2.06 to 27.51°	
Index ranges	$-22 \leq h \leq 23$, $-15 \leq k \leq 15$, $-18 \leq l \leq 21$	
Reflections collected	24924	
Independent reflections	4024 [<i>R</i> (int) = 0.0430]	
Observed reflections	3185	
Completeness to theta = 27.51°	99.4%	
Absorption correction	Multi-scan	
Max. and min. transmission	1.000000 and 0.862428	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	4024 / 0 / 213	
Goodness-of-fit on <i>F</i> ²	1.024	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0424, <i>wR</i> 2 = 0.0752	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0635, <i>wR</i> 2 = 0.0815	
Largest diff. peak and hole	0.254 and -0.369 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04051. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	7500	2500	3003(1)	19(1)
C1	6923(1)	3821(2)	2508(1)	24(1)
C2	6719(1)	2804(2)	2120(1)	23(1)
C3	5976(1)	2200(2)	2244(1)	26(1)
C4	6067(1)	1241(2)	2862(1)	27(1)
C5	6662(1)	1534(2)	3482(1)	23(1)
C6	6692(1)	2582(2)	3885(1)	24(1)
C7	6140(1)	3547(2)	3764(1)	29(1)
C8	6432(1)	4394(2)	3133(1)	31(1)
K1	7500	7500	4654(1)	21(1)
O1	6480(1)	5863(1)	5226(1)	25(1)
O2	8022(1)	5605(1)	5507(1)	27(1)
O3	8222(1)	7025(1)	3186(1)	27(1)
N1	9130(1)	7009(1)	4691(1)	22(1)
C9	5438(1)	6940(2)	4779(1)	28(1)
C10	5735(1)	6171(2)	5432(1)	27(1)
C11	6767(1)	5020(2)	5755(1)	27(1)
C12	7521(1)	4667(2)	5460(1)	26(1)
C13	8780(1)	5241(2)	5435(1)	29(1)
C14	9283(1)	6259(2)	5378(1)	28(1)
C15	9316(1)	6453(2)	3921(1)	25(1)
C16	9020(1)	7046(2)	3178(1)	26(1)
C17	7917(1)	7575(2)	2494(1)	27(1)

Table 3. Bond lengths [Å] and angles [°] for 04051.

Co(1)-C(5)#1	2.0472(19)	K(1)-N(1)	2.9733(16)
Co(1)-C(5)	2.0472(19)	K(1)-N(1)#2	2.9733(16)
Co(1)-C(1)#1	2.0481(19)	O(1)-C(10)	1.424(2)
Co(1)-C(1)	2.0481(19)	O(1)-C(11)	1.425(2)
Co(1)-C(2)#1	2.0546(19)	O(2)-C(13)	1.429(2)
Co(1)-C(2)	2.0546(19)	O(2)-C(12)	1.433(2)
Co(1)-C(6)#1	2.0574(19)	O(3)-C(17)	1.427(2)
Co(1)-C(6)	2.0574(19)	O(3)-C(16)	1.427(2)
C(1)-C(2)	1.415(3)	N(1)-C(14)	1.471(3)
C(1)-C(8)	1.517(3)	N(1)-C(15)	1.473(2)
C(1)-H(1A)	0.95(2)	N(1)-C(9)#2	1.474(2)
C(2)-C(3)	1.523(3)	C(9)-N(1)#2	1.474(2)
C(2)-H(2A)	1.0000	C(9)-C(10)	1.510(3)
C(3)-C(4)	1.539(3)	C(9)-H(9A)	0.9900
C(3)-H(3A)	0.9900	C(9)-H(9B)	0.9900
C(3)-H(3B)	0.9900	C(10)-H(10A)	0.9900
C(4)-C(5)	1.520(3)	C(10)-H(10B)	0.9900
C(4)-H(4A)	0.9900	C(11)-C(12)	1.494(3)
C(4)-H(4B)	0.9900	C(11)-H(11A)	0.9900
C(5)-C(6)	1.412(3)	C(11)-H(11B)	0.9900
C(5)-H(5A)	0.941(19)	C(12)-H(12A)	0.9900
C(6)-C(7)	1.524(3)	C(12)-H(12B)	0.9900
C(6)-H(6A)	0.96(2)	C(13)-C(14)	1.508(3)
C(7)-C(8)	1.541(3)	C(13)-H(13A)	0.9900
C(7)-H(7A)	0.9900	C(13)-H(13B)	0.9900
C(7)-H(7B)	0.9900	C(14)-H(14A)	0.9900
C(8)-H(8A)	0.9900	C(14)-H(14B)	0.9900
C(8)-H(8B)	0.9900	C(15)-C(16)	1.513(3)
K(1)-O(3)	2.8114(15)	C(15)-H(15A)	0.9900
K(1)-O(3)#2	2.8114(15)	C(15)-H(15B)	0.9900
K(1)-O(2)	2.8146(14)	C(16)-H(16A)	0.9900
K(1)-O(2)#2	2.8146(14)	C(16)-H(16B)	0.9900
K(1)-O(1)#2	2.8284(13)	C(17)-C(17)#2	1.501(4)
K(1)-O(1)	2.8284(13)	C(17)-H(17A)	0.9900

C(17)-H(17B)	0.9900	C(1)-C(2)-Co(1)	69.57(11)
C(5)#1-Co(1)-C(5)	134.38(11)	C(3)-C(2)-Co(1)	114.52(13)
C(5)#1-Co(1)-C(1)#1	102.36(8)	C(1)-C(2)-H(2A)	113.6
C(5)-Co(1)-C(1)#1	95.53(8)	C(3)-C(2)-H(2A)	113.6
C(5)#1-Co(1)-C(1)	95.53(8)	Co(1)-C(2)-H(2A)	113.6
C(5)-Co(1)-C(1)	102.36(8)	C(2)-C(3)-C(4)	110.17(16)
C(1)#1-Co(1)-C(1)	132.80(12)	C(2)-C(3)-H(3A)	109.6
C(5)#1-Co(1)-C(2)#1	82.87(8)	C(4)-C(3)-H(3A)	109.6
C(5)-Co(1)-C(2)#1	132.53(8)	C(2)-C(3)-H(3B)	109.6
C(1)#1-Co(1)-C(2)#1	40.35(8)	C(4)-C(3)-H(3B)	109.6
C(1)-Co(1)-C(2)#1	101.08(8)	H(3A)-C(3)-H(3B)	108.1
C(5)#1-Co(1)-C(2)	132.53(8)	C(5)-C(4)-C(3)	110.76(16)
C(5)-Co(1)-C(2)	82.87(8)	C(5)-C(4)-H(4A)	109.5
C(1)#1-Co(1)-C(2)	101.08(8)	C(3)-C(4)-H(4A)	109.5
C(1)-Co(1)-C(2)	40.35(8)	C(5)-C(4)-H(4B)	109.5
C(2)#1-Co(1)-C(2)	89.23(11)	C(3)-C(4)-H(4B)	109.5
C(5)#1-Co(1)-C(6)#1	40.25(8)	H(4A)-C(4)-H(4B)	108.1
C(5)-Co(1)-C(6)#1	102.29(8)	C(6)-C(5)-C(4)	123.22(18)
C(1)#1-Co(1)-C(6)#1	83.88(8)	C(6)-C(5)-Co(1)	70.26(11)
C(1)-Co(1)-C(6)#1	132.45(8)	C(4)-C(5)-Co(1)	112.26(13)
C(2)#1-Co(1)-C(6)#1	91.09(8)	C(6)-C(5)-H(5A)	118.9(11)
C(2)-Co(1)-C(6)#1	172.56(8)	C(4)-C(5)-H(5A)	112.0(12)
C(5)#1-Co(1)-C(6)	102.29(8)	Co(1)-C(5)-H(5A)	112.2(12)
C(5)-Co(1)-C(6)	40.25(8)	C(5)-C(6)-C(7)	125.03(18)
C(1)#1-Co(1)-C(6)	132.45(8)	C(5)-C(6)-Co(1)	69.49(11)
C(1)-Co(1)-C(6)	83.88(8)	C(7)-C(6)-Co(1)	113.40(13)
C(2)#1-Co(1)-C(6)	172.56(8)	C(5)-C(6)-H(6A)	116.0(12)
C(2)-Co(1)-C(6)	91.09(8)	C(7)-C(6)-H(6A)	113.2(12)
C(6)#1-Co(1)-C(6)	89.55(11)	Co(1)-C(6)-H(6A)	110.7(12)
C(2)-C(1)-C(8)	122.87(19)	C(6)-C(7)-C(8)	111.05(16)
C(2)-C(1)-Co(1)	70.07(11)	C(6)-C(7)-H(7A)	109.4
C(8)-C(1)-Co(1)	111.17(14)	C(8)-C(7)-H(7A)	109.4
C(2)-C(1)-H(1A)	116.5(12)	C(6)-C(7)-H(7B)	109.4
C(8)-C(1)-H(1A)	114.8(12)	C(8)-C(7)-H(7B)	109.4
Co(1)-C(1)-H(1A)	112.1(12)	H(7A)-C(7)-H(7B)	108.0
C(1)-C(2)-C(3)	124.39(18)	C(1)-C(8)-C(7)	111.49(17)

C(1)-C(8)-H(8A)	109.3	C(13)-O(2)-C(12)	110.78(15)
C(7)-C(8)-H(8A)	109.3	C(13)-O(2)-K(1)	120.97(11)
C(1)-C(8)-H(8B)	109.3	C(12)-O(2)-K(1)	112.66(11)
C(7)-C(8)-H(8B)	109.3	C(17)-O(3)-C(16)	111.58(15)
H(8A)-C(8)-H(8B)	108.0	C(17)-O(3)-K(1)	115.28(11)
O(3)-K(1)-O(3)#2	60.16(6)	C(16)-O(3)-K(1)	117.61(11)
O(3)-K(1)-O(2)	96.99(4)	C(14)-N(1)-C(15)	110.90(15)
O(3)#2-K(1)-O(2)	138.32(4)	C(14)-N(1)-C(9)#2	109.67(16)
O(3)-K(1)-O(2)#2	138.32(4)	C(15)-N(1)-C(9)#2	110.26(15)
O(3)#2-K(1)-O(2)#2	96.99(4)	C(14)-N(1)-K(1)	108.50(11)
O(2)-K(1)-O(2)#2	119.74(6)	C(15)-N(1)-K(1)	106.96(11)
O(3)-K(1)-O(1)#2	97.52(4)	C(9)#2-N(1)-K(1)	110.51(11)
O(3)#2-K(1)-O(1)#2	116.64(4)	N(1)#2-C(9)-C(10)	113.47(16)
O(2)-K(1)-O(1)#2	99.57(4)	N(1)#2-C(9)-H(9A)	108.9
O(2)#2-K(1)-O(1)#2	59.85(4)	C(10)-C(9)-H(9A)	108.9
O(3)-K(1)-O(1)	116.64(4)	N(1)#2-C(9)-H(9B)	108.9
O(3)#2-K(1)-O(1)	97.52(4)	C(10)-C(9)-H(9B)	108.9
O(2)-K(1)-O(1)	59.85(4)	H(9A)-C(9)-H(9B)	107.7
O(2)#2-K(1)-O(1)	99.57(4)	O(1)-C(10)-C(9)	108.24(16)
O(1)#2-K(1)-O(1)	140.89(6)	O(1)-C(10)-H(10A)	110.1
O(3)-K(1)-N(1)	61.83(4)	C(9)-C(10)-H(10A)	110.1
O(3)#2-K(1)-N(1)	120.47(4)	O(1)-C(10)-H(10B)	110.1
O(2)-K(1)-N(1)	60.52(4)	C(9)-C(10)-H(10B)	110.1
O(2)#2-K(1)-N(1)	118.15(4)	H(10A)-C(10)-H(10B)	108.4
O(1)#2-K(1)-N(1)	59.68(4)	O(1)-C(11)-C(12)	108.77(16)
O(1)-K(1)-N(1)	119.43(4)	O(1)-C(11)-H(11A)	109.9
O(3)-K(1)-N(1)#2	120.47(4)	C(12)-C(11)-H(11A)	109.9
O(3)#2-K(1)-N(1)#2	61.83(4)	O(1)-C(11)-H(11B)	109.9
O(2)-K(1)-N(1)#2	118.15(4)	C(12)-C(11)-H(11B)	109.9
O(2)#2-K(1)-N(1)#2	60.52(4)	H(11A)-C(11)-H(11B)	108.3
O(1)#2-K(1)-N(1)#2	119.43(4)	O(2)-C(12)-C(11)	109.18(15)
O(1)-K(1)-N(1)#2	59.68(4)	O(2)-C(12)-H(12A)	109.8
N(1)-K(1)-N(1)#2	177.68(7)	C(11)-C(12)-H(12A)	109.8
C(10)-O(1)-C(11)	111.80(15)	O(2)-C(12)-H(12B)	109.8
C(10)-O(1)-K(1)	120.51(11)	C(11)-C(12)-H(12B)	109.8
C(11)-O(1)-K(1)	117.04(11)	H(12A)-C(12)-H(12B)	108.3

O(2)-C(13)-C(14)	109.20(16)	N(1)-C(15)-H(15B)	108.6
O(2)-C(13)-H(13A)	109.8	C(16)-C(15)-H(15B)	108.6
C(14)-C(13)-H(13A)	109.8	H(15A)-C(15)-H(15B)	107.6
O(2)-C(13)-H(13B)	109.8	O(3)-C(16)-C(15)	109.55(16)
C(14)-C(13)-H(13B)	109.8	O(3)-C(16)-H(16A)	109.8
H(13A)-C(13)-H(13B)	108.3	C(15)-C(16)-H(16A)	109.8
N(1)-C(14)-C(13)	114.90(16)	O(3)-C(16)-H(16B)	109.8
N(1)-C(14)-H(14A)	108.5	C(15)-C(16)-H(16B)	109.8
C(13)-C(14)-H(14A)	108.5	H(16A)-C(16)-H(16B)	108.2
N(1)-C(14)-H(14B)	108.5	O(3)-C(17)-C(17)#2	109.01(14)
C(13)-C(14)-H(14B)	108.5	O(3)-C(17)-H(17A)	109.9
H(14A)-C(14)-H(14B)	107.5	C(17)#2-C(17)-H(17A)	109.9
N(1)-C(15)-C(16)	114.64(16)	O(3)-C(17)-H(17B)	109.9
N(1)-C(15)-H(15A)	108.6	C(17)#2-C(17)-H(17B)	109.9
C(16)-C(15)-H(15A)	108.6	H(17A)-C(17)-H(17B)	108.3

Symmetry transformations used to generate equivalent atoms:

#1 $-x+3/2, -y+1/2, z$ #2 $-x+3/2, -y+3/2, z$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04051. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	18(1)	20(1)	19(1)	0	0	-1(1)
C1	25(1)	22(1)	27(1)	6(1)	4(1)	1(1)
C2	21(1)	27(1)	21(1)	6(1)	-1(1)	1(1)
C3	22(1)	31(1)	25(1)	1(1)	-3(1)	-1(1)
C4	22(1)	30(1)	30(1)	1(1)	0(1)	-7(1)
C5	21(1)	25(1)	24(1)	7(1)	1(1)	-2(1)
C6	23(1)	29(1)	19(1)	3(1)	3(1)	-4(1)
C7	26(1)	32(1)	28(1)	-3(1)	6(1)	0(1)
C8	30(1)	26(1)	37(1)	3(1)	4(1)	5(1)
K1	18(1)	22(1)	24(1)	0	0	1(1)
O1	21(1)	26(1)	29(1)	9(1)	4(1)	2(1)
O2	21(1)	23(1)	38(1)	3(1)	1(1)	3(1)
O3	20(1)	36(1)	25(1)	3(1)	1(1)	1(1)
N1	19(1)	23(1)	25(1)	-4(1)	0(1)	-1(1)
C9	17(1)	32(1)	34(1)	7(1)	-2(1)	-4(1)
C10	20(1)	30(1)	33(1)	6(1)	3(1)	-4(1)
C11	30(1)	24(1)	26(1)	7(1)	3(1)	0(1)
C12	31(1)	20(1)	27(1)	5(1)	2(1)	2(1)
C13	25(1)	29(1)	32(1)	4(1)	-4(1)	9(1)
C14	20(1)	33(1)	30(1)	-2(1)	-6(1)	6(1)
C15	19(1)	25(1)	31(1)	-6(1)	1(1)	3(1)
C16	19(1)	33(1)	27(1)	-5(1)	3(1)	-1(1)
C17	28(1)	31(1)	21(1)	1(1)	3(1)	1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04051.

	x	y	z	U(eq)
H1A	7240(11)	4314(17)	2213(12)	20(5)
H2A	6921	2733	1560	23(5)
H3A	5801	1887	1723	31
H3B	5597	2742	2439	31
H4A	5585	1108	3139	33
H4B	6210	539	2578	33
H5A	6847(11)	890(16)	3746(11)	16(5)
H6A	6915(11)	2576(17)	4414(12)	21(5)
H7A	6059	3939	4284	34
H7B	5654	3239	3582	34
H8A	6003	4756	2860	37
H8B	6723	4989	3409	37
H9A	5443	6531	4259	33
H9B	4913	7133	4905	33
H10A	5728	6564	5959	33
H10B	5418	5490	5473	33
H11A	6426	4364	5765	32
H11B	6807	5324	6310	32
H12A	7711	4038	5794	31
H12B	7484	4402	4894	31
H13A	8838	4770	4945	34
H13B	8920	4782	5910	34
H14A	9234	6699	5883	33
H14B	9807	5998	5341	33
H15A	9114	5677	3931	30
H15B	9866	6397	3877	30
H16A	9198	7836	3170	32
H16B	9207	6665	2686	32
H17A	8132	7248	1996	32
H17B	8042	8388	2508	32

Table 6. Torsion angles [°] for 04051.

C5#1-Co1-C1-C2	159.23(12)	C5#1-Co1-C5-C6	45.96(10)
C5-Co1-C1-C2	-62.99(13)	C1#1-Co1-C5-C6	159.26(12)
C1#1-Co1-C1-C2	46.72(10)	C1-Co1-C5-C6	-64.68(13)
C2#1-Co1-C1-C2	75.43(15)	C2#1-Co1-C5-C6	177.42(12)
C6#1-Co1-C1-C2	177.29(12)	C2-Co1-C5-C6	-100.22(12)
C6-Co1-C1-C2	-98.96(12)	C6#1-Co1-C5-C6	74.34(16)
C5#1-Co1-C1-C8	-82.17(15)	C5#1-Co1-C5-C4	164.78(16)
C5-Co1-C1-C8	55.61(16)	C1#1-Co1-C5-C4	-81.92(15)
C1#1-Co1-C1-C8	165.33(16)	C1-Co1-C5-C4	54.14(16)
C2#1-Co1-C1-C8	-165.96(15)	C2#1-Co1-C5-C4	-63.76(18)
C2-Co1-C1-C8	118.6(2)	C2-Co1-C5-C4	18.60(14)
C6#1-Co1-C1-C8	-64.11(18)	C6#1-Co1-C5-C4	-166.84(14)
C6-Co1-C1-C8	19.64(15)	C6-Co1-C5-C4	118.82(19)
C8-C1-C2-C3	3.5(3)	C4-C5-C6-C7	0.6(3)
Co1-C1-C2-C3	106.37(18)	Co1-C5-C6-C7	104.80(18)
C8-C1-C2-Co1	-102.89(19)	C4-C5-C6-Co1	-104.25(18)
C5#1-Co1-C2-C1	-28.62(16)	C5#1-Co1-C6-C5	-148.28(11)
C5-Co1-C2-C1	118.71(13)	C1#1-Co1-C6-C5	-28.53(16)
C1#1-Co1-C2-C1	-147.02(11)	C1-Co1-C6-C5	117.37(13)
C2#1-Co1-C2-C1	-108.21(13)	C2#1-Co1-C6-C5	-14.8(7)
C6#1-Co1-C2-C1	-15.6(7)	C2-Co1-C6-C5	77.60(12)
C6-Co1-C2-C1	79.22(13)	C6#1-Co1-C6-C5	-109.81(14)
C5#1-Co1-C2-C3	-148.13(13)	C5#1-Co1-C6-C7	91.33(15)
C5-Co1-C2-C3	-0.80(14)	C5-Co1-C6-C7	-120.4(2)
C1#1-Co1-C2-C3	93.47(15)	C1#1-Co1-C6-C7	-148.92(14)
C1-Co1-C2-C3	-119.5(2)	C1-Co1-C6-C7	-3.02(15)
C2#1-Co1-C2-C3	132.28(17)	C2#1-Co1-C6-C7	-135.2(6)
C6#1-Co1-C2-C3	-135.2(6)	C2-Co1-C6-C7	-42.79(15)
C6-Co1-C2-C3	-40.29(15)	C6#1-Co1-C6-C7	129.80(18)
C1-C2-C3-C4	-97.9(2)	C5-C6-C7-C8	-94.6(2)
Co1-C2-C3-C4	-16.7(2)	Co1-C6-C7-C8	-13.9(2)
C2-C3-C4-C5	31.3(2)	C2-C1-C8-C7	46.8(3)
C3-C4-C5-C6	47.6(3)	Co1-C1-C8-C7	-32.5(2)
C3-C4-C5-Co1	-32.7(2)	C6-C7-C8-C1	30.0(2)

O3-K1-O1-C10	-126.76(13)	O2-K1-O3-C16	-65.11(13)
O3#2-K1-O1-C10	-66.46(14)	O2#2-K1-O3-C16	87.71(14)
O2-K1-O1-C10	150.93(15)	O1#2-K1-O3-C16	35.56(13)
O2#2-K1-O1-C10	31.99(14)	O1-K1-O3-C16	-124.81(13)
O1#2-K1-O1-C10	85.11(13)	N1-K1-O3-C16	-14.02(13)
N1-K1-O1-C10	162.11(13)	N1#2-K1-O3-C16	166.30(12)
N1#2-K1-O1-C10	-15.42(13)	O3-K1-N1-C14	-137.12(13)
O3-K1-O1-C11	91.54(13)	O3#2-K1-N1-C14	-151.15(11)
O3#2-K1-O1-C11	151.85(12)	O2-K1-N1-C14	-19.63(11)
O2-K1-O1-C11	9.23(12)	O2#2-K1-N1-C14	90.48(12)
O2#2-K1-O1-C11	-109.71(13)	O1#2-K1-N1-C14	103.86(12)
O1#2-K1-O1-C11	-56.58(12)	O1-K1-N1-C14	-30.74(13)
N1-K1-O1-C11	20.41(14)	N1#2-K1-N1-C14	35.95(12)
N1#2-K1-O1-C11	-157.12(14)	O3-K1-N1-C15	-17.42(11)
O3-K1-O2-C13	42.00(14)	O3#2-K1-N1-C15	-31.46(13)
O3#2-K1-O2-C13	93.97(14)	O2-K1-N1-C15	100.06(12)
O2#2-K1-O2-C13	-117.52(14)	O2#2-K1-N1-C15	-149.83(11)
O1#2-K1-O2-C13	-56.88(14)	O1#2-K1-N1-C15	-136.45(13)
O1-K1-O2-C13	158.83(15)	O1-K1-N1-C15	88.95(12)
N1-K1-O2-C13	-9.99(13)	N1#2-K1-N1-C15	155.64(11)
N1#2-K1-O2-C13	172.18(13)	O3-K1-N1-C9#2	102.61(13)
O3-K1-O2-C12	-92.33(12)	O3#2-K1-N1-C9#2	88.58(12)
O3#2-K1-O2-C12	-40.36(14)	O2-K1-N1-C9#2	-139.91(13)
O2#2-K1-O2-C12	108.15(12)	O2#2-K1-N1-C9#2	-29.79(13)
O1#2-K1-O2-C12	168.79(12)	O1#2-K1-N1-C9#2	-16.41(11)
O1-K1-O2-C12	24.49(11)	O1-K1-N1-C9#2	-151.01(11)
N1-K1-O2-C12	-144.32(13)	N1#2-K1-N1-C9#2	-84.32(12)
N1#2-K1-O2-C12	37.85(13)	C11-O1-C10-C9	-172.30(16)
O3#2-K1-O3-C17	17.12(10)	K1-O1-C10-C9	44.2(2)
O2-K1-O3-C17	159.98(12)	N1#2-C9-C10-O1	-61.0(2)
O2#2-K1-O3-C17	-47.21(14)	C10-O1-C11-C12	175.00(16)
O1#2-K1-O3-C17	-99.35(12)	K1-O1-C11-C12	-40.11(19)
O1-K1-O3-C17	100.28(12)	C13-O2-C12-C11	164.92(16)
N1-K1-O3-C17	-148.94(13)	K1-O2-C12-C11	-56.08(17)
N1#2-K1-O3-C17	31.39(14)	O1-C11-C12-O2	64.1(2)
O3#2-K1-O3-C16	152.03(16)	C12-O2-C13-C14	172.67(16)

K1-O2-C13-C14	37.6(2)	K1-N1-C15-C16	48.86(18)
C15-N1-C14-C13	-67.8(2)	C17-O3-C16-C15	-179.97(16)
C9#2-N1-C14-C13	170.19(17)	K1-O3-C16-C15	43.56(19)
K1-N1-C14-C13	49.40(19)	N1-C15-C16-O3	-64.8(2)
O2-C13-C14-N1	-59.6(2)	C16-O3-C17-C17#2	174.39(18)
C14-N1-C15-C16	166.99(17)	K1-O3-C17-C17#2	-48.1(2)
C9#2-N1-C15-C16	-71.3(2)		

Symmetry transformations used to generate equivalent atoms:

#1 $-x+3/2, -y+1/2, z$ #2 $-x+3/2, -y+3/2, z$

REFERENCE NUMBER: 04347 [10a]

CRYSTAL STRUCTURE REPORT

$C_{30} H_{44} Co K O_6$

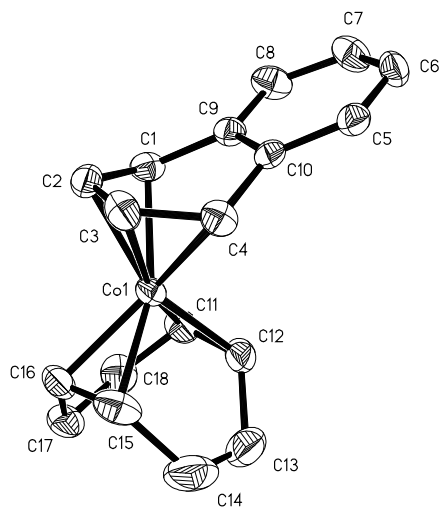
or

$[K(18\text{-crown-6})][Co(\eta^4\text{-}C_{10}H_8)(1,5\text{-COD})]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

December 12, 2004



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Data collection

A crystal (approximate dimensions 0.50 x 0.20 x 0.08 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 94 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 20 seconds and a detector distance of 4.81 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 3487 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ 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. Hydrogen atoms on metal-coordinated carbon atoms were found from the difference map and refined with individual isotropic displacement parameters. The remaining 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 $R1 = 0.0491$ and $wR2 = 0.1301$ (F^2 , all data).

Structure description

The structure is the one suggested. There are two independent cation-anion pairs in the asymmetric unit with all atoms on general positions. All cation-anion pairs are well separated from one another. One of the anions (Co1) has close contact to its potassium cation (K1) through the 1,5-COD ligand; the other (Co2) has close contact to its potassium cation (K2) through the naphthalene ligand. The initial synthesis involved 1,3-COD, which apparently isomerized to 1,5-COD. The fold (dihedral) angles on the naphthalene ligands are 32.4(2)° and 27.8(2)° for naphthalene ligands bound to Co1 and Co2, respectively. The respective twist angles are 69.6° and 69.1°: the overall geometry is closer to tetrahedral than to square planar.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-

- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
- ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
- ³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
- ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
- ⁵ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

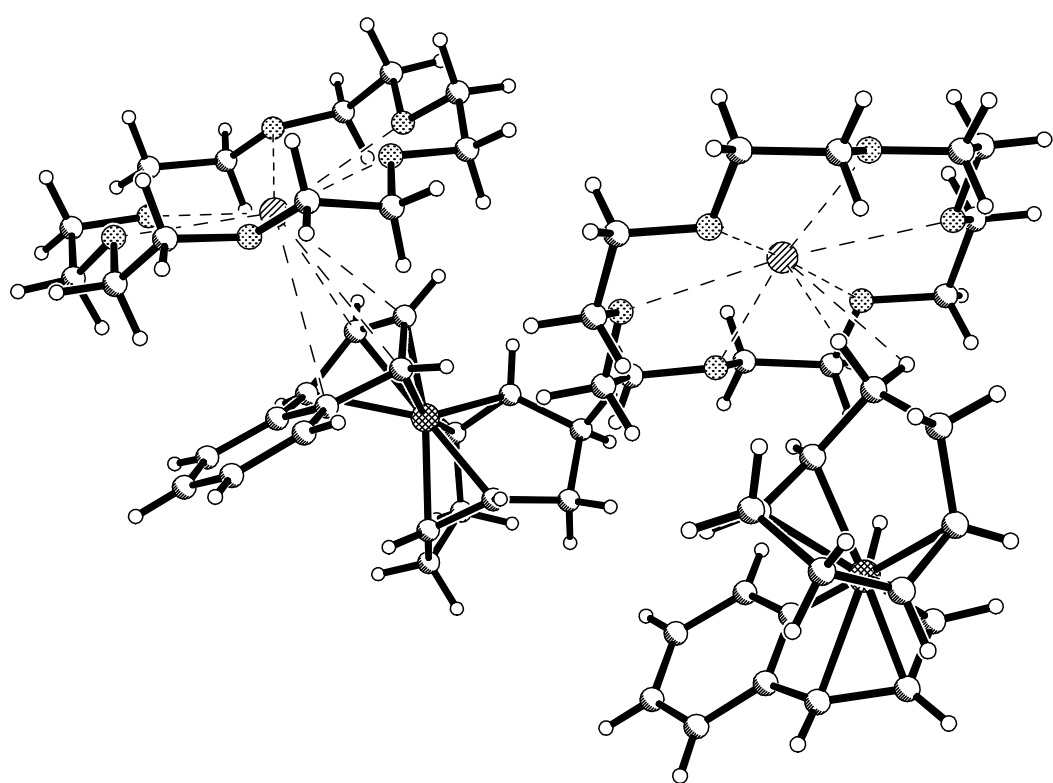
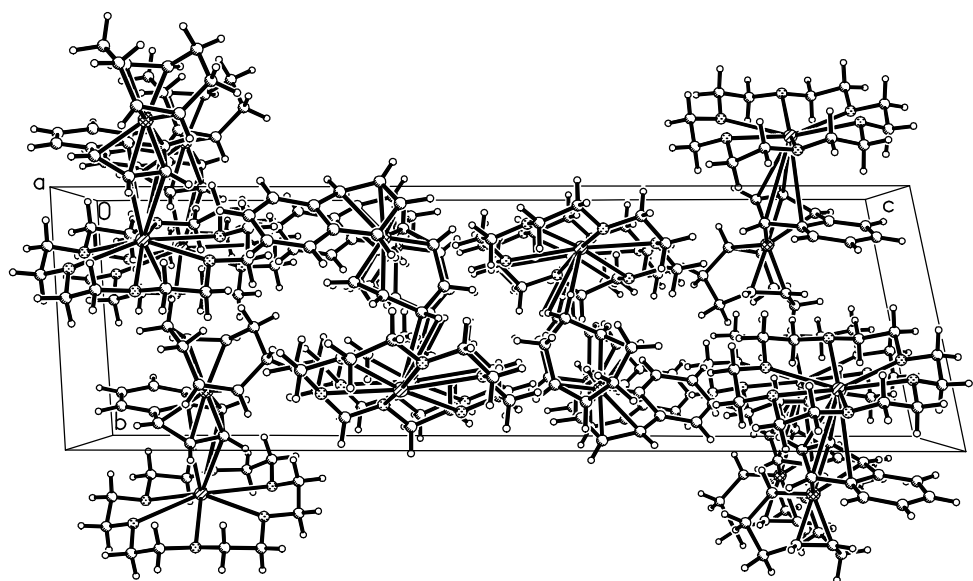
$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2 (F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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



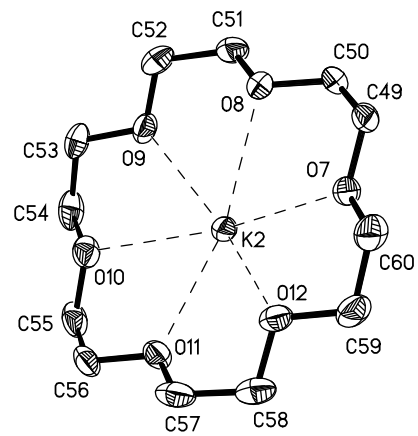
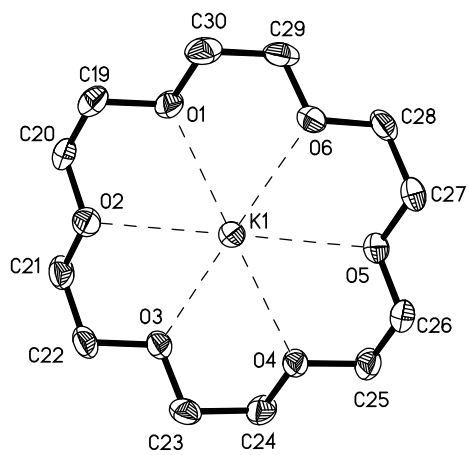
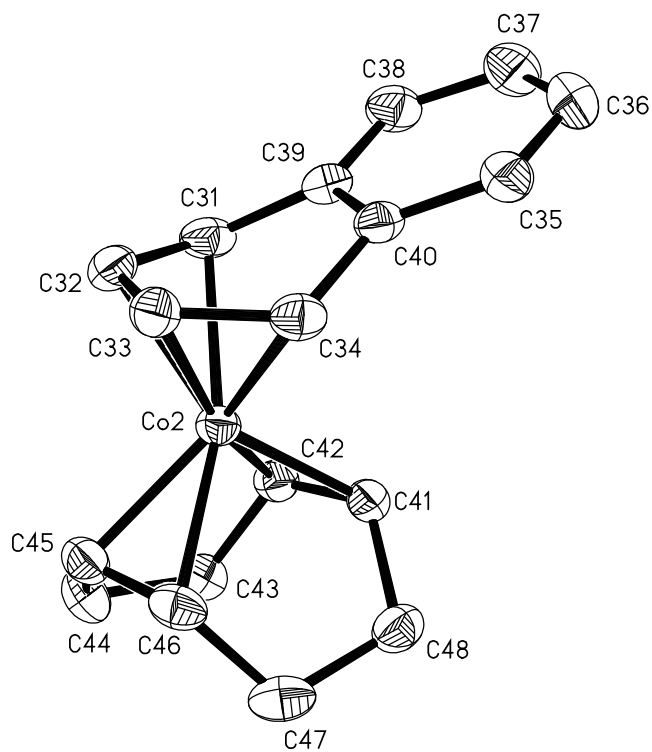


Table 1. Crystal data and structure refinement for 04344.

Identification code	04344	
Empirical formula	C ₃₀ H ₄₄ Co K O ₆	
Formula weight	598.68	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 10.040(2) Å	α = 82.405(3)°
	<i>b</i> = 10.195(2) Å	β = 88.299(3)°
	<i>c</i> = 30.618(5) Å	γ = 68.125(3)°
Volume	2882.2(9) Å ³	
<i>Z</i>	4	
Density (calculated)	1.380 Mg/m ³	
Absorption coefficient	0.781 mm ⁻¹	
<i>F</i> (000)	1272	
Crystal color, morphology	red-brown, plate	
Crystal size	0.50 x 0.20 x 0.08 mm ³	
Theta range for data collection	1.34 to 27.52°	
Index ranges	-13 ≤ <i>h</i> ≤ 12, -13 ≤ <i>k</i> ≤ 13, -39 ≤ <i>l</i> ≤ 39	
Reflections collected	34032	
Independent reflections	13089 [<i>R</i> (int) = 0.0413]	
Observed reflections	9905	
Completeness to theta = 27.52°	98.6%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9402 and 0.6961	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	13089 / 0 / 749	
Goodness-of-fit on <i>F</i> ²	1.033	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0491, <i>wR</i> 2 = 0.1201	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0709, <i>wR</i> 2 = 0.1301	
Largest diff. peak and hole	1.059 and -0.369 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04344. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	3433(1)	2123(1)	3888(1)	24(1)
C1	5547(3)	2105(3)	3851(1)	28(1)
C2	5405(3)	951(3)	4137(1)	32(1)
C3	4820(3)	113(3)	3935(1)	32(1)
C4	4498(3)	469(3)	3478(1)	29(1)
C5	5774(3)	771(3)	2768(1)	29(1)
C6	6564(3)	1453(3)	2518(1)	32(1)
C7	7033(4)	2372(3)	2700(1)	38(1)
C8	6755(3)	2585(3)	3141(1)	37(1)
C9	5946(3)	1928(3)	3391(1)	26(1)
C10	5418(3)	1031(3)	3197(1)	24(1)
C11	2647(4)	4261(3)	3792(1)	34(1)
C12	2060(3)	3761(4)	3476(1)	39(1)
C13	539(4)	3786(5)	3498(1)	55(1)
C14	437(4)	2482(5)	3771(2)	62(1)
C15	1684(4)	1724(4)	4093(1)	40(1)
C16	2121(3)	2356(4)	4416(1)	33(1)
C17	1290(4)	3904(4)	4470(1)	39(1)
C18	1882(4)	4887(4)	4191(1)	43(1)
K1	2813(1)	7676(1)	3871(1)	35(1)
O1	7(2)	8330(2)	3619(1)	36(1)
C19	-1068(3)	9185(4)	3884(1)	40(1)
C20	-746(3)	8537(4)	4354(1)	36(1)
O2	598(2)	8557(2)	4482(1)	34(1)
C21	989(4)	7964(4)	4925(1)	39(1)
C22	2383(4)	8073(4)	5033(1)	38(1)
O3	3486(2)	7176(2)	4784(1)	32(1)
C23	4857(3)	7170(4)	4891(1)	37(1)
C24	5965(3)	6164(4)	4627(1)	39(1)
O4	5661(2)	6657(2)	4173(1)	30(1)
C25	6738(3)	5838(4)	3902(1)	37(1)

C26	6398(3)	6510(4)	3432(1)	36(1)
O5	5043(2)	6501(2)	3314(1)	33(1)
C27	4710(4)	6939(4)	2855(1)	39(1)
C28	3304(4)	6840(4)	2761(1)	37(1)
O6	2206(2)	7840(2)	2985(1)	34(1)
C29	831(4)	7788(4)	2909(1)	38(1)
C30	-268(4)	8813(4)	3162(1)	41(1)
Co2	6785(1)	7935(1)	1499(1)	23(1)
C31	4508(3)	8733(3)	1574(1)	31(1)
C32	5149(3)	9746(3)	1598(1)	32(1)
C33	5931(3)	9981(3)	1229(1)	29(1)
C34	5977(3)	9209(3)	870(1)	27(1)
C35	4386(3)	8610(3)	368(1)	32(1)
C36	3284(4)	8118(4)	324(1)	40(1)
C37	2519(3)	7884(4)	684(1)	41(1)
C38	2850(3)	8128(3)	1098(1)	34(1)
C39	3983(3)	8564(3)	1151(1)	26(1)
C40	4770(3)	8824(3)	779(1)	25(1)
C41	7437(3)	5919(3)	1354(1)	27(1)
C42	7066(3)	5966(3)	1799(1)	26(1)
C43	8174(3)	5453(3)	2176(1)	30(1)
C44	8534(4)	6668(4)	2311(1)	35(1)
C45	8310(3)	7858(3)	1934(1)	29(1)
C46	8906(3)	7629(3)	1513(1)	30(1)
C47	9839(3)	6168(4)	1401(1)	38(1)
C48	8976(3)	5416(3)	1209(1)	32(1)
K2	2359(1)	12173(1)	1158(1)	29(1)
O7	3018(2)	13276(2)	341(1)	32(1)
C49	2133(3)	13481(4)	-35(1)	35(1)
C50	1482(3)	12379(4)	20(1)	35(1)
O8	567(2)	12588(2)	387(1)	33(1)
C51	-129(4)	11604(4)	440(1)	44(1)
C52	-1005(4)	11808(5)	846(1)	48(1)
O9	-58(2)	11423(2)	1215(1)	36(1)
C53	-779(4)	11444(4)	1623(1)	42(1)
C54	324(4)	10951(4)	1985(1)	45(1)

O10	974(2)	11978(2)	1979(1)	39(1)
C55	1932(4)	11716(4)	2341(1)	46(1)
C56	2434(4)	12921(4)	2319(1)	45(1)
O11	3197(2)	12984(2)	1923(1)	37(1)
C57	3680(4)	14138(4)	1872(1)	46(1)
C58	4596(4)	14029(4)	1476(1)	45(1)
O12	3775(2)	14107(2)	1099(1)	37(1)
C59	4567(4)	14075(4)	709(1)	46(1)
C60	3589(4)	14357(4)	321(1)	44(1)

Table 3. Bond lengths [Å] and angles [°] for 04344.

Co(1)-C(3)	1.992(3)	C(13)-H(13B)	0.9900
Co(1)-C(2)	2.004(3)	C(14)-C(15)	1.512(6)
Co(1)-C(11)	2.006(3)	C(14)-H(14A)	0.9900
Co(1)-C(15)	2.010(3)	C(14)-H(14B)	0.9900
Co(1)-C(12)	2.027(3)	C(15)-C(16)	1.411(5)
Co(1)-C(16)	2.038(3)	C(15)-H(15)	0.96(4)
Co(1)-C(1)	2.116(3)	C(16)-C(17)	1.514(5)
Co(1)-C(4)	2.168(3)	C(16)-H(16)	0.88(3)
C(1)-C(2)	1.421(5)	C(17)-C(18)	1.508(5)
C(1)-C(9)	1.466(4)	C(17)-H(17A)	0.9900
C(1)-H(1)	0.98(3)	C(17)-H(17B)	0.9900
C(2)-C(3)	1.411(5)	C(18)-K(1)	3.333(4)
C(2)-H(2)	1.03(4)	C(18)-H(18A)	0.9900
C(3)-C(4)	1.415(4)	C(18)-H(18B)	0.9900
C(3)-H(3)	0.92(3)	K(1)-O(1)	2.751(2)
C(4)-C(10)	1.462(4)	K(1)-O(6)	2.766(2)
C(4)-H(4)	0.92(4)	K(1)-O(5)	2.769(2)
C(5)-C(10)	1.384(4)	K(1)-O(4)	2.793(2)
C(5)-C(6)	1.391(4)	K(1)-O(2)	2.821(2)
C(5)-H(5)	0.9500	K(1)-O(3)	2.832(2)
C(6)-C(7)	1.376(5)	O(1)-C(30)	1.420(4)
C(6)-H(6)	0.9500	O(1)-C(19)	1.422(4)
C(7)-C(8)	1.398(5)	C(19)-C(20)	1.491(5)
C(7)-H(7)	0.9500	C(19)-H(19A)	0.9900
C(8)-C(9)	1.389(4)	C(19)-H(19B)	0.9900
C(8)-H(8)	0.9500	C(20)-O(2)	1.424(4)
C(9)-C(10)	1.412(4)	C(20)-H(20A)	0.9900
C(11)-C(12)	1.389(5)	C(20)-H(20B)	0.9900
C(11)-C(18)	1.509(4)	O(2)-C(21)	1.416(4)
C(11)-H(11)	0.98(3)	C(21)-C(22)	1.494(5)
C(12)-C(13)	1.518(5)	C(21)-H(21A)	0.9900
C(12)-H(12)	0.94(4)	C(21)-H(21B)	0.9900
C(13)-C(14)	1.510(6)	C(22)-O(3)	1.423(4)
C(13)-H(13A)	0.9900	C(22)-H(22A)	0.9900

C(22)-H(22B)	0.9900	C(31)-C(32)	1.416(5)
O(3)-C(23)	1.421(4)	C(31)-C(39)	1.467(4)
C(23)-C(24)	1.502(5)	C(31)-K(2)	3.452(3)
C(23)-H(23A)	0.9900	C(31)-H(31)	1.07(3)
C(23)-H(23B)	0.9900	C(32)-C(33)	1.404(4)
C(24)-O(4)	1.416(4)	C(32)-K(2)	3.157(3)
C(24)-H(24A)	0.9900	C(32)-H(32)	0.93(4)
C(24)-H(24B)	0.9900	C(33)-C(34)	1.424(4)
O(4)-C(25)	1.419(4)	C(33)-K(2)	3.443(3)
C(25)-C(26)	1.499(5)	C(33)-H(33)	0.89(3)
C(25)-H(25A)	0.9900	C(34)-C(40)	1.451(4)
C(25)-H(25B)	0.9900	C(34)-H(34)	0.89(3)
C(26)-O(5)	1.421(4)	C(35)-C(36)	1.390(4)
C(26)-H(26A)	0.9900	C(35)-C(40)	1.394(4)
C(26)-H(26B)	0.9900	C(35)-H(35)	0.9500
O(5)-C(27)	1.427(4)	C(36)-C(37)	1.371(5)
C(27)-C(28)	1.492(5)	C(36)-H(36)	0.9500
C(27)-H(27A)	0.9900	C(37)-C(38)	1.394(5)
C(27)-H(27B)	0.9900	C(37)-H(37)	0.9500
C(28)-O(6)	1.424(4)	C(38)-C(39)	1.388(4)
C(28)-H(28A)	0.9900	C(38)-H(38)	0.9500
C(28)-H(28B)	0.9900	C(39)-C(40)	1.420(4)
O(6)-C(29)	1.428(4)	C(39)-K(2)	3.427(3)
C(29)-C(30)	1.487(5)	C(41)-C(42)	1.404(4)
C(29)-H(29A)	0.9900	C(41)-C(48)	1.509(4)
C(29)-H(29B)	0.9900	C(41)-H(41)	0.95(4)
C(30)-H(30A)	0.9900	C(42)-C(43)	1.525(4)
C(30)-H(30B)	0.9900	C(42)-H(42)	0.94(4)
Co(2)-C(33)	2.006(3)	C(43)-C(44)	1.521(4)
Co(2)-C(32)	2.014(3)	C(43)-H(43A)	0.9900
Co(2)-C(42)	2.014(3)	C(43)-H(43B)	0.9900
Co(2)-C(41)	2.018(3)	C(44)-C(45)	1.514(4)
Co(2)-C(45)	2.031(3)	C(44)-H(44A)	0.9900
Co(2)-C(46)	2.035(3)	C(44)-H(44B)	0.9900
Co(2)-C(31)	2.138(3)	C(45)-C(46)	1.415(4)
Co(2)-C(34)	2.169(3)	C(45)-H(45)	0.93(3)

C(46)-C(47)	1.513(5)	C(55)-C(56)	1.485(6)
C(46)-H(46)	0.93(3)	C(55)-H(55A)	0.9900
C(47)-C(48)	1.526(5)	C(55)-H(55B)	0.9900
C(47)-H(47A)	0.9900	C(56)-O(11)	1.422(4)
C(47)-H(47B)	0.9900	C(56)-H(56A)	0.9900
C(48)-H(48A)	0.9900	C(56)-H(56B)	0.9900
C(48)-H(48B)	0.9900	O(11)-C(57)	1.420(4)
K(2)-O(7)	2.770(2)	C(57)-C(58)	1.491(5)
K(2)-O(9)	2.797(2)	C(57)-H(57A)	0.9900
K(2)-O(12)	2.815(2)	C(57)-H(57B)	0.9900
K(2)-O(11)	2.832(2)	C(58)-O(12)	1.414(4)
K(2)-O(10)	2.857(2)	C(58)-H(58A)	0.9900
K(2)-O(8)	2.899(2)	C(58)-H(58B)	0.9900
O(7)-C(60)	1.413(4)	O(12)-C(59)	1.413(4)
O(7)-C(49)	1.421(4)	C(59)-C(60)	1.491(5)
C(49)-C(50)	1.487(5)	C(59)-H(59A)	0.9900
C(49)-H(49A)	0.9900	C(59)-H(59B)	0.9900
C(49)-H(49B)	0.9900	C(60)-H(60A)	0.9900
C(50)-O(8)	1.419(4)	C(60)-H(60B)	0.9900
C(50)-H(50A)	0.9900	C(3)-Co(1)-C(2)	41.36(13)
C(50)-H(50B)	0.9900	C(3)-Co(1)-C(11)	160.64(14)
O(8)-C(51)	1.411(4)	C(2)-Co(1)-C(11)	123.21(14)
C(51)-C(52)	1.493(5)	C(3)-Co(1)-C(15)	97.89(14)
C(51)-H(51A)	0.9900	C(2)-Co(1)-C(15)	122.63(15)
C(51)-H(51B)	0.9900	C(11)-Co(1)-C(15)	101.39(14)
C(52)-O(9)	1.417(4)	C(3)-Co(1)-C(12)	144.55(14)
C(52)-H(52A)	0.9900	C(2)-Co(1)-C(12)	151.72(14)
C(52)-H(52B)	0.9900	C(11)-Co(1)-C(12)	40.29(14)
O(9)-C(53)	1.422(4)	C(15)-Co(1)-C(12)	85.64(15)
C(53)-C(54)	1.489(5)	C(3)-Co(1)-C(16)	109.11(13)
C(53)-H(53A)	0.9900	C(2)-Co(1)-C(16)	105.09(13)
C(53)-H(53B)	0.9900	C(11)-Co(1)-C(16)	84.81(13)
C(54)-O(10)	1.423(4)	C(15)-Co(1)-C(16)	40.81(13)
C(54)-H(54A)	0.9900	C(12)-Co(1)-C(16)	96.56(14)
C(54)-H(54B)	0.9900	C(3)-Co(1)-C(1)	70.87(13)
O(10)-C(55)	1.419(4)	C(2)-Co(1)-C(1)	40.23(13)

C(11)-Co(1)-C(1)	89.99(13)	C(10)-C(5)-H(5)	119.6
C(15)-Co(1)-C(1)	162.23(14)	C(6)-C(5)-H(5)	119.6
C(12)-Co(1)-C(1)	111.58(14)	C(7)-C(6)-C(5)	120.0(3)
C(16)-Co(1)-C(1)	128.59(12)	C(7)-C(6)-H(6)	120.0
C(3)-Co(1)-C(4)	39.50(12)	C(5)-C(6)-H(6)	120.0
C(2)-Co(1)-C(4)	70.72(12)	C(6)-C(7)-C(8)	119.9(3)
C(11)-Co(1)-C(4)	134.74(12)	C(6)-C(7)-H(7)	120.0
C(15)-Co(1)-C(4)	103.62(13)	C(8)-C(7)-H(7)	120.0
C(12)-Co(1)-C(4)	105.28(13)	C(9)-C(8)-C(7)	120.5(3)
C(16)-Co(1)-C(4)	136.75(12)	C(9)-C(8)-H(8)	119.7
C(1)-Co(1)-C(4)	76.78(11)	C(7)-C(8)-H(8)	119.7
C(2)-C(1)-C(9)	119.6(3)	C(8)-C(9)-C(10)	119.2(3)
C(2)-C(1)-Co(1)	65.66(17)	C(8)-C(9)-C(1)	125.4(3)
C(9)-C(1)-Co(1)	104.66(19)	C(10)-C(9)-C(1)	115.4(3)
C(2)-C(1)-H(1)	118.8(18)	C(5)-C(10)-C(9)	119.3(3)
C(9)-C(1)-H(1)	117.2(18)	C(5)-C(10)-C(4)	125.5(3)
Co(1)-C(1)-H(1)	118.7(18)	C(9)-C(10)-C(4)	115.1(3)
C(3)-C(2)-C(1)	114.6(3)	C(12)-C(11)-C(18)	125.4(3)
C(3)-C(2)-Co(1)	68.85(17)	C(12)-C(11)-Co(1)	70.67(19)
C(1)-C(2)-Co(1)	74.11(17)	C(18)-C(11)-Co(1)	111.9(2)
C(3)-C(2)-H(2)	123(2)	C(12)-C(11)-H(11)	114(2)
C(1)-C(2)-H(2)	123(2)	C(18)-C(11)-H(11)	116(2)
Co(1)-C(2)-H(2)	122(2)	Co(1)-C(11)-H(11)	108(2)
C(2)-C(3)-C(4)	117.6(3)	C(11)-C(12)-C(13)	122.7(3)
C(2)-C(3)-Co(1)	69.79(17)	C(11)-C(12)-Co(1)	69.04(18)
C(4)-C(3)-Co(1)	76.97(18)	C(13)-C(12)-Co(1)	112.2(3)
C(2)-C(3)-H(3)	119(2)	C(11)-C(12)-H(12)	120(2)
C(4)-C(3)-H(3)	123(2)	C(13)-C(12)-H(12)	112(2)
Co(1)-C(3)-H(3)	124(2)	Co(1)-C(12)-H(12)	112(2)
C(3)-C(4)-C(10)	118.6(3)	C(14)-C(13)-C(12)	112.8(3)
C(3)-C(4)-Co(1)	63.53(16)	C(14)-C(13)-H(13A)	109.0
C(10)-C(4)-Co(1)	104.31(19)	C(12)-C(13)-H(13A)	109.0
C(3)-C(4)-H(4)	119(2)	C(14)-C(13)-H(13B)	109.0
C(10)-C(4)-H(4)	116(2)	C(12)-C(13)-H(13B)	109.0
Co(1)-C(4)-H(4)	125(2)	H(13A)-C(13)-H(13B)	107.8
C(10)-C(5)-C(6)	120.8(3)	C(13)-C(14)-C(15)	113.3(3)

C(13)-C(14)-H(14A)	108.9	O(1)-K(1)-O(4)	172.39(7)
C(15)-C(14)-H(14A)	108.9	O(6)-K(1)-O(4)	120.02(6)
C(13)-C(14)-H(14B)	108.9	O(5)-K(1)-O(4)	59.45(6)
C(15)-C(14)-H(14B)	108.9	O(1)-K(1)-O(2)	59.89(6)
H(14A)-C(14)-H(14B)	107.7	O(6)-K(1)-O(2)	121.20(7)
C(16)-C(15)-C(14)	125.3(3)	O(5)-K(1)-O(2)	173.56(7)
C(16)-C(15)-Co(1)	70.64(18)	O(4)-K(1)-O(2)	118.77(6)
C(14)-C(15)-Co(1)	111.1(3)	O(1)-K(1)-O(3)	117.94(7)
C(16)-C(15)-H(15)	118(2)	O(6)-K(1)-O(3)	173.51(7)
C(14)-C(15)-H(15)	113(2)	O(5)-K(1)-O(3)	116.88(7)
Co(1)-C(15)-H(15)	109(2)	O(4)-K(1)-O(3)	59.15(6)
C(15)-C(16)-C(17)	120.0(3)	O(2)-K(1)-O(3)	60.14(6)
C(15)-C(16)-Co(1)	68.56(18)	O(1)-K(1)-C(18)	70.58(8)
C(17)-C(16)-Co(1)	112.6(2)	O(6)-K(1)-C(18)	95.47(8)
C(15)-C(16)-H(16)	117(2)	O(5)-K(1)-C(18)	100.71(8)
C(17)-C(16)-H(16)	117(2)	O(4)-K(1)-C(18)	101.80(8)
Co(1)-C(16)-H(16)	112(2)	O(2)-K(1)-C(18)	73.32(7)
C(18)-C(17)-C(16)	111.9(3)	O(3)-K(1)-C(18)	78.71(8)
C(18)-C(17)-H(17A)	109.2	C(30)-O(1)-C(19)	112.4(2)
C(16)-C(17)-H(17A)	109.2	C(30)-O(1)-K(1)	113.37(18)
C(18)-C(17)-H(17B)	109.2	C(19)-O(1)-K(1)	116.61(18)
C(16)-C(17)-H(17B)	109.2	O(1)-C(19)-C(20)	108.4(2)
H(17A)-C(17)-H(17B)	107.9	O(1)-C(19)-H(19A)	110.0
C(17)-C(18)-C(11)	112.6(3)	C(20)-C(19)-H(19A)	110.0
C(17)-C(18)-K(1)	160.2(2)	O(1)-C(19)-H(19B)	110.0
C(11)-C(18)-K(1)	87.0(2)	C(20)-C(19)-H(19B)	110.0
C(17)-C(18)-H(18A)	109.1	H(19A)-C(19)-H(19B)	108.4
C(11)-C(18)-H(18A)	109.1	O(2)-C(20)-C(19)	108.9(3)
K(1)-C(18)-H(18A)	59.5	O(2)-C(20)-H(20A)	109.9
C(17)-C(18)-H(18B)	109.1	C(19)-C(20)-H(20A)	109.9
C(11)-C(18)-H(18B)	109.1	O(2)-C(20)-H(20B)	109.9
K(1)-C(18)-H(18B)	64.1	C(19)-C(20)-H(20B)	109.9
H(18A)-C(18)-H(18B)	107.8	H(20A)-C(20)-H(20B)	108.3
O(1)-K(1)-O(6)	61.96(6)	C(21)-O(2)-C(20)	112.8(2)
O(1)-K(1)-O(5)	120.93(7)	C(21)-O(2)-K(1)	115.22(17)
O(6)-K(1)-O(5)	61.04(6)	C(20)-O(2)-K(1)	115.25(17)

O(2)-C(21)-C(22)	108.9(3)	O(5)-C(26)-C(25)	108.1(3)
O(2)-C(21)-H(21A)	109.9	O(5)-C(26)-H(26A)	110.1
C(22)-C(21)-H(21A)	109.9	C(25)-C(26)-H(26A)	110.1
O(2)-C(21)-H(21B)	109.9	O(5)-C(26)-H(26B)	110.1
C(22)-C(21)-H(21B)	109.9	C(25)-C(26)-H(26B)	110.1
H(21A)-C(21)-H(21B)	108.3	H(26A)-C(26)-H(26B)	108.4
O(3)-C(22)-C(21)	109.0(3)	C(26)-O(5)-C(27)	112.4(2)
O(3)-C(22)-H(22A)	109.9	C(26)-O(5)-K(1)	115.84(17)
C(21)-C(22)-H(22A)	109.9	C(27)-O(5)-K(1)	115.14(18)
O(3)-C(22)-H(22B)	109.9	O(5)-C(27)-C(28)	108.4(3)
C(21)-C(22)-H(22B)	109.9	O(5)-C(27)-H(27A)	110.0
H(22A)-C(22)-H(22B)	108.3	C(28)-C(27)-H(27A)	110.0
C(23)-O(3)-C(22)	111.8(2)	O(5)-C(27)-H(27B)	110.0
C(23)-O(3)-K(1)	114.62(17)	C(28)-C(27)-H(27B)	110.0
C(22)-O(3)-K(1)	112.90(17)	H(27A)-C(27)-H(27B)	108.4
O(3)-C(23)-C(24)	108.6(3)	O(6)-C(28)-C(27)	109.1(3)
O(3)-C(23)-H(23A)	110.0	O(6)-C(28)-H(28A)	109.9
C(24)-C(23)-H(23A)	110.0	C(27)-C(28)-H(28A)	109.9
O(3)-C(23)-H(23B)	110.0	O(6)-C(28)-H(28B)	109.9
C(24)-C(23)-H(23B)	110.0	C(27)-C(28)-H(28B)	109.9
H(23A)-C(23)-H(23B)	108.3	H(28A)-C(28)-H(28B)	108.3
O(4)-C(24)-C(23)	108.9(3)	C(28)-O(6)-C(29)	111.6(2)
O(4)-C(24)-H(24A)	109.9	C(28)-O(6)-K(1)	113.85(17)
C(23)-C(24)-H(24A)	109.9	C(29)-O(6)-K(1)	112.63(17)
O(4)-C(24)-H(24B)	109.9	O(6)-C(29)-C(30)	109.5(3)
C(23)-C(24)-H(24B)	109.9	O(6)-C(29)-H(29A)	109.8
H(24A)-C(24)-H(24B)	108.3	C(30)-C(29)-H(29A)	109.8
C(24)-O(4)-C(25)	112.3(2)	O(6)-C(29)-H(29B)	109.8
C(24)-O(4)-K(1)	118.77(17)	C(30)-C(29)-H(29B)	109.8
C(25)-O(4)-K(1)	117.89(17)	H(29A)-C(29)-H(29B)	108.2
O(4)-C(25)-C(26)	108.7(2)	O(1)-C(30)-C(29)	108.7(3)
O(4)-C(25)-H(25A)	110.0	O(1)-C(30)-H(30A)	110.0
C(26)-C(25)-H(25A)	110.0	C(29)-C(30)-H(30A)	110.0
O(4)-C(25)-H(25B)	110.0	O(1)-C(30)-H(30B)	110.0
C(26)-C(25)-H(25B)	110.0	C(29)-C(30)-H(30B)	110.0
H(25A)-C(25)-H(25B)	108.3	H(30A)-C(30)-H(30B)	108.3

C(33)-Co(2)-C(32)	40.88(13)	Co(2)-C(31)-H(31)	119.0(17)
C(33)-Co(2)-C(42)	164.11(12)	K(2)-C(31)-H(31)	110.8(17)
C(32)-Co(2)-C(42)	125.71(13)	C(33)-C(32)-C(31)	115.5(3)
C(33)-Co(2)-C(41)	142.62(12)	C(33)-C(32)-Co(2)	69.28(17)
C(32)-Co(2)-C(41)	148.36(13)	C(31)-C(32)-Co(2)	74.89(18)
C(42)-Co(2)-C(41)	40.75(12)	C(33)-C(32)-K(2)	89.45(18)
C(33)-Co(2)-C(45)	105.08(12)	C(31)-C(32)-K(2)	89.68(18)
C(32)-Co(2)-C(45)	102.49(13)	Co(2)-C(32)-K(2)	143.80(14)
C(42)-Co(2)-C(45)	85.10(12)	C(33)-C(32)-H(32)	119(2)
C(41)-Co(2)-C(45)	103.68(12)	C(31)-C(32)-H(32)	125(2)
C(33)-Co(2)-C(46)	100.79(13)	Co(2)-C(32)-H(32)	122(2)
C(32)-Co(2)-C(46)	125.67(13)	K(2)-C(32)-H(32)	93(2)
C(42)-Co(2)-C(46)	94.88(12)	C(32)-C(33)-C(34)	117.4(3)
C(41)-Co(2)-C(46)	85.94(12)	C(32)-C(33)-Co(2)	69.84(18)
C(45)-Co(2)-C(46)	40.73(13)	C(34)-C(33)-Co(2)	76.37(18)
C(33)-Co(2)-C(31)	70.18(12)	C(32)-C(33)-K(2)	66.49(16)
C(32)-Co(2)-C(31)	39.72(13)	C(34)-C(33)-K(2)	99.19(18)
C(42)-Co(2)-C(31)	93.95(12)	Co(2)-C(33)-K(2)	127.47(13)
C(41)-Co(2)-C(31)	108.91(12)	C(32)-C(33)-H(33)	118(2)
C(45)-Co(2)-C(31)	127.90(12)	C(34)-C(33)-H(33)	125(2)
C(46)-Co(2)-C(31)	164.56(13)	Co(2)-C(33)-H(33)	123(2)
C(33)-Co(2)-C(34)	39.62(12)	K(2)-C(33)-H(33)	102(2)
C(32)-Co(2)-C(34)	70.46(12)	C(33)-C(34)-C(40)	120.0(3)
C(42)-Co(2)-C(34)	137.71(12)	C(33)-C(34)-Co(2)	64.01(16)
C(41)-Co(2)-C(34)	103.02(12)	C(40)-C(34)-Co(2)	102.31(19)
C(45)-Co(2)-C(34)	133.17(12)	C(33)-C(34)-H(34)	117(2)
C(46)-Co(2)-C(34)	104.76(12)	C(40)-C(34)-H(34)	119(2)
C(31)-Co(2)-C(34)	76.61(11)	Co(2)-C(34)-H(34)	122(2)
C(32)-C(31)-C(39)	120.7(3)	C(36)-C(35)-C(40)	120.9(3)
C(32)-C(31)-Co(2)	65.39(16)	C(36)-C(35)-H(35)	119.6
C(39)-C(31)-Co(2)	102.78(19)	C(40)-C(35)-H(35)	119.6
C(32)-C(31)-K(2)	66.12(16)	C(37)-C(36)-C(35)	120.3(3)
C(39)-C(31)-K(2)	76.71(16)	C(37)-C(36)-H(36)	119.9
Co(2)-C(31)-K(2)	121.84(12)	C(35)-C(36)-H(36)	119.9
C(32)-C(31)-H(31)	117.7(17)	C(36)-C(37)-C(38)	120.1(3)
C(39)-C(31)-H(31)	118.0(16)	C(36)-C(37)-H(37)	119.9

C(38)-C(37)-H(37)	119.9	H(44A)-C(44)-H(44B)	107.9
C(39)-C(38)-C(37)	120.4(3)	C(46)-C(45)-C(44)	123.2(3)
C(39)-C(38)-H(38)	119.8	C(46)-C(45)-Co(2)	69.77(17)
C(37)-C(38)-H(38)	119.8	C(44)-C(45)-Co(2)	111.2(2)
C(38)-C(39)-C(40)	119.7(3)	C(46)-C(45)-H(45)	116(2)
C(38)-C(39)-C(31)	125.2(3)	C(44)-C(45)-H(45)	116(2)
C(40)-C(39)-C(31)	115.0(2)	Co(2)-C(45)-H(45)	111(2)
C(38)-C(39)-K(2)	103.94(19)	C(45)-C(46)-C(47)	122.8(3)
C(40)-C(39)-K(2)	89.00(16)	C(45)-C(46)-Co(2)	69.50(16)
C(31)-C(39)-K(2)	78.66(16)	C(47)-C(46)-Co(2)	111.7(2)
C(35)-C(40)-C(39)	118.5(3)	C(45)-C(46)-H(46)	118(2)
C(35)-C(40)-C(34)	125.7(3)	C(47)-C(46)-H(46)	112(2)
C(39)-C(40)-C(34)	115.7(3)	Co(2)-C(46)-H(46)	115(2)
C(42)-C(41)-C(48)	122.4(3)	C(46)-C(47)-C(48)	112.6(2)
C(42)-C(41)-Co(2)	69.47(16)	C(46)-C(47)-H(47A)	109.1
C(48)-C(41)-Co(2)	110.7(2)	C(48)-C(47)-H(47A)	109.1
C(42)-C(41)-H(41)	117(2)	C(46)-C(47)-H(47B)	109.1
C(48)-C(41)-H(41)	117(2)	C(48)-C(47)-H(47B)	109.1
Co(2)-C(41)-H(41)	108(2)	H(47A)-C(47)-H(47B)	107.8
C(41)-C(42)-C(43)	123.1(3)	C(41)-C(48)-C(47)	112.7(3)
C(41)-C(42)-Co(2)	69.78(17)	C(41)-C(48)-H(48A)	109.0
C(43)-C(42)-Co(2)	113.17(19)	C(47)-C(48)-H(48A)	109.0
C(41)-C(42)-H(42)	121(2)	C(41)-C(48)-H(48B)	109.0
C(43)-C(42)-H(42)	110(2)	C(47)-C(48)-H(48B)	109.0
Co(2)-C(42)-H(42)	114(2)	H(48A)-C(48)-H(48B)	107.8
C(44)-C(43)-C(42)	111.7(2)	O(7)-K(2)-O(9)	118.10(6)
C(44)-C(43)-H(43A)	109.3	O(7)-K(2)-O(12)	59.95(6)
C(42)-C(43)-H(43A)	109.3	O(9)-K(2)-O(12)	154.28(7)
C(44)-C(43)-H(43B)	109.3	O(7)-K(2)-O(11)	118.58(7)
C(42)-C(43)-H(43B)	109.3	O(9)-K(2)-O(11)	117.29(7)
H(43A)-C(43)-H(43B)	107.9	O(12)-K(2)-O(11)	58.65(7)
C(45)-C(44)-C(43)	112.2(2)	O(7)-K(2)-O(10)	160.79(7)
C(45)-C(44)-H(44A)	109.2	O(9)-K(2)-O(10)	59.17(7)
C(43)-C(44)-H(44A)	109.2	O(12)-K(2)-O(10)	113.24(7)
C(45)-C(44)-H(44B)	109.2	O(11)-K(2)-O(10)	58.38(7)
C(43)-C(44)-H(44B)	109.2	O(7)-K(2)-O(8)	59.02(6)

O(9)-K(2)-O(8)	59.09(6)	C(49)-O(7)-K(2)	120.69(17)
O(12)-K(2)-O(8)	112.42(7)	O(7)-C(49)-C(50)	108.5(2)
O(11)-K(2)-O(8)	154.67(7)	O(7)-C(49)-H(49A)	110.0
O(10)-K(2)-O(8)	114.52(7)	C(50)-C(49)-H(49A)	110.0
O(7)-K(2)-C(32)	109.36(8)	O(7)-C(49)-H(49B)	110.0
O(9)-K(2)-C(32)	113.40(8)	C(50)-C(49)-H(49B)	110.0
O(12)-K(2)-C(32)	89.59(8)	H(49A)-C(49)-H(49B)	108.4
O(11)-K(2)-C(32)	69.28(7)	O(8)-C(50)-C(49)	109.2(3)
O(10)-K(2)-C(32)	87.74(7)	O(8)-C(50)-H(50A)	109.8
O(8)-K(2)-C(32)	136.05(8)	C(49)-C(50)-H(50A)	109.8
O(7)-K(2)-C(39)	103.01(7)	O(8)-C(50)-H(50B)	109.8
O(9)-K(2)-C(39)	80.15(7)	C(49)-C(50)-H(50B)	109.8
O(12)-K(2)-C(39)	125.55(7)	H(50A)-C(50)-H(50B)	108.3
O(11)-K(2)-C(39)	110.51(7)	C(51)-O(8)-C(50)	111.2(2)
O(10)-K(2)-C(39)	95.32(7)	C(51)-O(8)-K(2)	109.67(18)
O(8)-K(2)-C(39)	93.95(7)	C(50)-O(8)-K(2)	106.98(16)
C(32)-K(2)-C(39)	44.51(8)	O(8)-C(51)-C(52)	109.1(3)
O(7)-K(2)-C(33)	85.29(7)	O(8)-C(51)-H(51A)	109.9
O(9)-K(2)-C(33)	128.76(7)	C(52)-C(51)-H(51A)	109.9
O(12)-K(2)-C(33)	76.83(7)	O(8)-C(51)-H(51B)	109.9
O(11)-K(2)-C(33)	80.16(7)	C(52)-C(51)-H(51B)	109.9
O(10)-K(2)-C(33)	111.46(7)	H(51A)-C(51)-H(51B)	108.3
O(8)-K(2)-C(33)	122.75(7)	O(9)-C(52)-C(51)	108.2(3)
C(32)-K(2)-C(33)	24.07(8)	O(9)-C(52)-H(52A)	110.0
C(39)-K(2)-C(33)	49.24(7)	C(51)-C(52)-H(52A)	110.0
O(7)-K(2)-C(31)	117.73(7)	O(9)-C(52)-H(52B)	110.0
O(9)-K(2)-C(31)	90.39(7)	C(51)-C(52)-H(52B)	110.0
O(12)-K(2)-C(31)	113.59(7)	H(52A)-C(52)-H(52B)	108.4
O(11)-K(2)-C(31)	85.90(7)	C(52)-O(9)-C(53)	112.7(2)
O(10)-K(2)-C(31)	81.45(7)	C(52)-O(9)-K(2)	119.08(18)
O(8)-K(2)-C(31)	118.24(7)	C(53)-O(9)-K(2)	119.00(19)
C(32)-K(2)-C(31)	24.21(8)	O(9)-C(53)-C(54)	107.9(3)
C(39)-K(2)-C(31)	24.63(7)	O(9)-C(53)-H(53A)	110.1
C(33)-K(2)-C(31)	40.48(7)	C(54)-C(53)-H(53A)	110.1
C(60)-O(7)-C(49)	110.9(2)	O(9)-C(53)-H(53B)	110.1
C(60)-O(7)-K(2)	118.45(18)	C(54)-C(53)-H(53B)	110.1

H(53A)-C(53)-H(53B)	108.4	O(11)-C(57)-H(57A)	110.0
O(10)-C(54)-C(53)	108.3(3)	C(58)-C(57)-H(57A)	110.0
O(10)-C(54)-H(54A)	110.0	O(11)-C(57)-H(57B)	110.0
C(53)-C(54)-H(54A)	110.0	C(58)-C(57)-H(57B)	110.0
O(10)-C(54)-H(54B)	110.0	H(57A)-C(57)-H(57B)	108.3
C(53)-C(54)-H(54B)	110.0	O(12)-C(58)-C(57)	109.3(3)
H(54A)-C(54)-H(54B)	108.4	O(12)-C(58)-H(58A)	109.8
C(55)-O(10)-C(54)	113.8(3)	C(57)-C(58)-H(58A)	109.8
C(55)-O(10)-K(2)	111.32(18)	O(12)-C(58)-H(58B)	109.8
C(54)-O(10)-K(2)	109.34(18)	C(57)-C(58)-H(58B)	109.8
O(10)-C(55)-C(56)	108.5(3)	H(58A)-C(58)-H(58B)	108.3
O(10)-C(55)-H(55A)	110.0	C(59)-O(12)-C(58)	112.0(3)
C(56)-C(55)-H(55A)	110.0	C(59)-O(12)-K(2)	111.88(19)
O(10)-C(55)-H(55B)	110.0	C(58)-O(12)-K(2)	115.6(2)
C(56)-C(55)-H(55B)	110.0	O(12)-C(59)-C(60)	109.2(3)
H(55A)-C(55)-H(55B)	108.4	O(12)-C(59)-H(59A)	109.8
O(11)-C(56)-C(55)	109.1(3)	C(60)-C(59)-H(59A)	109.8
O(11)-C(56)-H(56A)	109.9	O(12)-C(59)-H(59B)	109.8
C(55)-C(56)-H(56A)	109.9	C(60)-C(59)-H(59B)	109.8
O(11)-C(56)-H(56B)	109.9	H(59A)-C(59)-H(59B)	108.3
C(55)-C(56)-H(56B)	109.9	O(7)-C(60)-C(59)	109.7(3)
H(56A)-C(56)-H(56B)	108.3	O(7)-C(60)-H(60A)	109.7
C(57)-O(11)-C(56)	112.4(3)	C(59)-C(60)-H(60A)	109.7
C(57)-O(11)-K(2)	118.46(19)	O(7)-C(60)-H(60B)	109.7
C(56)-O(11)-K(2)	119.35(19)	C(59)-C(60)-H(60B)	109.7
O(11)-C(57)-C(58)	108.7(3)	H(60A)-C(60)-H(60B)	108.2

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04344. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	23(1)	26(1)	23(1)	-6(1)	5(1)	-8(1)
C1	24(1)	29(2)	33(2)	-14(1)	1(1)	-7(1)
C2	28(2)	34(2)	25(2)	-7(1)	-1(1)	1(1)
C3	39(2)	22(1)	29(2)	-2(1)	8(1)	-6(1)
C4	31(2)	26(2)	31(2)	-8(1)	4(1)	-11(1)
C5	25(1)	29(2)	27(2)	-6(1)	-2(1)	-4(1)
C6	35(2)	35(2)	21(1)	0(1)	5(1)	-7(1)
C7	40(2)	34(2)	38(2)	-3(1)	14(1)	-15(1)
C8	34(2)	35(2)	47(2)	-12(1)	8(1)	-17(1)
C9	23(1)	24(1)	28(1)	-5(1)	1(1)	-5(1)
C10	20(1)	21(1)	25(1)	0(1)	-3(1)	-1(1)
C11	35(2)	24(2)	35(2)	0(1)	7(1)	-3(1)
C12	32(2)	45(2)	26(2)	-1(1)	3(1)	2(1)
C13	35(2)	72(3)	45(2)	-14(2)	-9(2)	-2(2)
C14	36(2)	92(3)	71(3)	-37(3)	6(2)	-32(2)
C15	34(2)	40(2)	53(2)	-16(2)	15(2)	-21(2)
C16	33(2)	38(2)	28(2)	-3(1)	10(1)	-14(1)
C17	32(2)	47(2)	36(2)	-17(2)	10(1)	-10(2)
C18	46(2)	31(2)	41(2)	-10(1)	4(2)	-1(2)
K1	26(1)	55(1)	24(1)	-8(1)	1(1)	-13(1)
O1	25(1)	44(1)	29(1)	-1(1)	-3(1)	-2(1)
C19	24(2)	40(2)	45(2)	-5(2)	-2(1)	-1(1)
C20	24(2)	40(2)	39(2)	-11(1)	8(1)	-4(1)
O2	32(1)	38(1)	26(1)	-2(1)	0(1)	-9(1)
C21	39(2)	45(2)	25(2)	-6(1)	8(1)	-7(2)
C22	43(2)	43(2)	22(2)	-10(1)	3(1)	-7(2)
O3	33(1)	35(1)	24(1)	-7(1)	1(1)	-9(1)
C23	39(2)	50(2)	25(2)	-4(1)	-5(1)	-19(2)
C24	29(2)	45(2)	32(2)	2(1)	-5(1)	-4(1)
O4	27(1)	33(1)	26(1)	-4(1)	0(1)	-4(1)
C25	29(2)	37(2)	38(2)	-8(1)	3(1)	-2(1)

C26	29(2)	41(2)	35(2)	-10(1)	9(1)	-9(1)
O5	33(1)	43(1)	26(1)	-7(1)	7(1)	-16(1)
C27	40(2)	54(2)	24(2)	-9(1)	11(1)	-17(2)
C28	46(2)	49(2)	22(2)	-11(1)	7(1)	-22(2)
O6	35(1)	45(1)	27(1)	-10(1)	-1(1)	-18(1)
C29	40(2)	52(2)	27(2)	1(1)	-10(1)	-24(2)
C30	36(2)	45(2)	37(2)	6(2)	-13(1)	-10(2)
Co2	19(1)	24(1)	24(1)	-3(1)	0(1)	-8(1)
C31	21(1)	38(2)	26(2)	-1(1)	3(1)	-5(1)
C32	27(2)	32(2)	29(2)	-10(1)	0(1)	-1(1)
C33	28(2)	24(2)	36(2)	-5(1)	-4(1)	-9(1)
C34	22(1)	30(2)	28(2)	-1(1)	3(1)	-9(1)
C35	29(2)	37(2)	28(2)	-5(1)	-2(1)	-8(1)
C36	36(2)	48(2)	36(2)	-12(2)	-7(1)	-15(2)
C37	30(2)	46(2)	51(2)	-11(2)	-2(2)	-19(2)
C38	24(1)	40(2)	38(2)	-5(1)	4(1)	-12(1)
C39	21(1)	23(1)	30(2)	-2(1)	2(1)	-4(1)
C40	21(1)	23(1)	27(1)	-2(1)	0(1)	-4(1)
C41	24(1)	26(1)	32(2)	-7(1)	-4(1)	-8(1)
C42	24(1)	24(1)	33(2)	-4(1)	0(1)	-10(1)
C43	30(2)	32(2)	28(2)	-2(1)	1(1)	-13(1)
C44	39(2)	42(2)	28(2)	-1(1)	-7(1)	-20(2)
C45	27(2)	29(2)	35(2)	-4(1)	-5(1)	-13(1)
C46	23(1)	32(2)	37(2)	1(1)	-1(1)	-14(1)
C47	23(2)	42(2)	46(2)	-2(2)	7(1)	-10(1)
C48	29(2)	34(2)	27(2)	-5(1)	4(1)	-6(1)
K2	26(1)	39(1)	25(1)	0(1)	0(1)	-15(1)
O7	32(1)	38(1)	26(1)	2(1)	1(1)	-18(1)
C49	32(2)	45(2)	22(1)	3(1)	0(1)	-11(1)
C50	35(2)	48(2)	21(1)	-8(1)	1(1)	-14(2)
O8	27(1)	42(1)	31(1)	-6(1)	3(1)	-16(1)
C51	41(2)	66(2)	39(2)	-9(2)	-4(2)	-34(2)
C52	32(2)	67(3)	55(2)	-8(2)	2(2)	-31(2)
O9	29(1)	44(1)	36(1)	-3(1)	9(1)	-16(1)
C53	35(2)	48(2)	46(2)	-4(2)	17(2)	-21(2)
C54	50(2)	40(2)	39(2)	6(2)	18(2)	-14(2)

O10	37(1)	41(1)	30(1)	3(1)	3(1)	-8(1)
C55	41(2)	56(2)	22(2)	4(1)	3(1)	1(2)
C56	33(2)	61(2)	22(2)	-13(2)	-4(1)	8(2)
O11	34(1)	44(1)	29(1)	-14(1)	-1(1)	-7(1)
C57	39(2)	45(2)	52(2)	-22(2)	-16(2)	-7(2)
C58	40(2)	47(2)	56(2)	-11(2)	-11(2)	-22(2)
O12	31(1)	45(1)	39(1)	-5(1)	-5(1)	-20(1)
C59	39(2)	61(2)	48(2)	2(2)	1(2)	-33(2)
C60	46(2)	48(2)	43(2)	5(2)	4(2)	-29(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04344.

	x	y	z	U(eq)
H1	5760(30)	2840(30)	3978(10)	27(8)
H2	5640(40)	790(40)	4469(12)	41(9)
H3	4680(30)	-640(40)	4102(11)	28(8)
H4	4050(40)	-20(40)	3345(11)	37(9)
H5	5475	118	2643	35
H6	6780	1285	2222	39
H7	7546	2863	2526	45
H8	7121	3183	3269	44
H11	3420(40)	4580(40)	3685(11)	35(9)
H12	2380(40)	3780(40)	3185(14)	54(11)
H13A	-84	4647	3625	66
H13B	177	3853	3195	66
H14A	393	1810	3572	74
H14B	-466	2771	3937	74
H15	1920(40)	710(40)	4142(12)	50(11)
H16	2550(40)	1790(40)	4654(11)	31(9)
H17A	271	4160	4386	47
H17B	1330	4033	4783	47
H18A	2559	5098	4372	51
H18B	1084	5798	4093	51
H19A	-2025	9230	3795	48
H19B	-1075	10167	3847	48
H20A	-1512	9083	4543	43
H20B	-704	7543	4388	43
H21A	1087	6953	4968	46
H21B	236	8486	5123	46
H22A	2314	9072	4961	45
H22B	2609	7777	5352	45
H23A	5072	6859	5209	45
H23B	4867	8142	4820	45

H24A	6934	6119	4704	46
H24B	5947	5194	4695	46
H25A	6767	4849	3933	44
H25B	7689	5809	3991	44
H26A	6364	7501	3400	43
H26B	7148	5967	3237	43
H27A	5470	6316	2679	47
H27B	4653	7932	2775	47
H28A	3095	7050	2440	44
H28B	3341	5864	2862	44
H29A	856	6811	3003	46
H29B	580	8034	2591	46
H30A	-223	9772	3092	50
H30B	-1239	8878	3080	50
H31	4070(30)	8380(30)	1868(10)	27(8)
H32	5130(40)	10220(40)	1841(12)	39(9)
H33	6370(40)	10600(40)	1235(11)	32(9)
H34	6560(30)	9280(30)	652(10)	23(8)
H35	4884	8804	114	39
H36	3061	7942	43	48
H37	1762	7555	652	49
H38	2296	7995	1344	41
H41	6750(40)	5870(40)	1157(12)	42(10)
H42	6210(40)	5860(40)	1898(12)	45(10)
H43A	7796	5013	2433	36
H43B	9061	4714	2084	36
H44A	7922	7055	2559	42
H44B	9547	6296	2415	42
H45	8140(30)	8750(40)	2016(11)	31(9)
H46	9140(40)	8350(40)	1352(11)	33(9)
H47A	10358	5573	1671	46
H47B	10562	6265	1186	46
H48A	8991	5587	883	38
H48B	9439	4377	1300	38
H49A	2713	13396	-305	42
H49B	1370	14445	-64	42

H50A	924	12451	-250	42
H50B	2246	11417	66	42
H51A	592	10619	465	53
H51B	-757	11756	180	53
H52A	-1665	12816	834	57
H52B	-1587	11203	869	57
H53A	-1323	10805	1638	50
H53B	-1462	12422	1650	50
H54A	-130	10850	2272	54
H54B	1059	10013	1941	54
H55A	2761	10812	2327	55
H55B	1437	11631	2622	55
H56A	1601	13826	2325	54
H56B	3067	12783	2576	54
H57A	4240	14102	2138	55
H57B	2848	15055	1836	55
H58A	4960	14816	1439	54
H58B	5431	13114	1514	54
H59A	5350	13130	712	55
H59B	5000	14807	689	55
H60A	2798	15296	321	52
H60B	4126	14379	46	52

Table 6. Torsion angles [°] for 04344.

C3-Co1-C1-C2	-34.92(18)	C16-Co1-C3-C2	-91.3(2)
C11-Co1-C1-C2	148.02(19)	C1-Co1-C3-C2	34.02(18)
C15-Co1-C1-C2	17.7(5)	C4-Co1-C3-C2	126.3(3)
C12-Co1-C1-C2	-177.10(18)	C2-Co1-C3-C4	-126.3(3)
C16-Co1-C1-C2	64.7(2)	C11-Co1-C3-C4	-83.4(4)
C4-Co1-C1-C2	-75.67(18)	C15-Co1-C3-C4	101.9(2)
C3-Co1-C1-C9	81.3(2)	C12-Co1-C3-C4	8.3(3)
C2-Co1-C1-C9	116.2(3)	C16-Co1-C3-C4	142.33(19)
C11-Co1-C1-C9	-95.8(2)	C1-Co1-C3-C4	-92.3(2)
C15-Co1-C1-C9	134.0(4)	C2-C3-C4-C10	33.9(4)
C12-Co1-C1-C9	-60.9(2)	Co1-C3-C4-C10	92.5(2)
C16-Co1-C1-C9	-179.12(18)	C2-C3-C4-Co1	-58.6(2)
C4-Co1-C1-C9	40.54(19)	C2-Co1-C4-C3	34.3(2)
C9-C1-C2-C3	-36.5(4)	C11-Co1-C4-C3	152.4(2)
Co1-C1-C2-C3	57.1(2)	C15-Co1-C4-C3	-85.9(2)
C9-C1-C2-Co1	-93.6(2)	C12-Co1-C4-C3	-175.0(2)
C11-Co1-C2-C3	-164.35(18)	C16-Co1-C4-C3	-57.4(3)
C15-Co1-C2-C3	61.3(2)	C1-Co1-C4-C3	75.8(2)
C12-Co1-C2-C3	-119.4(3)	C3-Co1-C4-C10	-115.1(3)
C16-Co1-C2-C3	101.95(19)	C2-Co1-C4-C10	-80.8(2)
C1-Co1-C2-C3	-125.1(3)	C11-Co1-C4-C10	37.2(3)
C4-Co1-C2-C3	-32.87(18)	C15-Co1-C4-C10	159.0(2)
C3-Co1-C2-C1	125.1(3)	C12-Co1-C4-C10	69.8(2)
C11-Co1-C2-C1	-39.3(2)	C16-Co1-C4-C10	-172.57(19)
C15-Co1-C2-C1	-173.66(17)	C1-Co1-C4-C10	-39.29(19)
C12-Co1-C2-C1	5.7(4)	C10-C5-C6-C7	1.6(4)
C16-Co1-C2-C1	-132.97(18)	C5-C6-C7-C8	2.1(5)
C4-Co1-C2-C1	92.20(18)	C6-C7-C8-C9	-3.2(5)
C1-C2-C3-C4	2.4(4)	C7-C8-C9-C10	0.6(5)
Co1-C2-C3-C4	62.4(3)	C7-C8-C9-C1	-177.9(3)
C1-C2-C3-Co1	-60.0(2)	C2-C1-C9-C8	-147.7(3)
C11-Co1-C3-C2	42.9(5)	Co1-C1-C9-C8	142.3(3)
C15-Co1-C3-C2	-131.8(2)	C2-C1-C9-C10	33.7(4)
C12-Co1-C3-C2	134.6(3)	Co1-C1-C9-C10	-36.3(3)

C6-C5-C10-C9	-4.2(4)	C16-Co1-C12-C13	-44.0(3)
C6-C5-C10-C4	174.7(3)	C1-Co1-C12-C13	179.9(2)
C8-C9-C10-C5	3.0(4)	C4-Co1-C12-C13	98.3(3)
C1-C9-C10-C5	-178.3(3)	C11-C12-C13-C14	-86.6(4)
C8-C9-C10-C4	-175.9(3)	Co1-C12-C13-C14	-7.9(4)
C1-C9-C10-C4	2.8(4)	C12-C13-C14-C15	21.3(5)
C3-C4-C10-C5	145.0(3)	C13-C14-C15-C16	55.9(5)
Co1-C4-C10-C5	-147.6(2)	C13-C14-C15-Co1	-24.7(4)
C3-C4-C10-C9	-36.1(4)	C3-Co1-C15-C16	110.2(2)
Co1-C4-C10-C9	31.3(3)	C2-Co1-C15-C16	74.4(2)
C3-Co1-C11-C12	116.3(4)	C11-Co1-C15-C16	-68.0(2)
C2-Co1-C11-C12	148.8(2)	C12-Co1-C15-C16	-105.3(2)
C15-Co1-C11-C12	-69.1(2)	C1-Co1-C15-C16	60.9(5)
C16-Co1-C11-C12	-106.5(2)	C4-Co1-C15-C16	150.0(2)
C1-Co1-C11-C12	124.7(2)	C3-Co1-C15-C14	-128.4(3)
C4-Co1-C11-C12	53.5(3)	C2-Co1-C15-C14	-164.2(2)
C3-Co1-C11-C18	-122.4(4)	C11-Co1-C15-C14	53.4(3)
C2-Co1-C11-C18	-89.9(3)	C12-Co1-C15-C14	16.1(3)
C15-Co1-C11-C18	52.3(3)	C16-Co1-C15-C14	121.4(4)
C12-Co1-C11-C18	121.3(3)	C1-Co1-C15-C14	-177.7(3)
C16-Co1-C11-C18	14.8(3)	C4-Co1-C15-C14	-88.6(3)
C1-Co1-C11-C18	-114.0(3)	C14-C15-C16-C17	1.8(5)
C4-Co1-C11-C18	174.8(2)	Co1-C15-C16-C17	104.5(3)
C18-C11-C12-C13	0.0(5)	C14-C15-C16-Co1	-102.6(4)
Co1-C11-C12-C13	103.6(3)	C3-Co1-C16-C15	-79.7(2)
C18-C11-C12-Co1	-103.7(3)	C2-Co1-C16-C15	-122.8(2)
C3-Co1-C12-C11	-149.2(2)	C11-Co1-C16-C15	114.1(2)
C2-Co1-C12-C11	-66.1(3)	C12-Co1-C16-C15	75.5(2)
C15-Co1-C12-C11	113.3(2)	C1-Co1-C16-C15	-160.0(2)
C16-Co1-C12-C11	73.9(2)	C4-Co1-C16-C15	-45.1(3)
C1-Co1-C12-C11	-62.2(2)	C3-Co1-C16-C17	165.6(2)
C4-Co1-C12-C11	-143.73(19)	C2-Co1-C16-C17	122.4(2)
C3-Co1-C12-C13	92.9(3)	C11-Co1-C16-C17	-0.6(2)
C2-Co1-C12-C13	175.9(3)	C15-Co1-C16-C17	-114.7(3)
C11-Co1-C12-C13	-118.0(3)	C12-Co1-C16-C17	-39.2(3)
C15-Co1-C12-C13	-4.6(3)	C1-Co1-C16-C17	85.2(3)

C4-Co1-C16-C17	-159.9(2)	C19-C20-O2-C21	179.7(3)
C15-C16-C17-C18	-91.1(4)	C19-C20-O2-K1	-45.1(3)
Co1-C16-C17-C18	-13.7(4)	O1-K1-O2-C21	148.5(2)
C16-C17-C18-C11	25.9(4)	O6-K1-O2-C21	157.9(2)
C16-C17-C18-K1	-146.8(6)	O5-K1-O2-C21	49.4(7)
C12-C11-C18-C17	54.9(4)	O4-K1-O2-C21	-22.9(2)
Co1-C11-C18-C17	-26.4(4)	O3-K1-O2-C21	-14.7(2)
C12-C11-C18-K1	-127.6(3)	C18-K1-O2-C21	71.7(2)
Co1-C11-C18-K1	151.13(17)	O1-K1-O2-C20	14.47(19)
C17-C18-K1-O1	-86.9(7)	O6-K1-O2-C20	23.9(2)
C11-C18-K1-O1	99.9(2)	O5-K1-O2-C20	-84.7(6)
C17-C18-K1-O6	-144.6(7)	O4-K1-O2-C20	-156.92(19)
C11-C18-K1-O6	42.2(2)	O3-K1-O2-C20	-148.7(2)
C17-C18-K1-O5	153.9(7)	C18-K1-O2-C20	-62.4(2)
C11-C18-K1-O5	-19.3(2)	C20-O2-C21-C22	-178.2(3)
C17-C18-K1-O4	93.2(7)	K1-O2-C21-C22	46.6(3)
C11-C18-K1-O4	-80.05(19)	O2-C21-C22-O3	-66.7(3)
C17-C18-K1-O2	-23.6(7)	C21-C22-O3-C23	-176.7(3)
C11-C18-K1-O2	163.2(2)	C21-C22-O3-K1	52.3(3)
C17-C18-K1-O3	38.4(7)	O1-K1-O3-C23	-166.22(19)
C11-C18-K1-O3	-134.9(2)	O6-K1-O3-C23	106.4(6)
O6-K1-O1-C30	-18.2(2)	O5-K1-O3-C23	36.7(2)
O5-K1-O1-C30	-34.8(2)	O4-K1-O3-C23	21.86(19)
O4-K1-O1-C30	-125.3(5)	O2-K1-O3-C23	-149.8(2)
O2-K1-O1-C30	152.6(2)	C18-K1-O3-C23	133.1(2)
O3-K1-O1-C30	169.1(2)	O1-K1-O3-C22	-36.6(2)
C18-K1-O1-C30	-125.8(2)	O6-K1-O3-C22	-124.0(6)
O6-K1-O1-C19	-151.1(2)	O5-K1-O3-C22	166.29(19)
O5-K1-O1-C19	-167.6(2)	O4-K1-O3-C22	151.4(2)
O4-K1-O1-C19	101.8(5)	O2-K1-O3-C22	-20.20(19)
O2-K1-O1-C19	19.8(2)	C18-K1-O3-C22	-97.3(2)
O3-K1-O1-C19	36.3(2)	C22-O3-C23-C24	178.1(3)
C18-K1-O1-C19	101.3(2)	K1-O3-C23-C24	-51.8(3)
C30-O1-C19-C20	176.0(3)	O3-C23-C24-O4	61.5(3)
K1-O1-C19-C20	-50.8(3)	C23-C24-O4-C25	174.4(3)
O1-C19-C20-O2	62.8(3)	C23-C24-O4-K1	-42.2(3)

O1-K1-O4-C24	-57.5(6)	O4-K1-O6-C28	26.9(2)
O6-K1-O4-C24	-160.5(2)	O2-K1-O6-C28	-153.92(18)
O5-K1-O4-C24	-152.6(2)	O3-K1-O6-C28	-53.9(6)
O2-K1-O4-C24	20.3(2)	C18-K1-O6-C28	-80.1(2)
O3-K1-O4-C24	12.0(2)	O1-K1-O6-C29	-16.37(19)
C18-K1-O4-C24	-57.0(2)	O5-K1-O6-C29	147.4(2)
O1-K1-O4-C25	83.8(5)	O4-K1-O6-C29	155.22(19)
O6-K1-O4-C25	-19.2(2)	O2-K1-O6-C29	-25.6(2)
O5-K1-O4-C25	-11.2(2)	O3-K1-O6-C29	74.4(6)
O2-K1-O4-C25	161.6(2)	C18-K1-O6-C29	48.2(2)
O3-K1-O4-C25	153.4(2)	C28-O6-C29-C30	178.1(3)
C18-K1-O4-C25	84.3(2)	K1-O6-C29-C30	48.6(3)
C24-O4-C25-C26	-175.0(3)	C19-O1-C30-C29	-175.0(3)
K1-O4-C25-C26	41.3(3)	K1-O1-C30-C29	50.2(3)
O4-C25-C26-O5	-60.9(3)	O6-C29-C30-O1	-67.1(3)
C25-C26-O5-C27	-171.9(3)	C33-Co2-C31-C32	-34.53(18)
C25-C26-O5-K1	52.8(3)	C42-Co2-C31-C32	146.34(19)
O1-K1-O5-C26	166.10(19)	C41-Co2-C31-C32	-174.83(18)
O6-K1-O5-C26	149.4(2)	C45-Co2-C31-C32	59.5(2)
O4-K1-O5-C26	-22.75(19)	C46-Co2-C31-C32	21.6(5)
O2-K1-O5-C26	-98.5(6)	C34-Co2-C31-C32	-75.43(19)
O3-K1-O5-C26	-37.6(2)	C33-Co2-C31-C39	83.7(2)
C18-K1-O5-C26	-120.2(2)	C32-Co2-C31-C39	118.2(3)
O1-K1-O5-C27	32.1(2)	C42-Co2-C31-C39	-95.5(2)
O6-K1-O5-C27	15.4(2)	C41-Co2-C31-C39	-56.6(2)
O4-K1-O5-C27	-156.8(2)	C45-Co2-C31-C39	177.66(18)
O2-K1-O5-C27	127.5(6)	C46-Co2-C31-C39	139.7(4)
O3-K1-O5-C27	-171.58(19)	C34-Co2-C31-C39	42.76(19)
C18-K1-O5-C27	105.8(2)	C33-Co2-C31-K2	1.51(13)
C26-O5-C27-C28	177.8(3)	C32-Co2-C31-K2	36.03(16)
K1-O5-C27-C28	-46.6(3)	C42-Co2-C31-K2	-177.62(14)
O5-C27-C28-O6	65.0(3)	C41-Co2-C31-K2	-138.79(13)
C27-C28-O6-C29	-179.7(3)	C45-Co2-C31-K2	95.51(16)
C27-C28-O6-K1	-50.8(3)	C46-Co2-C31-K2	57.6(5)
O1-K1-O6-C28	-144.7(2)	C34-Co2-C31-K2	-39.39(13)
O5-K1-O6-C28	19.09(18)	C39-C31-C32-C33	-33.0(4)

Co2-C31-C32-C33	57.6(2)	C31-Co2-C33-C32	33.61(18)
K2-C31-C32-C33	-89.2(2)	C34-Co2-C33-C32	126.4(3)
C39-C31-C32-Co2	-90.6(3)	C32-Co2-C33-C34	-126.4(3)
K2-C31-C32-Co2	-146.87(12)	C42-Co2-C33-C34	-89.7(5)
C39-C31-C32-K2	56.3(3)	C41-Co2-C33-C34	2.7(3)
Co2-C31-C32-K2	146.87(12)	C45-Co2-C33-C34	141.79(18)
C42-Co2-C32-C33	-168.35(17)	C46-Co2-C33-C34	100.17(19)
C41-Co2-C32-C33	-116.1(3)	C31-Co2-C33-C34	-92.83(19)
C45-Co2-C32-C33	98.70(19)	C32-Co2-C33-K2	-35.22(16)
C46-Co2-C32-C33	61.5(2)	C42-Co2-C33-K2	1.6(5)
C31-Co2-C32-C33	-125.4(3)	C41-Co2-C33-K2	93.9(2)
C34-Co2-C32-C33	-32.99(17)	C45-Co2-C33-K2	-127.00(15)
C33-Co2-C32-C31	125.4(3)	C46-Co2-C33-K2	-168.62(15)
C42-Co2-C32-C31	-42.9(2)	C31-Co2-C33-K2	-1.62(13)
C41-Co2-C32-C31	9.4(3)	C34-Co2-C33-K2	91.2(2)
C45-Co2-C32-C31	-135.87(18)	C32-C33-C34-C40	31.2(4)
C46-Co2-C32-C31	-173.08(17)	Co2-C33-C34-C40	89.6(3)
C34-Co2-C32-C31	92.45(19)	K2-C33-C34-C40	-37.0(3)
C33-Co2-C32-K2	57.7(2)	C32-C33-C34-Co2	-58.3(2)
C42-Co2-C32-K2	-110.6(2)	K2-C33-C34-Co2	-126.51(13)
C41-Co2-C32-K2	-58.4(4)	C32-Co2-C34-C33	33.97(19)
C45-Co2-C32-K2	156.4(2)	C42-Co2-C34-C33	155.99(19)
C46-Co2-C32-K2	119.2(2)	C41-Co2-C34-C33	-178.34(18)
C31-Co2-C32-K2	-67.7(2)	C45-Co2-C34-C33	-55.0(2)
C34-Co2-C32-K2	24.7(2)	C46-Co2-C34-C33	-89.16(19)
C31-C32-C33-C34	1.1(4)	C31-Co2-C34-C33	74.99(19)
Co2-C32-C33-C34	61.7(2)	C33-Co2-C34-C40	-117.6(3)
K2-C32-C33-C34	-88.3(3)	C32-Co2-C34-C40	-83.6(2)
C31-C32-C33-Co2	-60.7(2)	C42-Co2-C34-C40	38.4(3)
K2-C32-C33-Co2	-150.05(11)	C41-Co2-C34-C40	64.1(2)
C31-C32-C33-K2	89.4(2)	C45-Co2-C34-C40	-172.59(18)
Co2-C32-C33-K2	150.05(11)	C46-Co2-C34-C40	153.24(19)
C42-Co2-C33-C32	36.8(5)	C31-Co2-C34-C40	-42.62(19)
C41-Co2-C33-C32	129.1(2)	C40-C35-C36-C37	2.5(5)
C45-Co2-C33-C32	-91.8(2)	C35-C36-C37-C38	-0.5(5)
C46-Co2-C33-C32	-133.40(19)	C36-C37-C38-C39	-2.1(5)

C37-C38-C39-C40	2.8(5)	C48-C41-C42-C43	-3.0(4)
C37-C38-C39-C31	-174.4(3)	Co2-C41-C42-C43	-105.1(3)
C37-C38-C39-K2	99.8(3)	C48-C41-C42-Co2	102.1(3)
C32-C31-C39-C38	-150.5(3)	C33-Co2-C42-C41	111.7(4)
Co2-C31-C39-C38	140.7(3)	C32-Co2-C42-C41	140.54(18)
K2-C31-C39-C38	-99.2(3)	C45-Co2-C42-C41	-117.59(18)
C32-C31-C39-C40	32.1(4)	C46-Co2-C42-C41	-78.00(18)
Co2-C31-C39-C40	-36.7(3)	C31-Co2-C42-C41	114.67(18)
K2-C31-C39-C40	83.5(2)	C34-Co2-C42-C41	40.3(2)
C32-C31-C39-K2	-51.4(2)	C33-Co2-C42-C43	-129.9(4)
Co2-C31-C39-K2	-120.15(13)	C32-Co2-C42-C43	-101.0(2)
C36-C35-C40-C39	-1.7(4)	C41-Co2-C42-C43	118.4(3)
C36-C35-C40-C34	174.1(3)	C45-Co2-C42-C43	0.8(2)
C38-C39-C40-C35	-0.9(4)	C46-Co2-C42-C43	40.4(2)
C31-C39-C40-C35	176.6(3)	C31-Co2-C42-C43	-126.9(2)
K2-C39-C40-C35	-106.4(2)	C34-Co2-C42-C43	158.71(19)
C38-C39-C40-C34	-177.2(3)	C41-C42-C43-C44	94.3(3)
C31-C39-C40-C34	0.3(4)	Co2-C42-C43-C44	14.1(3)
K2-C39-C40-C34	77.3(2)	C42-C43-C44-C45	-26.9(4)
C33-C34-C40-C35	152.6(3)	C43-C44-C45-C46	-51.6(4)
Co2-C34-C40-C35	-140.5(3)	C43-C44-C45-Co2	27.4(3)
C33-C34-C40-C39	-31.4(4)	C33-Co2-C45-C46	-89.1(2)
Co2-C34-C40-C39	35.5(3)	C32-Co2-C45-C46	-131.16(19)
C33-Co2-C41-C42	-155.2(2)	C42-Co2-C45-C46	103.32(19)
C32-Co2-C41-C42	-79.7(3)	C41-Co2-C45-C46	66.8(2)
C45-Co2-C41-C42	65.35(19)	C31-Co2-C45-C46	-165.48(18)
C46-Co2-C41-C42	102.30(18)	C34-Co2-C45-C46	-56.3(2)
C31-Co2-C41-C42	-73.38(19)	C33-Co2-C45-C44	152.0(2)
C34-Co2-C41-C42	-153.48(17)	C32-Co2-C45-C44	109.9(2)
C33-Co2-C41-C48	86.7(3)	C42-Co2-C45-C44	-15.6(2)
C32-Co2-C41-C48	162.2(2)	C41-Co2-C45-C44	-52.2(2)
C42-Co2-C41-C48	-118.1(3)	C46-Co2-C45-C44	-118.9(3)
C45-Co2-C41-C48	-52.7(2)	C31-Co2-C45-C44	75.6(3)
C46-Co2-C41-C48	-15.8(2)	C34-Co2-C45-C44	-175.3(2)
C31-Co2-C41-C48	168.5(2)	C44-C45-C46-C47	-0.6(4)
C34-Co2-C41-C48	88.5(2)	Co2-C45-C46-C47	-103.3(3)

C44-C45-C46-Co2	102.6(3)	Co2-C32-K2-O8	13.5(3)
C33-Co2-C46-C45	100.64(19)	C33-C32-K2-C39	89.7(2)
C32-Co2-C46-C45	64.8(2)	C31-C32-K2-C39	-25.89(16)
C42-Co2-C46-C45	-76.67(19)	Co2-C32-K2-C39	37.4(2)
C41-Co2-C46-C45	-116.47(19)	C31-C32-K2-C33	-115.6(3)
C31-Co2-C46-C45	48.0(5)	Co2-C32-K2-C33	-52.2(2)
C34-Co2-C46-C45	141.12(18)	C33-C32-K2-C31	115.6(3)
C33-Co2-C46-C47	-141.1(2)	Co2-C32-K2-C31	63.3(2)
C32-Co2-C46-C47	-176.9(2)	C38-C39-K2-O7	-106.3(2)
C42-Co2-C46-C47	41.6(2)	C40-C39-K2-O7	14.15(17)
C41-Co2-C46-C47	1.8(2)	C31-C39-K2-O7	129.94(16)
C45-Co2-C46-C47	118.2(3)	C38-C39-K2-O9	10.49(19)
C31-Co2-C46-C47	166.2(4)	C40-C39-K2-O9	130.93(17)
C34-Co2-C46-C47	-100.6(2)	C31-C39-K2-O9	-113.29(17)
C45-C46-C47-C48	91.6(4)	C38-C39-K2-O12	-168.48(18)
Co2-C46-C47-C48	12.6(3)	C40-C39-K2-O12	-48.04(19)
C42-C41-C48-C47	-51.4(4)	C31-C39-K2-O12	67.75(18)
Co2-C41-C48-C47	26.8(3)	C38-C39-K2-O11	126.07(19)
C46-C47-C48-C41	-25.9(4)	C40-C39-K2-O11	-113.49(16)
C33-C32-K2-O7	0.6(2)	C31-C39-K2-O11	2.30(18)
C31-C32-K2-O7	-114.91(18)	C38-C39-K2-O10	67.9(2)
Co2-C32-K2-O7	-51.6(3)	C40-C39-K2-O10	-171.66(16)
C33-C32-K2-O9	134.75(18)	C31-C39-K2-O10	-55.87(16)
C31-C32-K2-O9	19.2(2)	C38-C39-K2-O8	-47.2(2)
Co2-C32-K2-O9	82.5(3)	C40-C39-K2-O8	73.24(16)
C33-C32-K2-O12	-57.13(19)	C31-C39-K2-O8	-170.97(16)
C31-C32-K2-O12	-172.69(18)	C38-C39-K2-C32	149.2(2)
Co2-C32-K2-O12	-109.4(2)	C40-C39-K2-C32	-90.35(18)
C33-C32-K2-O11	-113.5(2)	C31-C39-K2-C32	25.44(16)
C31-C32-K2-O11	130.93(19)	C38-C39-K2-C33	-178.2(2)
Co2-C32-K2-O11	-165.8(3)	C40-C39-K2-C33	-57.78(16)
C33-C32-K2-O10	-170.41(19)	C31-C39-K2-C33	58.01(16)
C31-C32-K2-O10	74.03(18)	C38-C39-K2-C31	123.8(3)
Co2-C32-K2-O10	137.3(3)	C40-C39-K2-C31	-115.8(2)
C33-C32-K2-O8	65.7(2)	C32-C33-K2-O7	-179.39(19)
C31-C32-K2-O8	-49.8(2)	C34-C33-K2-O7	-63.38(19)

Co2-C33-K2-O7	-143.20(16)	C32-C31-K2-O10	-103.72(18)
C32-C33-K2-O9	-56.7(2)	C39-C31-K2-O10	123.55(17)
C34-C33-K2-O9	59.3(2)	Co2-C31-K2-O10	-139.52(15)
Co2-C33-K2-O9	-20.5(2)	C32-C31-K2-O8	142.98(17)
C32-C33-K2-O12	120.39(19)	C39-C31-K2-O8	10.24(18)
C34-C33-K2-O12	-123.6(2)	Co2-C31-K2-O8	107.18(14)
Co2-C33-K2-O12	156.58(17)	C39-C31-K2-C32	-132.7(3)
C32-C33-K2-O11	60.51(19)	Co2-C31-K2-C32	-35.80(16)
C34-C33-K2-O11	176.5(2)	C32-C31-K2-C39	132.7(3)
Co2-C33-K2-O11	96.70(16)	Co2-C31-K2-C39	96.9(2)
C32-C33-K2-O10	10.3(2)	C32-C31-K2-C33	34.52(17)
C34-C33-K2-O10	126.31(19)	C39-C31-K2-C33	-98.21(19)
Co2-C33-K2-O10	46.49(17)	Co2-C31-K2-C33	-1.27(11)
C32-C33-K2-O8	-131.23(18)	O9-K2-O7-C60	143.9(2)
C34-C33-K2-O8	-15.2(2)	O12-K2-O7-C60	-6.7(2)
Co2-C33-K2-O8	-95.04(16)	O11-K2-O7-C60	-8.1(2)
C34-C33-K2-C32	116.0(3)	O10-K2-O7-C60	67.4(3)
Co2-C33-K2-C32	36.19(17)	O8-K2-O7-C60	142.8(2)
C32-C33-K2-C39	-67.73(19)	C32-K2-O7-C60	-84.5(2)
C34-C33-K2-C39	48.28(18)	C39-K2-O7-C60	-130.5(2)
Co2-C33-K2-C39	-31.54(13)	C33-K2-O7-C60	-84.2(2)
C32-C33-K2-C31	-34.74(18)	C31-K2-O7-C60	-109.3(2)
C34-C33-K2-C31	81.3(2)	O9-K2-O7-C49	1.3(2)
Co2-C33-K2-C31	1.45(12)	O12-K2-O7-C49	-149.3(2)
C32-C31-K2-O7	75.17(19)	O11-K2-O7-C49	-150.7(2)
C39-C31-K2-O7	-57.57(18)	O10-K2-O7-C49	-75.2(3)
Co2-C31-K2-O7	39.37(16)	O8-K2-O7-C49	0.2(2)
C32-C31-K2-O9	-162.44(18)	C32-K2-O7-C49	133.0(2)
C39-C31-K2-O9	64.83(16)	C39-K2-O7-C49	87.0(2)
Co2-C31-K2-O9	161.77(14)	C33-K2-O7-C49	133.2(2)
C32-C31-K2-O12	8.0(2)	C31-K2-O7-C49	108.1(2)
C39-C31-K2-O12	-124.75(16)	C60-O7-C49-C50	-175.9(3)
Co2-C31-K2-O12	-27.81(16)	K2-O7-C49-C50	-30.8(3)
C32-C31-K2-O11	-45.11(18)	O7-C49-C50-O8	64.2(3)
C39-C31-K2-O11	-177.84(16)	C49-C50-O8-C51	177.3(3)
Co2-C31-K2-O11	-80.90(14)	C49-C50-O8-K2	-63.0(3)

O7-K2-O8-C51	152.5(2)	O8-K2-O9-C53	-152.3(2)
O9-K2-O8-C51	-26.3(2)	C32-K2-O9-C53	76.8(2)
O12-K2-O8-C51	-179.1(2)	C39-K2-O9-C53	107.0(2)
O11-K2-O8-C51	-115.4(2)	C33-K2-O9-C53	98.6(2)
O10-K2-O8-C51	-48.0(2)	C31-K2-O9-C53	84.5(2)
C32-K2-O8-C51	66.3(2)	C52-O9-C53-C54	177.1(3)
C39-K2-O8-C51	49.7(2)	K2-O9-C53-C54	-36.5(3)
C33-K2-O8-C51	92.5(2)	O9-C53-C54-O10	66.0(3)
C31-K2-O8-C51	45.4(2)	C53-C54-O10-C55	173.1(3)
O7-K2-O8-C50	31.78(18)	C53-C54-O10-K2	-61.7(3)
O9-K2-O8-C50	-147.1(2)	O7-K2-O10-C55	-116.7(3)
O12-K2-O8-C50	60.19(19)	O9-K2-O10-C55	155.9(2)
O11-K2-O8-C50	123.8(2)	O12-K2-O10-C55	-51.8(2)
O10-K2-O8-C50	-168.70(18)	O11-K2-O10-C55	-30.2(2)
C32-K2-O8-C50	-54.4(2)	O8-K2-O10-C55	177.5(2)
C39-K2-O8-C50	-71.03(19)	C32-K2-O10-C55	36.8(2)
C33-K2-O8-C50	-28.2(2)	C39-K2-O10-C55	80.7(2)
C31-K2-O8-C50	-75.29(19)	C33-K2-O10-C55	32.6(2)
C50-O8-C51-C52	176.5(3)	C31-K2-O10-C55	60.3(2)
K2-O8-C51-C52	58.4(3)	O7-K2-O10-C54	116.7(3)
O8-C51-C52-O9	-66.2(4)	O9-K2-O10-C54	29.35(19)
C51-C52-O9-C53	-174.1(3)	O12-K2-O10-C54	-178.34(19)
C51-C52-O9-K2	39.4(4)	O11-K2-O10-C54	-156.7(2)
O7-K2-O9-C52	-9.1(3)	O8-K2-O10-C54	51.0(2)
O12-K2-O9-C52	69.4(3)	C32-K2-O10-C54	-89.7(2)
O11-K2-O9-C52	143.3(2)	C39-K2-O10-C54	-45.8(2)
O10-K2-O9-C52	149.0(3)	C33-K2-O10-C54	-93.9(2)
O8-K2-O9-C52	-8.0(2)	C31-K2-O10-C54	-66.3(2)
C32-K2-O9-C52	-138.9(2)	C54-O10-C55-C56	-175.1(3)
C39-K2-O9-C52	-108.6(2)	K2-O10-C55-C56	60.9(3)
C33-K2-O9-C52	-117.1(2)	O10-C55-C56-O11	-62.2(3)
C31-K2-O9-C52	-131.2(2)	C55-C56-O11-C57	178.5(3)
O7-K2-O9-C53	-153.4(2)	C55-C56-O11-K2	33.0(3)
O12-K2-O9-C53	-74.9(3)	O7-K2-O11-C57	12.1(2)
O11-K2-O9-C53	-1.1(2)	O9-K2-O11-C57	-140.1(2)
O10-K2-O9-C53	4.7(2)	O12-K2-O11-C57	10.7(2)

O10-K2-O11-C57	-146.0(2)	O11-K2-O12-C59	152.5(2)
O8-K2-O11-C57	-65.3(3)	O10-K2-O12-C59	174.1(2)
C32-K2-O11-C57	113.5(2)	O8-K2-O12-C59	-54.1(2)
C39-K2-O11-C57	130.6(2)	C32-K2-O12-C59	86.8(2)
C33-K2-O11-C57	91.2(2)	C39-K2-O12-C59	58.6(2)
C31-K2-O11-C57	131.6(2)	C33-K2-O12-C59	66.2(2)
O7-K2-O11-C56	155.5(2)	C31-K2-O12-C59	83.5(2)
O9-K2-O11-C56	3.3(2)	O7-K2-O12-C58	-155.8(2)
O12-K2-O11-C56	154.1(2)	O9-K2-O12-C58	111.1(2)
O10-K2-O11-C56	-2.5(2)	O11-K2-O12-C58	22.7(2)
O8-K2-O11-C56	78.2(3)	O10-K2-O12-C58	44.3(2)
C32-K2-O11-C56	-103.1(2)	O8-K2-O12-C58	176.0(2)
C39-K2-O11-C56	-86.0(2)	C32-K2-O12-C58	-43.1(2)
C33-K2-O11-C56	-125.4(2)	C39-K2-O12-C58	-71.2(2)
C31-K2-O11-C56	-85.0(2)	C33-K2-O12-C58	-63.7(2)
C56-O11-C57-C58	174.0(3)	C31-K2-O12-C58	-46.3(2)
K2-O11-C57-C58	-40.2(3)	C58-O12-C59-C60	-172.4(3)
O11-C57-C58-O12	60.6(4)	K2-O12-C59-C60	55.9(3)
C57-C58-O12-C59	177.3(3)	C49-O7-C60-C59	-177.3(3)
C57-C58-O12-K2	-52.9(3)	K2-O7-C60-C59	36.7(4)
O7-K2-O12-C59	-26.0(2)	O12-C59-C60-O7	-61.9(4)
O9-K2-O12-C59	-119.0(2)		

Symmetry transformations used to generate equivalent atoms:

REFERENCE NUMBER: 05155 [**10b**]

CRYSTAL STRUCTURE REPORT

$C_{42.5} H_{66.5} Co K_{1.5} O_{10}$

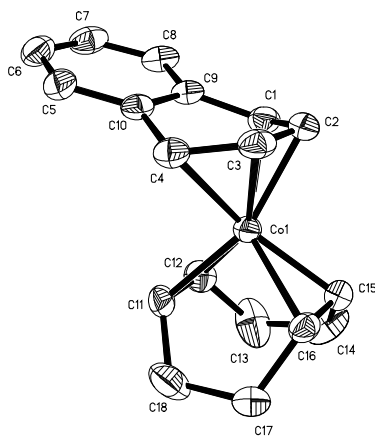
or

$0.5(\{[K(18\text{-crown-6})]_2[Cp]\}[K(18\text{-crown-6})(THF)_2][Co(1,5\text{-COD})(\eta^4\text{-}C_{10}H_8)_2])$

Report prepared for:

W. Brennessel, Prof. J. Ellis

June 03, 2005



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Data collection

A crystal (approximate dimensions 0.32 x 0.30 x 0.24 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Siemens SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 184 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 10 seconds and a detector distance of 4.92 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 3851 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ 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. Hydrogen atoms on carbon atoms attached to the cobalt center were found from the difference map and refined with individual isotropic displacement parameters. The remaining 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 $R1 = 0.0369$ and $wR2 = 0.0887$ (F^2 , all data).

Structure description

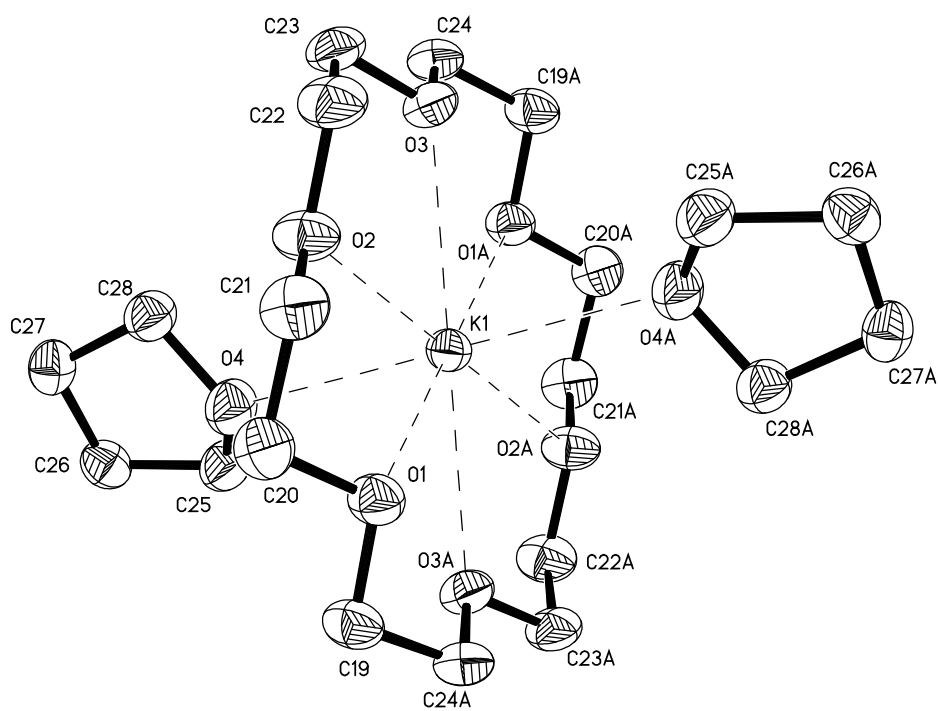
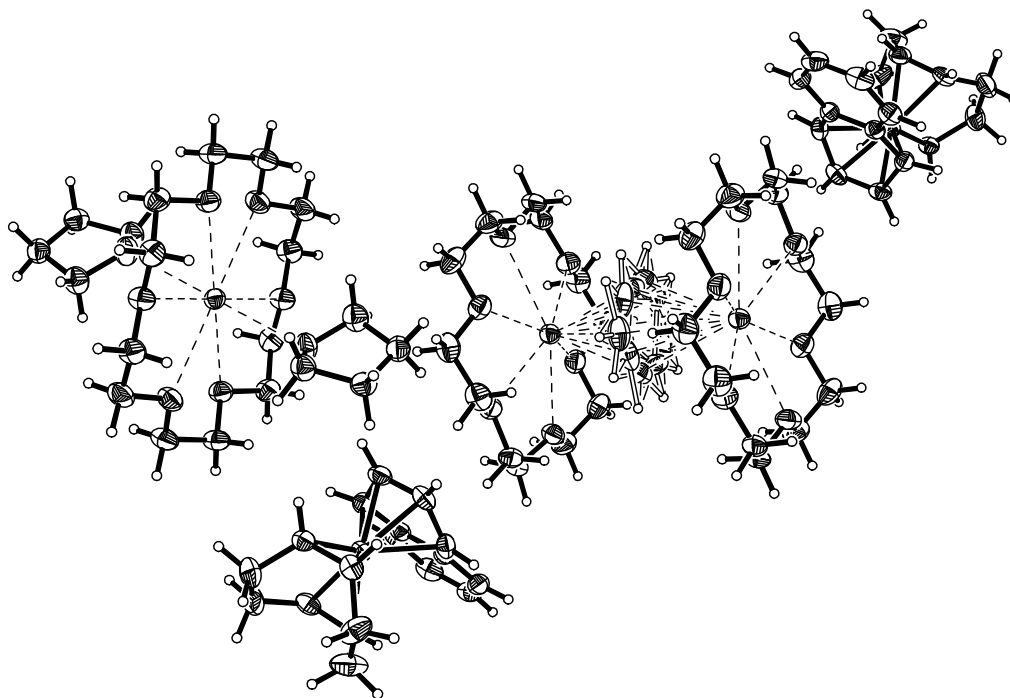
The structure is the one suggested. It is a double salt of naphthalenecyclooctadienecobaltate and cyclopentadienide, in a ratio of one to one half. The Cp anion is sandwiched between two K(18-crown-6) cations and lies on a crystallographic inversion center; thus, one half of this complex cation is unique and the disorder of the Cp anion is 50:50. The second cation, K(18-crown-6)(THF)₂⁺, also lies on a crystallographic inversion center, coincident with the potassium atom; thus, one half of this cation is unique. The atoms of the cobalt anion all lie on general positions; the twist angle is 81.4° (almost tetrahedral) and the dihedral (fold) angle is 27.4(1)°.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
 - ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
 - ³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
 - ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
 - ⁵ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

$$\begin{aligned}
 R_{\text{int}} &= \Sigma |F_o|^2 - \langle F_o|^2 \rangle / \Sigma |F_o|^2 \\
 R_1 &= \Sigma ||F_o| - |F_c|| / \Sigma |F_o| \\
 wR2 &= [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2} \\
 \text{where } w &= q / [\sigma^2(F_o^2) + (a^*P)^2 + b^*P + d + e^*\sin(\theta)] \\
 \text{GooF} = S &= [\Sigma [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}
 \end{aligned}$$



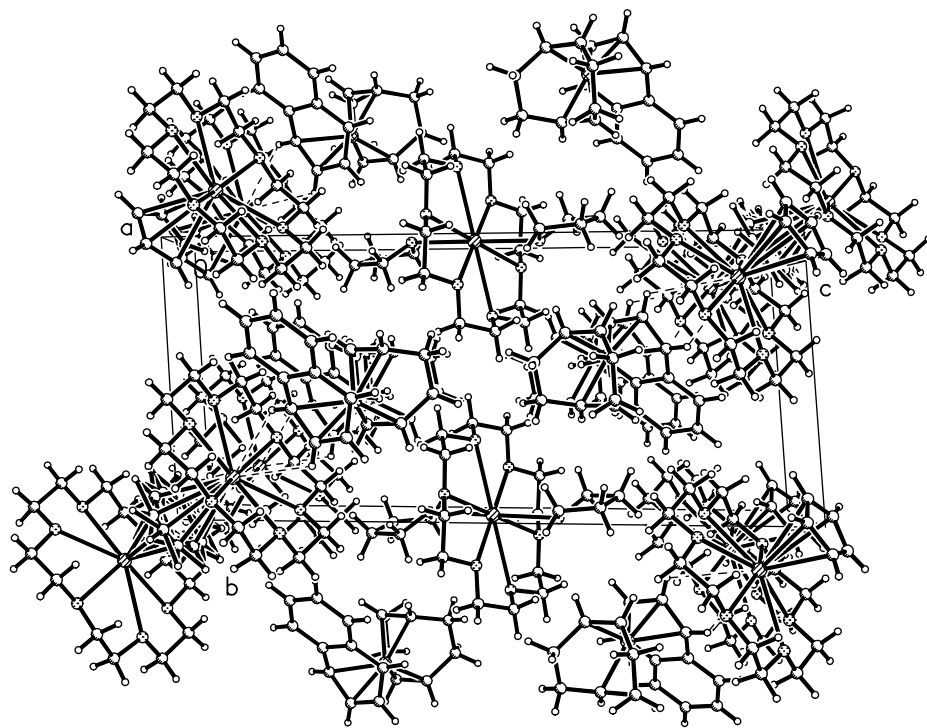
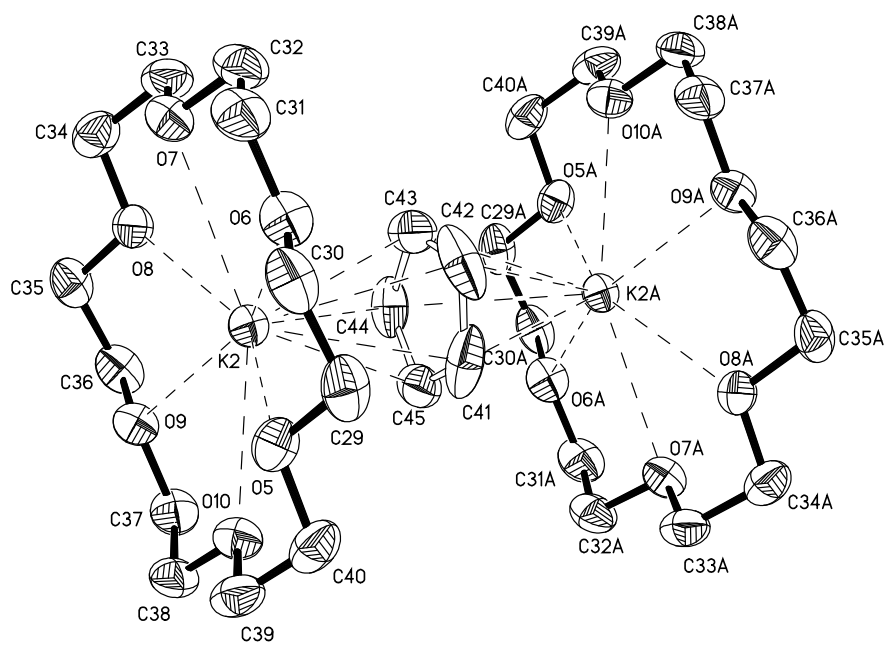


Table 1. Crystal data and structure refinement for 05155.

Identification code	05155	
Empirical formula	C _{42.50} H _{66.50} Co K _{1.50} O ₁₀	
Formula weight	855.04	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 9.7377(8) Å	α = 85.758(1)°
	<i>b</i> = 10.0468(8) Å	β = 79.304(1)°
	<i>c</i> = 22.625(2) Å	γ = 87.193(1)°
Volume	2167.6(3) Å ³	
<i>Z</i>	2	
Density (calculated)	1.310 Mg/m ³	
Absorption coefficient	0.594 mm ⁻¹	
<i>F</i> (000)	914	
Crystal color, morphology	deep red-orange, block	
Crystal size	0.32 x 0.30 x 0.24 mm ³	
Theta range for data collection	0.92 to 27.53°	
Index ranges	-12 ≤ <i>h</i> ≤ 12, -12 ≤ <i>k</i> ≤ 12, -29 ≤ <i>l</i> ≤ 29	
Reflections collected	25641	
Independent reflections	9840 [<i>R</i> (int) = 0.0293]	
Observed reflections	7569	
Completeness to theta = 27.53°	98.5%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8705 and 0.8326	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	9840 / 14 / 552	
Goodness-of-fit on <i>F</i> ²	1.039	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0369, <i>wR</i> 2 = 0.0815	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0557, <i>wR</i> 2 = 0.0887	
Largest diff. peak and hole	0.453 and -0.428 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05155. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	7433(1)	4223(1)	6992(1)	25(1)
C1	6523(2)	3970(2)	7934(1)	32(1)
C2	6463(2)	2836(2)	7598(1)	34(1)
C3	5787(2)	3019(2)	7101(1)	33(1)
C4	5234(2)	4327(2)	6983(1)	30(1)
C5	3672(2)	6175(2)	7473(1)	35(1)
C6	3326(2)	7016(2)	7953(1)	41(1)
C7	4002(2)	6842(2)	8435(1)	40(1)
C8	5026(2)	5825(2)	8456(1)	35(1)
C9	5402(2)	4998(2)	7980(1)	28(1)
C10	4710(2)	5182(2)	7479(1)	28(1)
C11	7761(2)	5978(2)	6507(1)	32(1)
C12	8362(2)	5966(2)	7020(1)	36(1)
C13	9929(3)	5754(2)	6995(1)	60(1)
C14	10431(2)	4336(2)	6989(1)	50(1)
C15	9377(2)	3394(2)	6859(1)	32(1)
C16	8837(2)	3437(2)	6320(1)	29(1)
C17	9293(2)	4461(2)	5801(1)	42(1)
C18	8543(3)	5785(2)	5879(1)	53(1)
K1	5000	0	5000	28(1)
C19	6353(2)	-2941(2)	4260(1)	38(1)
O1	5337(1)	-2742(1)	4790(1)	35(1)
C20	4043(2)	-3322(2)	4762(1)	40(1)
C21	3025(2)	-3053(2)	5329(1)	42(1)
O2	2667(1)	-1664(1)	5320(1)	39(1)
C22	1680(2)	-1309(2)	5836(1)	44(1)
C23	1346(2)	156(2)	5766(1)	40(1)
O3	2580(1)	857(1)	5755(1)	35(1)
C24	2337(2)	2268(2)	5698(1)	37(1)
O4	4088(2)	-34(2)	3945(1)	43(1)
C25	4820(2)	755(2)	3445(1)	43(1)

C26	3945(2)	782(2)	2955(1)	38(1)
C27	2481(2)	441(2)	3296(1)	37(1)
C28	2646(2)	296(2)	3952(1)	39(1)
K2	-932(1)	1539(1)	9022(1)	31(1)
O5	-1919(1)	-309(1)	8294(1)	40(1)
O6	-3796(1)	848(2)	9233(1)	42(1)
O7	-3235(1)	3439(2)	9537(1)	41(1)
O8	-436(1)	4206(1)	9279(1)	38(1)
O9	1406(1)	2880(1)	8380(1)	37(1)
O10	935(1)	341(1)	8053(1)	40(1)
C29	-3083(2)	-987(2)	8637(1)	47(1)
C30	-4228(2)	15(2)	8825(1)	45(1)
C31	-4847(2)	1811(2)	9455(1)	49(1)
C32	-4290(2)	2622(2)	9875(1)	48(1)
C33	-2651(2)	4258(2)	9903(1)	46(1)
C34	-1565(2)	5077(2)	9505(1)	46(1)
C35	636(2)	4861(2)	8866(1)	44(1)
C36	1835(2)	3893(2)	8707(1)	44(1)
C37	2524(2)	1976(2)	8163(1)	45(1)
C38	2050(2)	1119(2)	7735(1)	45(1)
C39	320(2)	-414(2)	7672(1)	45(1)
C40	-818(2)	-1205(2)	8053(1)	46(1)
C41	-100(30)	-931(11)	9772(10)	61(4)
C42	-1072(15)	-300(30)	10184(9)	66(4)
C43	-480(20)	820(20)	10327(7)	55(4)
C44	870(18)	862(14)	10021(9)	47(3)
C45	1110(20)	-210(20)	9671(8)	50(3)

Table 3. Bond lengths [Å] and angles [°] for 05155.

Co(1)-C(15)	2.0099(19)	C(13)-H(13B)	0.9900
Co(1)-C(11)	2.0134(18)	C(14)-C(15)	1.512(3)
Co(1)-C(2)	2.0199(18)	C(14)-H(14A)	0.9900
Co(1)-C(12)	2.0203(19)	C(14)-H(14B)	0.9900
Co(1)-C(3)	2.0228(19)	C(15)-C(16)	1.412(3)
Co(1)-C(16)	2.0252(18)	C(15)-H(15)	0.97(2)
Co(1)-C(4)	2.1427(19)	C(16)-C(17)	1.518(3)
Co(1)-C(1)	2.1528(18)	C(16)-H(16)	0.95(2)
C(1)-C(2)	1.425(3)	C(17)-C(18)	1.492(3)
C(1)-C(9)	1.460(3)	C(17)-H(17A)	0.9900
C(1)-H(1)	0.94(2)	C(17)-H(17B)	0.9900
C(2)-C(3)	1.402(3)	C(18)-H(18A)	0.9900
C(2)-H(2)	0.94(2)	C(18)-H(18B)	0.9900
C(3)-C(4)	1.421(3)	K(1)-O(4)	2.7001(14)
C(3)-H(3)	0.95(2)	K(1)-O(4)#1	2.7001(14)
C(4)-C(10)	1.465(3)	K(1)-O(3)	2.7809(12)
C(4)-H(4)	0.96(2)	K(1)-O(3)#1	2.7810(12)
C(5)-C(10)	1.387(3)	K(1)-O(1)#1	2.8231(13)
C(5)-C(6)	1.407(3)	K(1)-O(1)	2.8231(13)
C(5)-H(5)	0.9500	K(1)-O(2)	2.8398(13)
C(6)-C(7)	1.371(3)	K(1)-O(2)#1	2.8398(13)
C(6)-H(6)	0.9500	C(19)-O(1)	1.425(2)
C(7)-C(8)	1.396(3)	C(19)-C(24)#1	1.494(3)
C(7)-H(7)	0.9500	C(19)-H(19A)	0.9900
C(8)-C(9)	1.394(3)	C(19)-H(19B)	0.9900
C(8)-H(8)	0.9500	O(1)-C(20)	1.427(2)
C(9)-C(10)	1.419(3)	C(20)-C(21)	1.501(3)
C(11)-C(12)	1.392(3)	C(20)-H(20A)	0.9900
C(11)-C(18)	1.503(3)	C(20)-H(20B)	0.9900
C(11)-H(11)	0.96(2)	C(21)-O(2)	1.421(2)
C(12)-C(13)	1.522(3)	C(21)-H(21A)	0.9900
C(12)-H(12)	0.95(2)	C(21)-H(21B)	0.9900
C(13)-C(14)	1.483(3)	O(2)-C(22)	1.424(2)
C(13)-H(13A)	0.9900	C(22)-C(23)	1.495(3)

C(22)-H(22A)	0.9900	O(6)-C(31)	1.421(3)
C(22)-H(22B)	0.9900	O(6)-C(30)	1.422(2)
C(23)-O(3)	1.418(2)	O(7)-C(33)	1.417(3)
C(23)-H(23A)	0.9900	O(7)-C(32)	1.419(2)
C(23)-H(23B)	0.9900	O(8)-C(34)	1.414(2)
O(3)-C(24)	1.426(2)	O(8)-C(35)	1.417(2)
C(24)-C(19)#1	1.494(3)	O(9)-C(37)	1.422(2)
C(24)-H(24A)	0.9900	O(9)-C(36)	1.423(2)
C(24)-H(24B)	0.9900	O(10)-C(39)	1.416(2)
O(4)-C(28)	1.425(2)	O(10)-C(38)	1.421(2)
O(4)-C(25)	1.429(2)	C(29)-C(30)	1.488(3)
C(25)-C(26)	1.515(3)	C(29)-H(29A)	0.9900
C(25)-H(25A)	0.9900	C(29)-H(29B)	0.9900
C(25)-H(25B)	0.9900	C(30)-H(30A)	0.9900
C(26)-C(27)	1.532(3)	C(30)-H(30B)	0.9900
C(26)-H(26A)	0.9900	C(31)-C(32)	1.486(3)
C(26)-H(26B)	0.9900	C(31)-H(31A)	0.9900
C(27)-C(28)	1.518(3)	C(31)-H(31B)	0.9900
C(27)-H(27A)	0.9900	C(32)-H(32A)	0.9900
C(27)-H(27B)	0.9900	C(32)-H(32B)	0.9900
C(28)-H(28A)	0.9900	C(33)-C(34)	1.493(3)
C(28)-H(28B)	0.9900	C(33)-H(33A)	0.9900
K(2)-O(9)	2.8092(14)	C(33)-H(33B)	0.9900
K(2)-O(6)	2.8514(14)	C(34)-H(34A)	0.9900
K(2)-O(8)	2.8652(14)	C(34)-H(34B)	0.9900
K(2)-O(10)	2.8737(14)	C(35)-C(36)	1.491(3)
K(2)-O(5)	2.8812(14)	C(35)-H(35A)	0.9900
K(2)-O(7)	2.9948(15)	C(35)-H(35B)	0.9900
K(2)-C(42)#2	3.054(14)	C(36)-H(36A)	0.9900
K(2)-C(41)	3.066(15)	C(36)-H(36B)	0.9900
K(2)-C(42)	3.085(13)	C(37)-C(38)	1.491(3)
K(2)-C(41)#2	3.087(16)	C(37)-H(37A)	0.9900
K(2)-C(45)	3.09(2)	C(37)-H(37B)	0.9900
K(2)-C(43)	3.093(19)	C(38)-H(38A)	0.9900
O(5)-C(40)	1.421(3)	C(38)-H(38B)	0.9900
O(5)-C(29)	1.423(2)	C(39)-C(40)	1.495(3)

C(39)-H(39A)	0.9900	C(2)-Co(1)-C(4)	70.24(8)
C(39)-H(39B)	0.9900	C(12)-Co(1)-C(4)	116.99(8)
C(40)-H(40A)	0.9900	C(3)-Co(1)-C(4)	39.75(8)
C(40)-H(40B)	0.9900	C(16)-Co(1)-C(4)	122.04(8)
C(41)-C(42)	1.370(11)	C(15)-Co(1)-C(1)	109.19(8)
C(41)-C(45)	1.383(11)	C(11)-Co(1)-C(1)	125.93(8)
C(41)-K(2)#2	3.087(16)	C(2)-Co(1)-C(1)	39.78(8)
C(41)-H(41A)	0.9500	C(12)-Co(1)-C(1)	97.60(8)
C(42)-C(43)	1.370(11)	C(3)-Co(1)-C(1)	70.48(8)
C(42)-K(2)#2	3.054(14)	C(16)-Co(1)-C(1)	144.24(8)
C(42)-H(42A)	0.9500	C(4)-Co(1)-C(1)	77.16(7)
C(43)-C(44)	1.372(9)	C(2)-C(1)-C(9)	120.26(18)
C(43)-K(2)#2	3.100(19)	C(2)-C(1)-Co(1)	65.08(10)
C(43)-H(43A)	0.9500	C(9)-C(1)-Co(1)	101.16(12)
C(44)-C(45)	1.365(10)	C(2)-C(1)-H(1)	119.6(12)
C(44)-K(2)#2	3.127(17)	C(9)-C(1)-H(1)	115.4(12)
C(44)-H(44A)	0.9500	Co(1)-C(1)-H(1)	124.5(12)
C(45)-K(2)#2	3.13(2)	C(3)-C(2)-C(1)	117.08(18)
C(45)-H(45A)	0.9500	C(3)-C(2)-Co(1)	69.81(11)
C(15)-Co(1)-C(11)	100.81(8)	C(1)-C(2)-Co(1)	75.14(11)
C(15)-Co(1)-C(2)	99.21(8)	C(3)-C(2)-H(2)	121.8(13)
C(11)-Co(1)-C(2)	159.16(8)	C(1)-C(2)-H(2)	120.8(13)
C(15)-Co(1)-C(12)	85.93(8)	Co(1)-C(2)-H(2)	119.7(13)
C(11)-Co(1)-C(12)	40.37(8)	C(2)-C(3)-C(4)	116.23(18)
C(2)-Co(1)-C(12)	136.49(8)	C(2)-C(3)-Co(1)	69.59(11)
C(15)-Co(1)-C(3)	118.83(8)	C(4)-C(3)-Co(1)	74.68(11)
C(11)-Co(1)-C(3)	129.68(8)	C(2)-C(3)-H(3)	121.9(13)
C(2)-Co(1)-C(3)	40.59(8)	C(4)-C(3)-H(3)	121.8(13)
C(12)-Co(1)-C(3)	154.67(8)	Co(1)-C(3)-H(3)	123.5(12)
C(15)-Co(1)-C(16)	40.95(8)	C(3)-C(4)-C(10)	120.46(17)
C(11)-Co(1)-C(16)	85.58(8)	C(3)-C(4)-Co(1)	65.57(11)
C(2)-Co(1)-C(16)	113.65(8)	C(10)-C(4)-Co(1)	101.58(12)
C(12)-Co(1)-C(16)	98.44(8)	C(3)-C(4)-H(4)	118.0(11)
C(3)-Co(1)-C(16)	104.04(8)	C(10)-C(4)-H(4)	117.8(11)
C(15)-Co(1)-C(4)	155.76(8)	Co(1)-C(4)-H(4)	120.6(11)
C(11)-Co(1)-C(4)	93.16(8)	C(10)-C(5)-C(6)	120.44(19)

C(10)-C(5)-H(5)	119.8	C(13)-C(14)-H(14A)	108.8
C(6)-C(5)-H(5)	119.8	C(15)-C(14)-H(14A)	108.8
C(7)-C(6)-C(5)	119.91(19)	C(13)-C(14)-H(14B)	108.8
C(7)-C(6)-H(6)	120.0	C(15)-C(14)-H(14B)	108.8
C(5)-C(6)-H(6)	120.0	H(14A)-C(14)-H(14B)	107.7
C(6)-C(7)-C(8)	120.50(18)	C(16)-C(15)-C(14)	125.07(18)
C(6)-C(7)-H(7)	119.7	C(16)-C(15)-Co(1)	70.10(11)
C(8)-C(7)-H(7)	119.7	C(14)-C(15)-Co(1)	111.60(13)
C(9)-C(8)-C(7)	120.43(19)	C(16)-C(15)-H(15)	116.1(13)
C(9)-C(8)-H(8)	119.8	C(14)-C(15)-H(15)	113.5(13)
C(7)-C(8)-H(8)	119.8	Co(1)-C(15)-H(15)	111.2(13)
C(8)-C(9)-C(10)	119.17(17)	C(15)-C(16)-C(17)	121.92(18)
C(8)-C(9)-C(1)	125.14(18)	C(15)-C(16)-Co(1)	68.95(10)
C(10)-C(9)-C(1)	115.61(16)	C(17)-C(16)-Co(1)	112.16(13)
C(5)-C(10)-C(9)	119.51(17)	C(15)-C(16)-H(16)	117.1(12)
C(5)-C(10)-C(4)	124.95(18)	C(17)-C(16)-H(16)	115.0(12)
C(9)-C(10)-C(4)	115.43(16)	Co(1)-C(16)-H(16)	112.2(12)
C(12)-C(11)-C(18)	125.4(2)	C(18)-C(17)-C(16)	113.44(16)
C(12)-C(11)-Co(1)	70.08(11)	C(18)-C(17)-H(17A)	108.9
C(18)-C(11)-Co(1)	111.57(13)	C(16)-C(17)-H(17A)	108.9
C(12)-C(11)-H(11)	116.3(12)	C(18)-C(17)-H(17B)	108.9
C(18)-C(11)-H(11)	114.0(12)	C(16)-C(17)-H(17B)	108.9
Co(1)-C(11)-H(11)	109.1(12)	H(17A)-C(17)-H(17B)	107.7
C(11)-C(12)-C(13)	122.1(2)	C(17)-C(18)-C(11)	114.58(17)
C(11)-C(12)-Co(1)	69.55(11)	C(17)-C(18)-H(18A)	108.6
C(13)-C(12)-Co(1)	111.46(14)	C(11)-C(18)-H(18A)	108.6
C(11)-C(12)-H(12)	116.4(14)	C(17)-C(18)-H(18B)	108.6
C(13)-C(12)-H(12)	115.8(14)	C(11)-C(18)-H(18B)	108.6
Co(1)-C(12)-H(12)	111.5(14)	H(18A)-C(18)-H(18B)	107.6
C(14)-C(13)-C(12)	114.50(18)	O(4)-K(1)-O(4)#1	180.000(19)
C(14)-C(13)-H(13A)	108.6	O(4)-K(1)-O(3)	101.06(4)
C(12)-C(13)-H(13A)	108.6	O(4)#1-K(1)-O(3)	78.94(4)
C(14)-C(13)-H(13B)	108.6	O(4)-K(1)-O(3)#1	78.94(4)
C(12)-C(13)-H(13B)	108.6	O(4)#1-K(1)-O(3)#1	101.06(4)
H(13A)-C(13)-H(13B)	107.6	O(3)-K(1)-O(3)#1	180.0
C(13)-C(14)-C(15)	113.87(18)	O(4)-K(1)-O(1)#1	101.17(4)

O(4)#1-K(1)-O(1)#1	78.83(4)	O(2)-C(21)-C(20)	108.50(16)
O(3)-K(1)-O(1)#1	61.96(4)	O(2)-C(21)-H(21A)	110.0
O(3)#1-K(1)-O(1)#1	118.04(4)	C(20)-C(21)-H(21A)	110.0
O(4)-K(1)-O(1)	78.83(4)	O(2)-C(21)-H(21B)	110.0
O(4)#1-K(1)-O(1)	101.17(4)	C(20)-C(21)-H(21B)	110.0
O(3)-K(1)-O(1)	118.04(4)	H(21A)-C(21)-H(21B)	108.4
O(3)#1-K(1)-O(1)	61.96(4)	C(21)-O(2)-C(22)	112.85(15)
O(1)#1-K(1)-O(1)	180.0	C(21)-O(2)-K(1)	114.03(11)
O(4)-K(1)-O(2)	77.92(4)	C(22)-O(2)-K(1)	115.24(11)
O(4)#1-K(1)-O(2)	102.08(4)	O(2)-C(22)-C(23)	107.97(16)
O(3)-K(1)-O(2)	59.19(4)	O(2)-C(22)-H(22A)	110.1
O(3)#1-K(1)-O(2)	120.81(4)	C(23)-C(22)-H(22A)	110.1
O(1)#1-K(1)-O(2)	119.55(4)	O(2)-C(22)-H(22B)	110.1
O(1)-K(1)-O(2)	60.45(4)	C(23)-C(22)-H(22B)	110.1
O(4)-K(1)-O(2)#1	102.08(4)	H(22A)-C(22)-H(22B)	108.4
O(4)#1-K(1)-O(2)#1	77.92(4)	O(3)-C(23)-C(22)	108.70(16)
O(3)-K(1)-O(2)#1	120.80(4)	O(3)-C(23)-H(23A)	109.9
O(3)#1-K(1)-O(2)#1	59.19(4)	C(22)-C(23)-H(23A)	109.9
O(1)#1-K(1)-O(2)#1	60.45(4)	O(3)-C(23)-H(23B)	109.9
O(1)-K(1)-O(2)#1	119.55(4)	C(22)-C(23)-H(23B)	109.9
O(2)-K(1)-O(2)#1	180.00(4)	H(23A)-C(23)-H(23B)	108.3
O(1)-C(19)-C(24)#1	109.37(16)	C(23)-O(3)-C(24)	111.95(15)
O(1)-C(19)-H(19A)	109.8	C(23)-O(3)-K(1)	117.47(11)
C(24)#1-C(19)-H(19A)	109.8	C(24)-O(3)-K(1)	112.82(10)
O(1)-C(19)-H(19B)	109.8	O(3)-C(24)-C(19)#1	109.00(16)
C(24)#1-C(19)-H(19B)	109.8	O(3)-C(24)-H(24A)	109.9
H(19A)-C(19)-H(19B)	108.2	C(19)#1-C(24)-H(24A)	109.9
C(19)-O(1)-C(20)	111.59(14)	O(3)-C(24)-H(24B)	109.9
C(19)-O(1)-K(1)	110.34(10)	C(19)#1-C(24)-H(24B)	109.9
C(20)-O(1)-K(1)	112.19(11)	H(24A)-C(24)-H(24B)	108.3
O(1)-C(20)-C(21)	108.46(16)	C(28)-O(4)-C(25)	105.06(15)
O(1)-C(20)-H(20A)	110.0	C(28)-O(4)-K(1)	116.97(11)
C(21)-C(20)-H(20A)	110.0	C(25)-O(4)-K(1)	116.82(12)
O(1)-C(20)-H(20B)	110.0	O(4)-C(25)-C(26)	106.12(16)
C(21)-C(20)-H(20B)	110.0	O(4)-C(25)-H(25A)	110.5
H(20A)-C(20)-H(20B)	108.4	C(26)-C(25)-H(25A)	110.5

O(4)-C(25)-H(25B)	110.5	O(9)-K(2)-C(42)#2	85.4(2)
C(26)-C(25)-H(25B)	110.5	O(6)-K(2)-C(42)#2	121.2(2)
H(25A)-C(25)-H(25B)	108.7	O(8)-K(2)-C(42)#2	93.0(6)
C(25)-C(26)-C(27)	104.06(16)	O(10)-K(2)-C(42)#2	85.2(6)
C(25)-C(26)-H(26A)	110.9	O(5)-K(2)-C(42)#2	114.5(6)
C(27)-C(26)-H(26A)	110.9	O(7)-K(2)-C(42)#2	119.6(6)
C(25)-C(26)-H(26B)	110.9	O(9)-K(2)-C(41)	112.1(6)
C(27)-C(26)-H(26B)	110.9	O(6)-K(2)-C(41)	92.6(5)
H(26A)-C(26)-H(26B)	109.0	O(8)-K(2)-C(41)	122.7(2)
C(28)-C(27)-C(26)	103.88(16)	O(10)-K(2)-C(41)	83.7(5)
C(28)-C(27)-H(27A)	111.0	O(5)-K(2)-C(41)	86.2(2)
C(26)-C(27)-H(27A)	111.0	O(7)-K(2)-C(41)	121.1(6)
C(28)-C(27)-H(27B)	111.0	C(42)#2-K(2)-C(41)	33.0(3)
C(26)-C(27)-H(27B)	111.0	O(9)-K(2)-C(42)	127.0(2)
H(27A)-C(27)-H(27B)	109.0	O(6)-K(2)-C(42)	79.5(2)
O(4)-C(28)-C(27)	105.74(16)	O(8)-K(2)-C(42)	109.0(6)
O(4)-C(28)-H(28A)	110.6	O(10)-K(2)-C(42)	109.4(6)
C(27)-C(28)-H(28A)	110.6	O(5)-K(2)-C(42)	98.0(5)
O(4)-C(28)-H(28B)	110.6	O(7)-K(2)-C(42)	95.4(6)
C(27)-C(28)-H(28B)	110.6	C(42)#2-K(2)-C(42)	41.9(4)
H(28A)-C(28)-H(28B)	108.7	C(41)-K(2)-C(42)	25.7(2)
O(9)-K(2)-O(6)	153.45(4)	O(9)-K(2)-C(41)#2	98.5(5)
O(9)-K(2)-O(8)	59.53(4)	O(6)-K(2)-C(41)#2	106.5(6)
O(6)-K(2)-O(8)	115.41(4)	O(8)-K(2)-C(41)#2	80.78(19)
O(9)-K(2)-O(10)	58.81(4)	O(10)-K(2)-C(41)#2	110.9(6)
O(6)-K(2)-O(10)	117.73(4)	O(5)-K(2)-C(41)#2	128.01(19)
O(8)-K(2)-O(10)	118.26(4)	O(7)-K(2)-C(41)#2	94.1(5)
O(9)-K(2)-O(5)	111.54(4)	C(42)#2-K(2)-C(41)#2	25.8(2)
O(6)-K(2)-O(5)	58.81(4)	C(41)-K(2)-C(41)#2	42.6(4)
O(8)-K(2)-O(5)	151.08(4)	C(42)-K(2)-C(41)#2	32.7(3)
O(10)-K(2)-O(5)	58.92(4)	O(9)-K(2)-C(45)	87.5(4)
O(9)-K(2)-O(7)	112.03(4)	O(6)-K(2)-C(45)	118.2(4)
O(6)-K(2)-O(7)	58.16(4)	O(8)-K(2)-C(45)	103.7(5)
O(8)-K(2)-O(7)	57.32(4)	O(10)-K(2)-C(45)	76.5(2)
O(10)-K(2)-O(7)	154.01(4)	O(5)-K(2)-C(45)	103.2(4)
O(5)-K(2)-O(7)	111.13(4)	O(7)-K(2)-C(45)	129.1(2)

C(42)#2-K(2)-C(45)	11.5(4)	O(5)-C(29)-H(29B)	110.0
C(41)-K(2)-C(45)	26.0(2)	C(30)-C(29)-H(29B)	110.0
C(42)-K(2)-C(45)	42.2(3)	H(29A)-C(29)-H(29B)	108.3
C(41)#2-K(2)-C(45)	35.3(4)	O(6)-C(30)-C(29)	108.70(17)
O(9)-K(2)-C(43)	108.9(5)	O(6)-C(30)-H(30A)	109.9
O(6)-K(2)-C(43)	95.8(5)	C(29)-C(30)-H(30A)	109.9
O(8)-K(2)-C(43)	84.2(5)	O(6)-C(30)-H(30B)	109.9
O(10)-K(2)-C(43)	118.4(2)	C(29)-C(30)-H(30B)	109.9
O(5)-K(2)-C(43)	123.5(5)	H(30A)-C(30)-H(30B)	108.3
O(7)-K(2)-C(43)	87.4(2)	O(6)-C(31)-C(32)	108.31(18)
C(42)#2-K(2)-C(43)	34.2(4)	O(6)-C(31)-H(31A)	110.0
C(41)-K(2)-C(43)	42.1(3)	C(32)-C(31)-H(31A)	110.0
C(42)-K(2)-C(43)	25.6(2)	O(6)-C(31)-H(31B)	110.0
C(41)#2-K(2)-C(43)	10.8(3)	C(32)-C(31)-H(31B)	110.0
C(45)-K(2)-C(43)	41.9(3)	H(31A)-C(31)-H(31B)	108.4
C(40)-O(5)-C(29)	112.28(16)	O(7)-C(32)-C(31)	108.79(18)
C(40)-O(5)-K(2)	110.53(11)	O(7)-C(32)-H(32A)	109.9
C(29)-O(5)-K(2)	109.87(12)	C(31)-C(32)-H(32A)	109.9
C(31)-O(6)-C(30)	112.74(16)	O(7)-C(32)-H(32B)	109.9
C(31)-O(6)-K(2)	119.31(12)	C(31)-C(32)-H(32B)	109.9
C(30)-O(6)-K(2)	117.94(12)	H(32A)-C(32)-H(32B)	108.3
C(33)-O(7)-C(32)	112.59(16)	O(7)-C(33)-C(34)	108.24(17)
C(33)-O(7)-K(2)	106.27(12)	O(7)-C(33)-H(33A)	110.1
C(32)-O(7)-K(2)	105.27(12)	C(34)-C(33)-H(33A)	110.1
C(34)-O(8)-C(35)	113.08(16)	O(7)-C(33)-H(33B)	110.1
C(34)-O(8)-K(2)	120.46(12)	C(34)-C(33)-H(33B)	110.1
C(35)-O(8)-K(2)	115.52(11)	H(33A)-C(33)-H(33B)	108.4
C(37)-O(9)-C(36)	112.44(16)	O(8)-C(34)-C(33)	107.78(17)
C(37)-O(9)-K(2)	111.86(11)	O(8)-C(34)-H(34A)	110.2
C(36)-O(9)-K(2)	112.86(11)	C(33)-C(34)-H(34A)	110.2
C(39)-O(10)-C(38)	113.11(16)	O(8)-C(34)-H(34B)	110.2
C(39)-O(10)-K(2)	116.78(12)	C(33)-C(34)-H(34B)	110.2
C(38)-O(10)-K(2)	117.23(11)	H(34A)-C(34)-H(34B)	108.5
O(5)-C(29)-C(30)	108.60(17)	O(8)-C(35)-C(36)	108.76(17)
O(5)-C(29)-H(29A)	110.0	O(8)-C(35)-H(35A)	109.9
C(30)-C(29)-H(29A)	110.0	C(36)-C(35)-H(35A)	109.9

O(8)-C(35)-H(35B)	109.9	C(42)-C(41)-K(2)#2	75.8(8)
C(36)-C(35)-H(35B)	109.9	C(45)-C(41)-K(2)#2	79.0(11)
H(35A)-C(35)-H(35B)	108.3	K(2)-C(41)-K(2)#2	137.4(4)
O(9)-C(36)-C(35)	108.64(17)	C(42)-C(41)-H(41A)	126.2
O(9)-C(36)-H(36A)	110.0	C(45)-C(41)-H(41A)	126.2
C(35)-C(36)-H(36A)	110.0	K(2)-C(41)-H(41A)	110.8
O(9)-C(36)-H(36B)	110.0	K(2)#2-C(41)-H(41A)	111.7
C(35)-C(36)-H(36B)	110.0	C(41)-C(42)-C(43)	107.7(6)
H(36A)-C(36)-H(36B)	108.3	C(41)-C(42)-K(2)#2	78.5(9)
O(9)-C(37)-C(38)	108.46(17)	C(43)-C(42)-K(2)#2	79.0(10)
O(9)-C(37)-H(37A)	110.0	C(41)-C(42)-K(2)	76.4(8)
C(38)-C(37)-H(37A)	110.0	C(43)-C(42)-K(2)	77.5(9)
O(9)-C(37)-H(37B)	110.0	K(2)#2-C(42)-K(2)	138.1(4)
C(38)-C(37)-H(37B)	110.0	C(41)-C(42)-H(42A)	126.1
H(37A)-C(37)-H(37B)	108.4	C(43)-C(42)-H(42A)	126.1
O(10)-C(38)-C(37)	108.87(17)	K(2)#2-C(42)-H(42A)	109.3
O(10)-C(38)-H(38A)	109.9	K(2)-C(42)-H(42A)	112.5
C(37)-C(38)-H(38A)	109.9	C(42)-C(43)-C(44)	108.7(7)
O(10)-C(38)-H(38B)	109.9	C(42)-C(43)-K(2)	76.9(9)
C(37)-C(38)-H(38B)	109.9	C(44)-C(43)-K(2)	78.7(13)
H(38A)-C(38)-H(38B)	108.3	C(42)-C(43)-K(2)#2	75.2(9)
O(10)-C(39)-C(40)	108.51(18)	C(44)-C(43)-K(2)#2	78.4(13)
O(10)-C(39)-H(39A)	110.0	K(2)-C(43)-K(2)#2	135.6(4)
C(40)-C(39)-H(39A)	110.0	C(42)-C(43)-H(43A)	125.7
O(10)-C(39)-H(39B)	110.0	C(44)-C(43)-H(43A)	125.7
C(40)-C(39)-H(39B)	110.0	K(2)-C(43)-H(43A)	111.3
H(39A)-C(39)-H(39B)	108.4	K(2)#2-C(43)-H(43A)	113.0
O(5)-C(40)-C(39)	108.58(17)	C(45)-C(44)-C(43)	107.6(7)
O(5)-C(40)-H(40A)	110.0	C(45)-C(44)-K(2)#2	77.7(14)
C(39)-C(40)-H(40A)	110.0	C(43)-C(44)-K(2)#2	76.2(13)
O(5)-C(40)-H(40B)	110.0	C(45)-C(44)-K(2)	75.7(14)
C(39)-C(40)-H(40B)	110.0	C(43)-C(44)-K(2)	75.8(13)
H(40A)-C(40)-H(40B)	108.4	K(2)#2-C(44)-K(2)	132.9(2)
C(42)-C(41)-C(45)	107.7(5)	C(45)-C(44)-H(44A)	126.2
C(42)-C(41)-K(2)	77.9(8)	C(43)-C(44)-H(44A)	126.2
C(45)-C(41)-K(2)	77.9(11)	K(2)#2-C(44)-H(44A)	112.5

K(2)-C(44)-H(44A)	114.6	K(2)-C(45)-K(2)#2	134.3(4)
C(44)-C(45)-C(41)	108.3(7)	C(44)-C(45)-H(45A)	125.9
C(44)-C(45)-K(2)	78.9(14)	C(41)-C(45)-H(45A)	125.9
C(41)-C(45)-K(2)	76.1(10)	K(2)-C(45)-H(45A)	111.6
C(44)-C(45)-K(2)#2	77.2(14)	K(2)#2-C(45)-H(45A)	114.0
C(41)-C(45)-K(2)#2	75.3(10)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x,-y,-z+2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05155. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	25(1)	22(1)	26(1)	-1(1)	0(1)	-1(1)
C1	28(1)	41(1)	24(1)	3(1)	-3(1)	-1(1)
C2	32(1)	29(1)	36(1)	5(1)	5(1)	-1(1)
C3	31(1)	29(1)	37(1)	-7(1)	5(1)	-9(1)
C4	27(1)	37(1)	27(1)	-3(1)	-4(1)	-6(1)
C5	26(1)	37(1)	41(1)	0(1)	-4(1)	-3(1)
C6	30(1)	32(1)	55(1)	-5(1)	5(1)	1(1)
C7	35(1)	37(1)	44(1)	-16(1)	8(1)	-10(1)
C8	29(1)	45(1)	30(1)	-8(1)	1(1)	-11(1)
C9	23(1)	34(1)	25(1)	-2(1)	1(1)	-6(1)
C10	24(1)	30(1)	30(1)	-2(1)	0(1)	-7(1)
C11	32(1)	20(1)	43(1)	5(1)	-4(1)	0(1)
C12	44(1)	24(1)	38(1)	-6(1)	-2(1)	-5(1)
C13	57(2)	40(1)	93(2)	9(1)	-41(1)	-16(1)
C14	32(1)	68(2)	53(1)	-30(1)	-6(1)	1(1)
C15	30(1)	30(1)	33(1)	0(1)	-2(1)	4(1)
C16	28(1)	24(1)	33(1)	-6(1)	1(1)	-1(1)
C17	43(1)	47(1)	31(1)	2(1)	5(1)	3(1)
C18	80(2)	36(1)	36(1)	8(1)	-1(1)	-6(1)
K1	26(1)	30(1)	28(1)	-5(1)	-3(1)	-2(1)
C19	41(1)	30(1)	41(1)	-11(1)	-2(1)	2(1)
O1	33(1)	33(1)	39(1)	-8(1)	-2(1)	-4(1)
C20	41(1)	30(1)	49(1)	-7(1)	-7(1)	-7(1)
C21	42(1)	30(1)	52(1)	0(1)	-2(1)	-9(1)
O2	37(1)	32(1)	42(1)	-3(1)	6(1)	-5(1)
C22	36(1)	44(1)	47(1)	-5(1)	9(1)	-13(1)
C23	24(1)	46(1)	47(1)	-10(1)	4(1)	-4(1)
O3	26(1)	32(1)	45(1)	-6(1)	-2(1)	0(1)
C24	33(1)	34(1)	41(1)	-7(1)	0(1)	7(1)
O4	41(1)	53(1)	36(1)	3(1)	-12(1)	1(1)
C25	34(1)	52(1)	42(1)	1(1)	-6(1)	-2(1)

C26	45(1)	35(1)	34(1)	-2(1)	-6(1)	1(1)
C27	41(1)	31(1)	42(1)	0(1)	-16(1)	0(1)
C28	34(1)	44(1)	39(1)	0(1)	-5(1)	-2(1)
K2	28(1)	32(1)	33(1)	-1(1)	-6(1)	-4(1)
O5	41(1)	30(1)	49(1)	-2(1)	-12(1)	-8(1)
O6	32(1)	51(1)	46(1)	0(1)	-12(1)	-9(1)
O7	39(1)	50(1)	33(1)	-3(1)	-6(1)	-5(1)
O8	41(1)	31(1)	41(1)	-1(1)	-4(1)	-6(1)
O9	29(1)	45(1)	37(1)	-4(1)	-5(1)	-7(1)
O10	37(1)	47(1)	35(1)	-8(1)	-6(1)	-1(1)
C29	58(1)	37(1)	51(1)	4(1)	-19(1)	-23(1)
C30	40(1)	53(1)	44(1)	8(1)	-14(1)	-25(1)
C31	27(1)	67(2)	52(1)	2(1)	-3(1)	-5(1)
C32	35(1)	62(2)	42(1)	-3(1)	4(1)	0(1)
C33	50(1)	49(1)	39(1)	-14(1)	-4(1)	5(1)
C34	55(1)	35(1)	50(1)	-11(1)	-13(1)	2(1)
C35	57(1)	36(1)	41(1)	0(1)	-8(1)	-20(1)
C36	37(1)	54(1)	44(1)	-2(1)	-7(1)	-23(1)
C37	25(1)	57(1)	51(1)	2(1)	-1(1)	-1(1)
C38	35(1)	55(1)	40(1)	-4(1)	5(1)	7(1)
C39	52(1)	46(1)	41(1)	-17(1)	-15(1)	13(1)
C40	60(1)	31(1)	53(1)	-11(1)	-23(1)	5(1)
C41	101(14)	30(4)	67(14)	8(4)	-59(10)	-14(8)
C42	36(5)	106(18)	57(15)	44(9)	-23(4)	-30(9)
C43	60(8)	70(9)	32(3)	0(6)	-12(6)	27(6)
C44	47(5)	44(4)	56(8)	17(3)	-30(5)	-16(4)
C45	45(4)	63(8)	37(5)	8(4)	-4(4)	18(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05155.

	x	y	z	U(eq)
H1	7040(20)	3907(19)	8249(9)	34(5)
H2	6940(20)	2030(20)	7683(9)	43(6)
H3	5730(20)	2320(20)	6846(9)	40(6)
H4	4890(20)	4517(19)	6611(9)	30(5)
H5	3191	6289	7143	42
H6	2624	7704	7943	49
H7	3773	7417	8756	48
H8	5468	5697	8798	42
H11	6880(20)	6469(19)	6521(9)	32(5)
H12	7880(20)	6470(20)	7338(11)	54(7)
H13A	10425	6246	6628	72
H13B	10181	6144	7348	72
H14A	10678	4054	7386	60
H14B	11292	4262	6681	60
H15	9400(20)	2530(20)	7076(9)	42(6)
H16	8540(20)	2620(20)	6207(9)	35(5)
H17A	10310	4583	5761	51
H17B	9131	4111	5423	51
H18A	7873	5897	5598	63
H18B	9232	6494	5765	63
H19A	5987	-2565	3901	46
H19B	6553	-3908	4219	46
H20A	4186	-4296	4724	48
H20B	3675	-2927	4407	48
H21A	2175	-3571	5353	50
H21B	3451	-3326	5686	50
H22A	2078	-1520	6206	53
H22B	820	-1818	5871	53
H23A	989	370	5386	48
H23B	615	424	6106	48

H24A	1571	2544	6023	44
H24B	2057	2531	5306	44
H25A	5761	352	3303	51
H25B	4925	1671	3559	51
H26A	4308	112	2660	45
H26B	3936	1676	2740	45
H27A	1790	1166	3229	44
H27B	2179	-402	3168	44
H28A	2373	1142	4148	47
H28B	2055	-420	4174	47
H29A	-2811	-1473	8997	56
H29B	-3404	-1644	8392	56
H30A	-4436	560	8468	54
H30B	-5087	-444	9023	54
H31A	-5696	1358	9669	59
H31B	-5101	2393	9117	59
H32A	-5053	3186	10093	57
H32B	-3896	2028	10175	57
H33A	-2224	3697	10204	55
H33B	-3389	4847	10120	55
H34A	-1957	5539	9168	55
H34B	-1242	5759	9737	55
H35A	944	5632	9050	53
H35B	280	5196	8498	53
H36A	2638	4358	8458	53
H36B	2130	3490	9078	53
H37A	2797	1414	8504	54
H37B	3347	2477	7956	54
H38A	1730	1685	7406	54
H38B	2834	527	7554	54
H39A	1035	-1021	7452	54
H39B	-69	190	7374	54
H40A	-1168	-1841	7807	55
H40B	-454	-1721	8385	55
H41A	-222	-1726	9589	73
H42A	-1991	-582	10343	80

H43A	-939	1459	10593	65
H44A	1524	1516	10047	56
H45A	1951	-415	9405	60

Table 6. Torsion angles [°] for 05155.

C15-Co1-C1-C2	-81.19(13)	C16-Co1-C3-C2	110.11(12)
C11-Co1-C1-C2	158.98(12)	C4-Co1-C3-C2	-126.22(17)
C12-Co1-C1-C2	-169.50(13)	C1-Co1-C3-C2	-32.92(11)
C3-Co1-C1-C2	33.55(12)	C15-Co1-C3-C4	-164.99(11)
C16-Co1-C1-C2	-53.47(18)	C11-Co1-C3-C4	-27.69(16)
C4-Co1-C1-C2	74.45(12)	C2-Co1-C3-C4	126.22(17)
C15-Co1-C1-C9	160.47(12)	C12-Co1-C3-C4	28.2(2)
C11-Co1-C1-C9	40.64(16)	C16-Co1-C3-C4	-123.68(11)
C2-Co1-C1-C9	-118.34(18)	C1-Co1-C3-C4	93.30(12)
C12-Co1-C1-C9	72.16(13)	C2-C3-C4-C10	-31.9(2)
C3-Co1-C1-C9	-84.79(13)	Co1-C3-C4-C10	-89.35(16)
C16-Co1-C1-C9	-171.81(12)	C2-C3-C4-Co1	57.45(14)
C4-Co1-C1-C9	-43.89(12)	C15-Co1-C4-C3	33.5(2)
C9-C1-C2-C3	31.1(3)	C11-Co1-C4-C3	159.01(12)
Co1-C1-C2-C3	-57.55(14)	C2-Co1-C4-C3	-33.90(12)
C9-C1-C2-Co1	88.63(16)	C12-Co1-C4-C3	-166.89(12)
C15-Co1-C2-C3	-124.17(12)	C16-Co1-C4-C3	72.25(13)
C11-Co1-C2-C3	72.1(3)	C1-Co1-C4-C3	-74.81(12)
C12-Co1-C2-C3	142.02(13)	C15-Co1-C4-C10	151.92(16)
C16-Co1-C2-C3	-84.02(13)	C11-Co1-C4-C10	-82.61(13)
C4-Co1-C2-C3	33.24(11)	C2-Co1-C4-C10	84.47(13)
C1-Co1-C2-C3	126.82(17)	C12-Co1-C4-C10	-48.52(14)
C15-Co1-C2-C1	109.01(12)	C3-Co1-C4-C10	118.38(17)
C11-Co1-C2-C1	-54.7(3)	C16-Co1-C4-C10	-169.38(11)
C12-Co1-C2-C1	15.21(18)	C1-Co1-C4-C10	43.56(12)
C3-Co1-C2-C1	-126.82(17)	C10-C5-C6-C7	-1.0(3)
C16-Co1-C2-C1	149.16(11)	C5-C6-C7-C8	-0.6(3)
C4-Co1-C2-C1	-93.58(12)	C6-C7-C8-C9	1.9(3)
C1-C2-C3-C4	0.2(3)	C7-C8-C9-C10	-1.4(3)
Co1-C2-C3-C4	-60.16(15)	C7-C8-C9-C1	175.35(18)
C1-C2-C3-Co1	60.35(15)	C2-C1-C9-C8	152.85(18)
C15-Co1-C3-C2	68.79(13)	Co1-C1-C9-C8	-139.60(16)
C11-Co1-C3-C2	-153.91(12)	C2-C1-C9-C10	-30.3(2)
C12-Co1-C3-C2	-98.0(2)	Co1-C1-C9-C10	37.25(17)

C6-C5-C10-C9	1.4(3)	C16-Co1-C12-C13	-44.75(17)
C6-C5-C10-C4	-174.66(17)	C4-Co1-C12-C13	-177.39(15)
C8-C9-C10-C5	-0.2(3)	C1-Co1-C12-C13	103.19(17)
C1-C9-C10-C5	-177.30(16)	C11-C12-C13-C14	-81.8(3)
C8-C9-C10-C4	176.22(16)	Co1-C12-C13-C14	-3.1(3)
C1-C9-C10-C4	-0.8(2)	C12-C13-C14-C15	13.9(3)
C3-C4-C10-C5	-151.73(19)	C13-C14-C15-C16	62.1(3)
Co1-C4-C10-C5	139.93(16)	C13-C14-C15-Co1	-18.2(3)
C3-C4-C10-C9	32.0(2)	C11-Co1-C15-C16	-70.15(12)
Co1-C4-C10-C9	-36.31(17)	C2-Co1-C15-C16	115.68(12)
C15-Co1-C11-C12	-70.36(13)	C12-Co1-C15-C16	-107.85(12)
C2-Co1-C11-C12	93.3(3)	C3-Co1-C15-C16	77.76(13)
C3-Co1-C11-C12	146.85(12)	C4-Co1-C15-C16	54.0(2)
C16-Co1-C11-C12	-108.55(13)	C1-Co1-C15-C16	155.50(11)
C4-Co1-C11-C12	129.54(12)	C11-Co1-C15-C14	50.78(16)
C1-Co1-C11-C12	53.12(15)	C2-Co1-C15-C14	-123.40(15)
C15-Co1-C11-C18	50.91(17)	C12-Co1-C15-C14	13.07(15)
C2-Co1-C11-C18	-145.4(2)	C3-Co1-C15-C14	-161.31(14)
C12-Co1-C11-C18	121.3(2)	C16-Co1-C15-C14	120.93(19)
C3-Co1-C11-C18	-91.88(18)	C4-Co1-C15-C14	174.90(16)
C16-Co1-C11-C18	12.72(16)	C1-Co1-C15-C14	-83.57(16)
C4-Co1-C11-C18	-109.19(16)	C14-C15-C16-C17	0.7(3)
C1-Co1-C11-C18	174.39(15)	Co1-C15-C16-C17	103.68(17)
C18-C11-C12-C13	0.3(3)	C14-C15-C16-Co1	-102.95(18)
Co1-C11-C12-C13	103.11(18)	C11-Co1-C16-C15	112.09(12)
C18-C11-C12-Co1	-102.84(18)	C2-Co1-C16-C15	-76.22(13)
C15-Co1-C12-C11	111.96(13)	C12-Co1-C16-C15	73.71(12)
C2-Co1-C12-C11	-148.95(13)	C3-Co1-C16-C15	-118.06(12)
C3-Co1-C12-C11	-79.6(2)	C4-Co1-C16-C15	-156.94(11)
C16-Co1-C12-C11	72.86(13)	C1-Co1-C16-C15	-42.08(18)
C4-Co1-C12-C11	-59.78(14)	C15-Co1-C16-C17	-117.07(19)
C1-Co1-C12-C11	-139.20(12)	C11-Co1-C16-C17	-4.98(15)
C15-Co1-C12-C13	-5.65(17)	C2-Co1-C16-C17	166.71(14)
C11-Co1-C12-C13	-117.6(2)	C12-Co1-C16-C17	-43.36(16)
C2-Co1-C12-C13	93.45(19)	C3-Co1-C16-C17	124.87(15)
C3-Co1-C12-C13	162.80(19)	C4-Co1-C16-C17	85.99(16)

C1-Co1-C16-C17	-159.15(14)	O3-K1-O2-C22	-18.10(13)
C15-C16-C17-C18	-82.2(3)	O3#1-K1-O2-C22	161.90(13)
Co1-C16-C17-C18	-3.9(2)	O1#1-K1-O2-C22	-32.85(15)
C16-C17-C18-C11	14.6(3)	O1-K1-O2-C22	147.15(15)
C12-C11-C18-C17	61.9(3)	O2#1-K1-O2-C22	49(14)
Co1-C11-C18-C17	-18.4(3)	C21-O2-C22-C23	-177.89(17)
C24#1-C19-O1-C20	177.67(16)	K1-O2-C22-C23	48.7(2)
C24#1-C19-O1-K1	52.23(18)	O2-C22-C23-O3	-63.2(2)
O4-K1-O1-C19	64.28(12)	C22-C23-O3-C24	-179.02(16)
O4#1-K1-O1-C19	-115.72(12)	C22-C23-O3-K1	48.1(2)
O3-K1-O1-C19	160.97(11)	O4-K1-O3-C23	51.91(13)
O3#1-K1-O1-C19	-19.03(11)	O4#1-K1-O3-C23	-128.09(13)
O1#1-K1-O1-C19	79(7)	O3#1-K1-O3-C23	174(9)
O2-K1-O1-C19	146.63(13)	O1#1-K1-O3-C23	148.78(14)
O2#1-K1-O1-C19	-33.38(13)	O1-K1-O3-C23	-31.22(14)
O4-K1-O1-C20	-60.82(12)	O2-K1-O3-C23	-16.69(13)
O4#1-K1-O1-C20	119.18(12)	O2#1-K1-O3-C23	163.31(13)
O3-K1-O1-C20	35.87(13)	O4-K1-O3-C24	-80.60(12)
O3#1-K1-O1-C20	-144.13(13)	O4#1-K1-O3-C24	99.40(12)
O1#1-K1-O1-C20	-46(7)	O3#1-K1-O3-C24	41(9)
O2-K1-O1-C20	21.52(11)	O1#1-K1-O3-C24	16.26(11)
O2#1-K1-O1-C20	-158.48(11)	O1-K1-O3-C24	-163.74(11)
C19-O1-C20-C21	-179.09(16)	O2-K1-O3-C24	-149.21(13)
K1-O1-C20-C21	-54.69(18)	O2#1-K1-O3-C24	30.79(13)
O1-C20-C21-O2	69.2(2)	C23-O3-C24-C19#1	175.47(16)
C20-C21-O2-C22	178.93(17)	K1-O3-C24-C19#1	-49.37(18)
C20-C21-O2-K1	-47.08(19)	O4#1-K1-O4-C28	-51(54)
O4-K1-O2-C21	98.19(13)	O3-K1-O4-C28	-2.68(13)
O4#1-K1-O2-C21	-81.81(13)	O3#1-K1-O4-C28	177.32(13)
O3-K1-O2-C21	-150.95(14)	O1#1-K1-O4-C28	-65.97(13)
O3#1-K1-O2-C21	29.05(14)	O1-K1-O4-C28	114.03(13)
O1#1-K1-O2-C21	-165.70(12)	O2-K1-O4-C28	52.18(13)
O1-K1-O2-C21	14.30(12)	O2#1-K1-O4-C28	-127.82(13)
O2#1-K1-O2-C21	-84(14)	O4#1-K1-O4-C25	75(54)
O4-K1-O2-C22	-128.96(14)	O3-K1-O4-C25	123.05(13)
O4#1-K1-O2-C22	51.04(14)	O3#1-K1-O4-C25	-56.95(13)

O1#1-K1-O4-C25	59.76(13)	O5-K2-O6-C31	-148.11(15)
O1-K1-O4-C25	-120.24(13)	O7-K2-O6-C31	2.57(13)
O2-K1-O4-C25	177.91(14)	C42#2-K2-O6-C31	110.3(8)
O2#1-K1-O4-C25	-2.09(14)	C41-K2-O6-C31	128.0(4)
C28-O4-C25-C26	-37.6(2)	C42-K2-O6-C31	105.8(7)
K1-O4-C25-C26	-169.11(12)	C41#2-K2-O6-C31	87.0(3)
O4-C25-C26-C27	21.3(2)	C45-K2-O6-C31	123.2(4)
C25-C26-C27-C28	1.8(2)	C43-K2-O6-C31	85.9(4)
C25-O4-C28-C27	38.8(2)	O9-K2-O6-C30	70.43(17)
K1-O4-C28-C27	170.18(11)	O8-K2-O6-C30	142.67(13)
C26-C27-C28-O4	-24.4(2)	O10-K2-O6-C30	-4.67(15)
O9-K2-O5-C40	54.33(13)	O5-K2-O6-C30	-5.02(13)
O6-K2-O5-C40	-153.39(14)	O7-K2-O6-C30	145.66(15)
O8-K2-O5-C40	119.94(13)	C42#2-K2-O6-C30	-106.6(8)
O10-K2-O5-C40	26.97(12)	C41-K2-O6-C30	-88.9(4)
O7-K2-O5-C40	-179.88(12)	C42-K2-O6-C30	-111.1(7)
C42#2-K2-O5-C40	-40.5(3)	C41#2-K2-O6-C30	-129.9(3)
C41-K2-O5-C40	-58.0(6)	C45-K2-O6-C30	-93.7(4)
C42-K2-O5-C40	-80.9(4)	C43-K2-O6-C30	-131.0(4)
C41#2-K2-O5-C40	-66.4(8)	O9-K2-O7-C33	-56.80(13)
C45-K2-O5-C40	-38.2(3)	O6-K2-O7-C33	150.99(13)
C43-K2-O5-C40	-78.5(4)	O8-K2-O7-C33	-32.22(12)
O9-K2-O5-C29	178.78(12)	O10-K2-O7-C33	-120.37(14)
O6-K2-O5-C29	-28.94(12)	O5-K2-O7-C33	177.68(12)
O8-K2-O5-C29	-115.60(14)	C42#2-K2-O7-C33	40.7(4)
O10-K2-O5-C29	151.42(14)	C41-K2-O7-C33	79.1(4)
O7-K2-O5-C29	-55.43(13)	C42-K2-O7-C33	76.9(4)
C42#2-K2-O5-C29	83.9(3)	C41#2-K2-O7-C33	44.1(4)
C41-K2-O5-C29	66.5(6)	C45-K2-O7-C33	48.7(6)
C42-K2-O5-C29	43.6(4)	C43-K2-O7-C33	52.6(6)
C41#2-K2-O5-C29	58.1(8)	O9-K2-O7-C32	-176.43(12)
C45-K2-O5-C29	86.3(3)	O6-K2-O7-C32	31.36(12)
C43-K2-O5-C29	46.0(4)	O8-K2-O7-C32	-151.85(13)
O9-K2-O6-C31	-72.66(18)	O10-K2-O7-C32	120.00(14)
O8-K2-O6-C31	-0.42(15)	O5-K2-O7-C32	58.05(13)
O10-K2-O6-C31	-147.76(14)	C42#2-K2-O7-C32	-79.0(4)

C41-K2-O7-C32	-40.5(4)	C45-K2-O9-C37	45.4(4)
C42-K2-O7-C32	-42.7(4)	C43-K2-O9-C37	82.0(3)
C41#2-K2-O7-C32	-75.5(4)	O6-K2-O9-C36	111.33(15)
C45-K2-O7-C32	-70.9(6)	O8-K2-O9-C36	24.96(12)
C43-K2-O7-C32	-67.1(6)	O10-K2-O9-C36	-158.38(14)
O9-K2-O8-C34	151.52(15)	O5-K2-O9-C36	174.23(13)
O6-K2-O8-C34	1.12(15)	O7-K2-O9-C36	48.93(14)
O10-K2-O8-C34	148.27(13)	C42#2-K2-O9-C36	-71.2(7)
O5-K2-O8-C34	72.12(17)	C41-K2-O9-C36	-91.0(4)
O7-K2-O8-C34	-1.90(13)	C42-K2-O9-C36	-66.7(8)
C42#2-K2-O8-C34	-125.6(4)	C41#2-K2-O9-C36	-49.0(4)
C41-K2-O8-C34	-110.4(7)	C45-K2-O9-C36	-82.6(4)
C42-K2-O8-C34	-86.0(4)	C43-K2-O9-C36	-46.0(3)
C41#2-K2-O8-C34	-102.8(6)	O9-K2-O10-C39	-141.97(15)
C45-K2-O8-C34	-129.8(3)	O6-K2-O10-C39	7.70(15)
C43-K2-O8-C34	-92.5(4)	O8-K2-O10-C39	-138.70(13)
O9-K2-O8-C35	9.83(13)	O5-K2-O10-C39	8.04(13)
O6-K2-O8-C35	-140.57(13)	O7-K2-O10-C39	-65.94(17)
O10-K2-O8-C35	6.58(15)	C42#2-K2-O10-C39	130.5(4)
O5-K2-O8-C35	-69.57(16)	C41-K2-O10-C39	97.4(4)
O7-K2-O8-C35	-143.60(14)	C42-K2-O10-C39	95.8(4)
C42#2-K2-O8-C35	92.7(4)	C41#2-K2-O10-C39	130.7(4)
C41-K2-O8-C35	107.9(7)	C45-K2-O10-C39	122.7(5)
C42-K2-O8-C35	132.3(4)	C43-K2-O10-C39	122.1(6)
C41#2-K2-O8-C35	115.5(6)	O9-K2-O10-C38	-3.03(13)
C45-K2-O8-C35	88.5(3)	O6-K2-O10-C38	146.64(13)
C43-K2-O8-C35	125.8(4)	O8-K2-O10-C38	0.24(14)
O6-K2-O9-C37	-120.69(14)	O5-K2-O10-C38	146.99(14)
O8-K2-O9-C37	152.94(13)	O7-K2-O10-C38	73.00(16)
O10-K2-O9-C37	-30.40(12)	C42#2-K2-O10-C38	-90.5(4)
O5-K2-O9-C37	-57.79(13)	C41-K2-O10-C38	-123.7(4)
O7-K2-O9-C37	176.91(12)	C42-K2-O10-C38	-125.3(4)
C42#2-K2-O9-C37	56.7(7)	C41#2-K2-O10-C38	-90.4(4)
C41-K2-O9-C37	37.0(4)	C45-K2-O10-C38	-98.3(5)
C42-K2-O9-C37	61.3(8)	C43-K2-O10-C38	-99.0(6)
C41#2-K2-O9-C37	79.0(4)	C40-O5-C29-C30	-175.10(17)

K2-O5-C29-C30	61.46(18)	C41#2-K2-C41-C42	52.8(6)
C31-O6-C30-C29	-177.83(17)	C45-K2-C41-C42	111.3(8)
K2-O6-C30-C29	36.8(2)	C43-K2-C41-C42	36.7(4)
O5-C29-C30-O6	-66.3(2)	O9-K2-C41-C45	19.5(15)
C30-O6-C31-C32	179.96(17)	O6-K2-C41-C45	-170.3(13)
K2-O6-C31-C32	-35.2(2)	O8-K2-C41-C45	-47.6(17)
C33-O7-C32-C31	179.57(18)	O10-K2-C41-C45	72.1(14)
K2-O7-C32-C31	-65.09(18)	O5-K2-C41-C45	131.2(14)
O6-C31-C32-O7	69.9(2)	O7-K2-C41-C45	-116.3(15)
C32-O7-C33-C34	-179.68(17)	C42#2-K2-C41-C45	-18.7(7)
K2-O7-C33-C34	65.58(18)	C42-K2-C41-C45	-111.3(8)
C35-O8-C34-C33	176.74(17)	C41#2-K2-C41-C45	-58.6(6)
K2-O8-C34-C33	34.2(2)	C43-K2-C41-C45	-74.6(5)
O7-C33-C34-O8	-68.6(2)	O9-K2-C41-K2#2	78.1(17)
C34-O8-C35-C36	173.94(17)	O6-K2-C41-K2#2	-111.7(15)
K2-O8-C35-C36	-41.6(2)	O8-K2-C41-K2#2	11(2)
C37-O9-C36-C35	174.76(17)	O10-K2-C41-K2#2	130.7(16)
K2-O9-C36-C35	-57.56(18)	O5-K2-C41-K2#2	-170.2(16)
O8-C35-C36-O9	66.4(2)	O7-K2-C41-K2#2	-57.8(17)
C36-O9-C37-C38	-169.50(17)	C42#2-K2-C41-K2#2	39.8(4)
K2-O9-C37-C38	62.29(19)	C42-K2-C41-K2#2	-52.8(6)
C39-O10-C38-C37	174.28(17)	C41#2-K2-C41-K2#2	0.0
K2-O10-C38-C37	33.9(2)	C45-K2-C41-K2#2	58.6(6)
O9-C37-C38-O10	-63.8(2)	C43-K2-C41-K2#2	-16.0(4)
C38-O10-C39-C40	179.12(17)	C45-C41-C42-C43	1(3)
K2-O10-C39-C40	-40.3(2)	K2-C41-C42-C43	-71.9(13)
C29-O5-C40-C39	176.83(17)	K2#2-C41-C42-C43	74.4(13)
K2-O5-C40-C39	-60.10(18)	C45-C41-C42-K2#2	-73.3(14)
O10-C39-C40-O5	68.0(2)	K2-C41-C42-K2#2	-146.3(3)
O9-K2-C41-C42	130.9(14)	C45-C41-C42-K2	72.9(14)
O6-K2-C41-C42	-58.9(13)	K2#2-C41-C42-K2	146.3(3)
O8-K2-C41-C42	63.8(17)	O9-K2-C42-C41	-61.4(18)
O10-K2-C41-C42	-176.6(13)	O6-K2-C42-C41	119.5(14)
O5-K2-C41-C42	-117.4(13)	O8-K2-C42-C41	-127.1(14)
O7-K2-C41-C42	-5.0(15)	O10-K2-C42-C41	3.6(14)
C42#2-K2-C41-C42	92.6(8)	O5-K2-C42-C41	63.4(13)

O7-K2-C42-C41	175.7(13)	O10-K2-C43-C42	-75.2(17)
C42#2-K2-C42-C41	-54.6(6)	O5-K2-C43-C42	-5.4(16)
C41#2-K2-C42-C41	-95.2(8)	O7-K2-C43-C42	108.3(14)
C45-K2-C42-C41	-37.4(5)	C42#2-K2-C43-C42	-90.2(7)
C43-K2-C42-C41	-112.0(8)	C41-K2-C43-C42	-36.9(5)
O9-K2-C42-C43	50.7(18)	C41#2-K2-C43-C42	-123(2)
O6-K2-C42-C43	-128.5(15)	C45-K2-C43-C42	-76.1(6)
O8-K2-C42-C43	-15.0(15)	O9-K2-C43-C44	-26.8(15)
O10-K2-C42-C43	115.7(15)	O6-K2-C43-C44	163.1(13)
O5-K2-C42-C43	175.4(13)	O8-K2-C43-C44	-81.8(14)
O7-K2-C42-C43	-72.3(13)	O10-K2-C43-C44	37.3(17)
C42#2-K2-C42-C43	57.4(6)	O5-K2-C43-C44	107.0(15)
C41-K2-C42-C43	112.0(8)	O7-K2-C43-C44	-139.2(14)
C41#2-K2-C42-C43	16.8(7)	C42#2-K2-C43-C44	22.2(7)
C45-K2-C42-C43	74.6(5)	C41-K2-C43-C44	75.6(7)
O9-K2-C42-K2#2	-7(2)	C42-K2-C43-C44	112.4(10)
O6-K2-C42-K2#2	174.1(18)	C41#2-K2-C43-C44	-10.9(19)
O8-K2-C42-K2#2	-72.4(18)	C45-K2-C43-C44	36.3(6)
O10-K2-C42-K2#2	58.3(18)	O9-K2-C43-K2#2	-87.0(13)
O5-K2-C42-K2#2	118.1(16)	O6-K2-C43-K2#2	103.0(13)
O7-K2-C42-K2#2	-129.7(17)	O8-K2-C43-K2#2	-142.0(13)
C42#2-K2-C42-K2#2	0.001(2)	O10-K2-C43-K2#2	-22.9(16)
C41-K2-C42-K2#2	54.6(7)	O5-K2-C43-K2#2	46.9(15)
C41#2-K2-C42-K2#2	-40.6(4)	O7-K2-C43-K2#2	160.6(13)
C45-K2-C42-K2#2	17.2(5)	C42#2-K2-C43-K2#2	-37.9(4)
C43-K2-C42-K2#2	-57.4(6)	C41-K2-C43-K2#2	15.4(4)
C41-C42-C43-C44	-2(3)	C42-K2-C43-K2#2	52.3(6)
K2#2-C42-C43-C44	72.0(17)	C41#2-K2-C43-K2#2	-71(2)
K2-C42-C43-C44	-73.1(17)	C45-K2-C43-K2#2	-23.8(4)
C41-C42-C43-K2	71.1(12)	C42-C43-C44-C45	2(3)
K2#2-C42-C43-K2	145.1(4)	K2-C43-C44-C45	-69.7(19)
C41-C42-C43-K2#2	-74.0(12)	K2#2-C43-C44-C45	72.0(19)
K2-C42-C43-K2#2	-145.1(4)	C42-C43-C44-K2#2	-69.9(14)
O9-K2-C43-C42	-139.3(15)	K2-C43-C44-K2#2	-141.7(3)
O6-K2-C43-C42	50.7(14)	C42-C43-C44-K2	71.8(14)
O8-K2-C43-C42	165.7(15)	K2#2-C43-C44-K2	141.7(3)

O9-K2-C44-C45	-92.6(15)	K2-C44-C45-C41	-71.2(15)
O6-K2-C44-C45	93.2(16)	C43-C44-C45-K2	69.8(18)
O8-K2-C44-C45	-152.4(15)	K2#2-C44-C45-K2	140.8(2)
O10-K2-C44-C45	-34.8(14)	C43-C44-C45-K2#2	-71.0(18)
O5-K2-C44-C45	21.5(17)	K2-C44-C45-K2#2	-140.8(2)
O7-K2-C44-C45	155.6(14)	C42-C41-C45-C44	0(3)
C42#2-K2-C44-C45	-5.6(12)	K2-C41-C45-C44	73.2(18)
C41-K2-C44-C45	37.2(6)	K2#2-C41-C45-C44	-70.8(18)
C42-K2-C44-C45	76.0(7)	C42-C41-C45-K2	-72.9(12)
C41#2-K2-C44-C45	120.5(15)	K2#2-C41-C45-K2	-144.0(4)
C43-K2-C44-C45	112.7(11)	C42-C41-C45-K2#2	71.0(13)
O9-K2-C44-C43	154.7(15)	K2-C41-C45-K2#2	144.0(4)
O6-K2-C44-C43	-19.5(16)	O9-K2-C45-C44	85.9(14)
O8-K2-C44-C43	94.9(15)	O6-K2-C45-C44	-101.1(15)
O10-K2-C44-C43	-147.5(14)	O8-K2-C45-C44	28.1(15)
O5-K2-C44-C43	-91.2(17)	O10-K2-C45-C44	144.4(15)
O7-K2-C44-C43	42.9(14)	O5-K2-C45-C44	-162.6(14)
C42#2-K2-C44-C43	-118.3(15)	O7-K2-C45-C44	-30.7(18)
C41-K2-C44-C43	-75.5(7)	C42#2-K2-C45-C44	6.7(15)
C42-K2-C44-C43	-36.7(6)	C41-K2-C45-C44	-112.2(10)
C41#2-K2-C44-C43	7.8(13)	C42-K2-C45-C44	-75.2(7)
C45-K2-C44-C43	-112.7(11)	C41#2-K2-C45-C44	-22.7(6)
O9-K2-C44-K2#2	-150.1(10)	C43-K2-C45-C44	-36.5(6)
O6-K2-C44-K2#2	35.8(11)	O9-K2-C45-C41	-162.0(14)
O8-K2-C44-K2#2	150.1(10)	O6-K2-C45-C41	11.0(16)
O10-K2-C44-K2#2	-92.3(9)	O8-K2-C45-C41	140.3(14)
O5-K2-C44-K2#2	-36.0(12)	O10-K2-C45-C41	-103.5(15)
O7-K2-C44-K2#2	98.1(9)	O5-K2-C45-C41	-50.4(14)
C42#2-K2-C44-K2#2	-63.1(11)	O7-K2-C45-C41	81.4(17)
C41-K2-C44-K2#2	-20.3(5)	C42#2-K2-C45-C41	119(2)
C42-K2-C44-K2#2	18.6(5)	C42-K2-C45-C41	37.0(5)
C41#2-K2-C44-K2#2	63.1(10)	C41#2-K2-C45-C41	89.4(7)
C45-K2-C44-K2#2	-57.5(8)	C43-K2-C45-C41	75.7(6)
C43-K2-C44-K2#2	55.2(7)	O9-K2-C45-K2#2	145.4(11)
C43-C44-C45-C41	-1(3)	O6-K2-C45-K2#2	-41.6(13)
K2#2-C44-C45-C41	69.5(15)	O8-K2-C45-K2#2	87.6(11)

O10-K2-C45-K2#2	-156.1(12)	C41-K2-C45-K2#2	-52.6(6)
O5-K2-C45-K2#2	-103.1(11)	C42-K2-C45-K2#2	-15.6(4)
O7-K2-C45-K2#2	28.8(15)	C41#2-K2-C45-K2#2	36.8(4)
C42#2-K2-C45-K2#2	66.2(17)	C43-K2-C45-K2#2	23.0(4)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, -y, -z+1$ #2 $-x, -y, -z+2$

REFERENCE NUMBER: 05320 [13]

[Revised September 21, 2011]

CRYSTAL STRUCTURE REPORT

$C_{24} H_{42} Co K O_6$

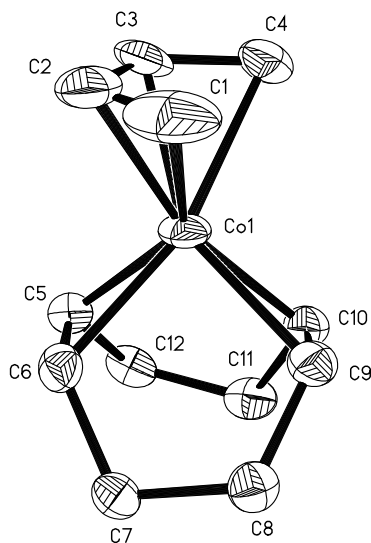
or

$[K(18\text{-crown-6})][Co(1,5\text{-COD})(C_4H_6)]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

October 30, 2005



William W. Brennessel

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Data collection

A crystal (0.32 x 0.30 x 0.24 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART CCD Platform diffractometer for a data collection at 123(2) K.¹ The lower temperature was applied after a previously applied crystal turned to powder after an hour at 173(2) K (this may have been specific to flaws in that one crystal). 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 MoK α radiation (graphite monochromator) with a frame time of 15 seconds and a detector distance of 4.98 cm. A randomly oriented region of reciprocal space was surveyed: three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption.² Final cell constants were calculated from the xyz centroids of 3182 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 SIR97⁴ and refined using SHELXL-97.⁵ The space group *P*-1 was determined based on 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 $R1 = 0.0401$ (F^2 , $I > 2\sigma(I)$) and $wR2 = 0.1016$ (F^2 , all data).

Structure description

The structure is the one suggested. The cation and anion form discrete units with all atoms on general positions. The butadiene ligand occupies an axial position of the potassium atom. It is also disordered and was modeled over two positions (51:49). The other axial position of the potassium atom is occupied by the symmetry equivalent of the C11 methylene group.

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

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

-
- ¹ SMART V5.629, Bruker Analytical X-ray Systems, Madison, WI (2003).
- ² SADABS V2.10, An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
- ³ SAINT V7.06A, Bruker Analytical X-ray Systems, Madison, WI (2003).
- ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
- ⁵ Sheldrick, G. M. *Acta. Cryst.* **2008**, *A64*, 112-122.

Some equations of interest:

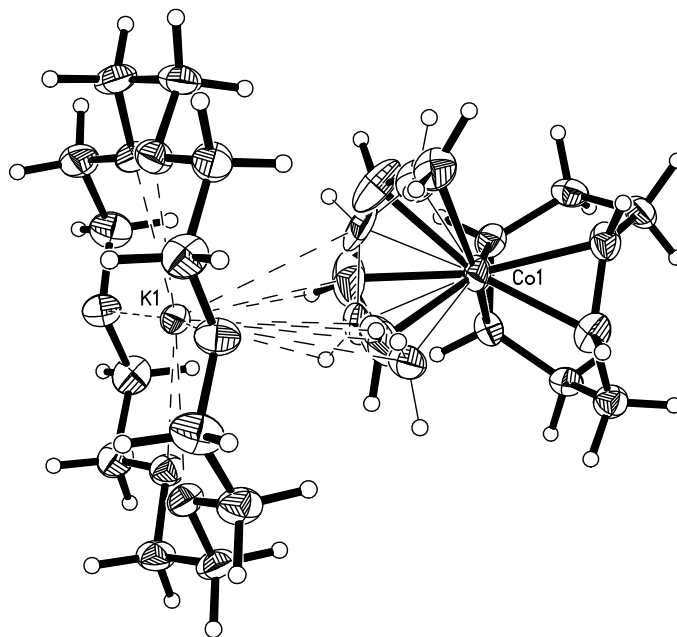
$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2(F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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



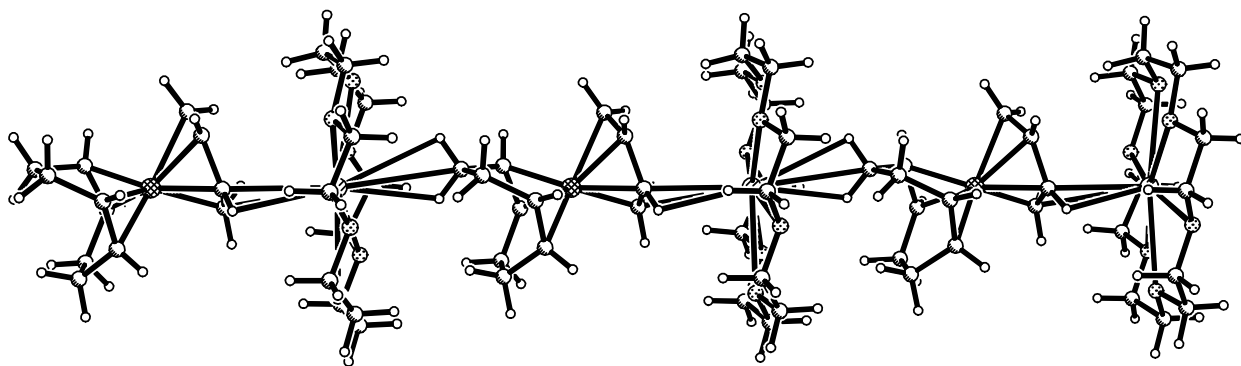
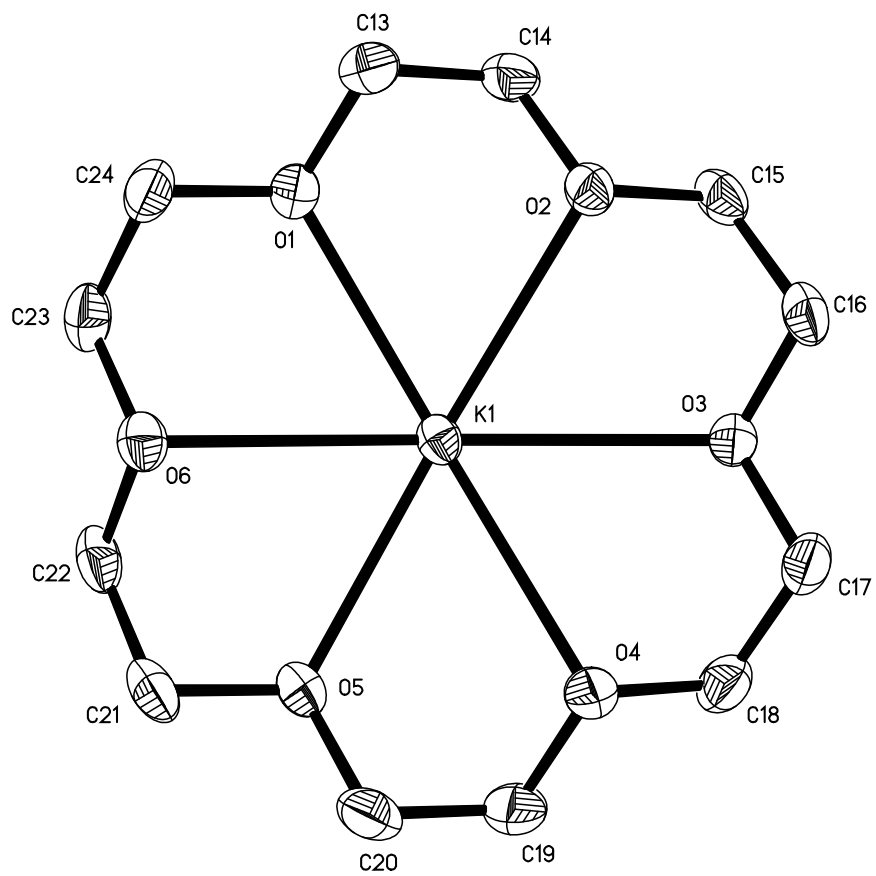


Table 1. Crystal data and structure refinement for 320.

Identification code	05320	
Empirical formula	C ₂₄ H ₄₂ Co K O ₆	
Formula weight	524.61	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 8.6632(7) Å	α = 90.9520(10)°
	<i>b</i> = 10.9612(9) Å	β = 93.5740(10)°
	<i>c</i> = 14.9236(12) Å	γ = 112.8260(10)°
Volume	1302.33(18) Å ³	
<i>Z</i>	2	
Density (calculated)	1.338 Mg/m ³	
Absorption coefficient	0.853 mm ⁻¹	
<i>F</i> (000)	560	
Crystal color, morphology	orange, block	
Crystal size	0.32 x 0.30 x 0.24 mm ³	
Theta range for data collection	1.37 to 27.10°	
Index ranges	-11 ≤ <i>h</i> ≤ 11, -14 ≤ <i>k</i> ≤ 14, -19 ≤ <i>l</i> ≤ 19	
Reflections collected	15009	
Independent reflections	5670 [<i>R</i> (int) = 0.0297]	
Observed reflections	4613	
Completeness to theta = 27.10°	99.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8214 and 0.7719	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	5670 / 18 / 302	
Goodness-of-fit on <i>F</i> ²	1.052	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0401, <i>wR</i> 2 = 0.0932	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0537, <i>wR</i> 2 = 0.1016	
Largest diff. peak and hole	1.210 and -0.777 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 320. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	2232(1)	3028(1)	2380(1)	27(1)
C1	2934(10)	4955(8)	2077(7)	38(2)
C2	2112(13)	4681(8)	2859(6)	48(2)
C3	365(13)	3644(13)	2785(8)	52(2)
C4	-240(20)	3090(30)	1950(11)	47(2)
C1'	3131(10)	4869(8)	1671(6)	38(2)
C2'	2798(13)	4952(8)	2561(6)	48(2)
C3'	1075(14)	4108(13)	2805(7)	52(2)
C4'	33(19)	3300(30)	2136(11)	47(2)
C5	2474(3)	2116(2)	3508(2)	29(1)
C6	4070(3)	2885(2)	3210(2)	28(1)
C7	5135(3)	2271(2)	2756(2)	26(1)
C8	4814(3)	2205(2)	1730(2)	29(1)
C9	3088(3)	2157(3)	1440(2)	31(1)
C10	1588(3)	1235(2)	1756(2)	30(1)
C11	1610(3)	175(2)	2400(2)	32(1)
C12	1668(3)	620(2)	3381(2)	30(1)
K1	2192(1)	7400(1)	2558(1)	22(1)
O1	1254(2)	7371(2)	746(1)	31(1)
O2	4666(2)	8722(2)	1392(1)	26(1)
O3	5651(2)	8484(2)	3185(1)	27(1)
O4	3163(2)	7980(2)	4420(1)	30(1)
O5	-196(2)	6545(2)	3797(1)	30(1)
O6	-1254(2)	6704(2)	1980(1)	28(1)
C13	2476(3)	8328(3)	250(2)	38(1)
C14	4145(3)	8248(3)	488(2)	34(1)
C15	6285(3)	8750(3)	1660(2)	30(1)
C16	6773(3)	9336(3)	2594(2)	32(1)
C17	6021(3)	8980(3)	4092(2)	33(1)
C18	4803(3)	8022(3)	4661(2)	35(1)
C19	1948(3)	7145(3)	4979(2)	37(1)

C20	259(3)	7127(3)	4678(2)	36(1)
C21	-1883(3)	6315(3)	3494(2)	34(1)
C22	-2224(3)	5723(3)	2556(2)	34(1)
C23	-1578(3)	6259(3)	1058(2)	34(1)
C24	-404(3)	7304(3)	518(2)	34(1)

Table 3. Bond lengths [Å] and angles [°] for 320.

Co(1)-C(3')	1.945(12)	C(4')-H(4D)	0.9900
Co(1)-C(2)	1.979(7)	C(5)-C(6)	1.417(3)
Co(1)-C(2')	1.981(8)	C(5)-C(12)	1.516(3)
Co(1)-C(6)	2.012(2)	C(5)-H(5A)	1.0000
Co(1)-C(5)	2.014(2)	C(6)-C(7)	1.519(3)
Co(1)-C(9)	2.016(2)	C(6)-H(6A)	1.0000
Co(1)-C(10)	2.016(2)	C(7)-C(8)	1.535(3)
Co(1)-C(1)	2.026(8)	C(7)-H(7A)	0.9900
Co(1)-C(4')	2.05(3)	C(7)-H(7B)	0.9900
Co(1)-C(3)	2.097(11)	C(8)-C(9)	1.511(3)
Co(1)-C(1')	2.180(8)	C(8)-H(8A)	0.9900
Co(1)-C(4)	2.22(3)	C(8)-H(8B)	0.9900
C(1)-C(2)	1.382(8)	C(9)-C(10)	1.417(4)
C(1)-K(1)	3.072(9)	C(9)-H(9A)	1.0000
C(1)-H(1A)	0.9900	C(10)-C(11)	1.524(4)
C(1)-H(1B)	0.9900	C(10)-H(10A)	1.0000
C(2)-C(3)	1.495(8)	C(11)-C(12)	1.526(4)
C(2)-K(1)	2.995(8)	C(11)-K(1)#1	3.281(2)
C(2)-H(2A)	1.0000	C(11)-H(11A)	0.9900
C(3)-C(4)	1.356(7)	C(11)-H(11B)	0.9900
C(3)-H(3A)	1.0000	C(12)-H(12A)	0.9900
C(4)-H(4A)	0.9900	C(12)-H(12B)	0.9900
C(4)-H(4B)	0.9900	K(1)-O(5)	2.7576(17)
C(1')-C(2')	1.387(8)	K(1)-O(1)	2.7711(17)
C(1')-K(1)	3.446(8)	K(1)-O(2)	2.8035(17)
C(1')-H(1C)	0.9900	K(1)-O(4)	2.8400(17)
C(1')-H(1D)	0.9900	K(1)-O(3)	2.8490(17)
C(2')-C(3')	1.491(8)	K(1)-O(6)	2.8513(17)
C(2')-K(1)	2.926(7)	K(1)-C(11)#2	3.281(2)
C(2')-H(2B)	1.0000	O(1)-C(13)	1.425(3)
C(3')-C(4')	1.355(7)	O(1)-C(24)	1.428(3)
C(3')-K(1)	3.386(13)	O(2)-C(14)	1.420(3)
C(3')-H(3B)	1.0000	O(2)-C(15)	1.422(3)
C(4')-H(4C)	0.9900	O(3)-C(17)	1.421(3)

O(3)-C(16)	1.423(3)	C(24)-H(24B)	0.9900
O(4)-C(19)	1.424(3)	C(3')-Co(1)-C(2)	25.6(4)
O(4)-C(18)	1.427(3)	C(3')-Co(1)-C(2')	44.6(3)
O(5)-C(20)	1.415(3)	C(2)-Co(1)-C(2')	21.37(19)
O(5)-C(21)	1.426(3)	C(3')-Co(1)-C(6)	117.3(4)
O(6)-C(22)	1.422(3)	C(2)-Co(1)-C(6)	101.4(2)
O(6)-C(23)	1.426(3)	C(2')-Co(1)-C(6)	98.6(2)
C(13)-C(14)	1.503(4)	C(3')-Co(1)-C(5)	100.8(3)
C(13)-H(13A)	0.9900	C(2)-Co(1)-C(5)	102.4(3)
C(13)-H(13B)	0.9900	C(2')-Co(1)-C(5)	114.3(3)
C(14)-H(14A)	0.9900	C(6)-Co(1)-C(5)	41.21(10)
C(14)-H(14B)	0.9900	C(3')-Co(1)-C(9)	155.0(3)
C(15)-C(16)	1.490(4)	C(2)-Co(1)-C(9)	147.3(3)
C(15)-H(15A)	0.9900	C(2')-Co(1)-C(9)	126.4(3)
C(15)-H(15B)	0.9900	C(6)-Co(1)-C(9)	85.41(10)
C(16)-H(16A)	0.9900	C(5)-Co(1)-C(9)	103.45(10)
C(16)-H(16B)	0.9900	C(3')-Co(1)-C(10)	136.9(4)
C(17)-C(18)	1.489(4)	C(2)-Co(1)-C(10)	161.6(3)
C(17)-H(17A)	0.9900	C(2')-Co(1)-C(10)	160.4(3)
C(17)-H(17B)	0.9900	C(6)-Co(1)-C(10)	95.36(10)
C(18)-H(18A)	0.9900	C(5)-Co(1)-C(10)	85.26(10)
C(18)-H(18B)	0.9900	C(9)-Co(1)-C(10)	41.13(10)
C(19)-C(20)	1.496(4)	C(3')-Co(1)-C(1)	58.1(3)
C(19)-H(19A)	0.9900	C(2)-Co(1)-C(1)	40.3(2)
C(19)-H(19B)	0.9900	C(2')-Co(1)-C(1)	21.2(3)
C(20)-H(20A)	0.9900	C(6)-Co(1)-C(1)	107.7(3)
C(20)-H(20B)	0.9900	C(5)-Co(1)-C(1)	133.5(3)
C(21)-C(22)	1.496(4)	C(9)-Co(1)-C(1)	107.1(3)
C(21)-H(21A)	0.9900	C(10)-Co(1)-C(1)	139.6(3)
C(21)-H(21B)	0.9900	C(3')-Co(1)-C(4')	39.5(5)
C(22)-H(22A)	0.9900	C(2)-Co(1)-C(4')	61.8(7)
C(22)-H(22B)	0.9900	C(2')-Co(1)-C(4')	73.6(7)
C(23)-C(24)	1.491(4)	C(6)-Co(1)-C(4')	152.3(4)
C(23)-H(23A)	0.9900	C(5)-Co(1)-C(4')	117.1(6)
C(23)-H(23B)	0.9900	C(9)-Co(1)-C(4')	120.9(4)
C(24)-H(24A)	0.9900	C(10)-Co(1)-C(4')	99.7(6)

C(1)-Co(1)-C(4')	74.7(8)	K(1)-C(1)-H(1A)	89.5
C(3')-Co(1)-C(3)	17.3(4)	C(2)-C(1)-H(1B)	116.9
C(2)-Co(1)-C(3)	42.9(3)	Co(1)-C(1)-H(1B)	116.9
C(2')-Co(1)-C(3)	61.6(4)	K(1)-C(1)-H(1B)	71.7
C(6)-Co(1)-C(3)	124.6(4)	H(1A)-C(1)-H(1B)	113.9
C(5)-Co(1)-C(3)	97.1(3)	C(1)-C(2)-C(3)	116.7(5)
C(9)-Co(1)-C(3)	149.2(4)	C(1)-C(2)-Co(1)	71.6(5)
C(10)-Co(1)-C(3)	120.1(4)	C(3)-C(2)-Co(1)	72.7(6)
C(1)-Co(1)-C(3)	72.9(4)	C(1)-C(2)-K(1)	80.0(6)
C(4')-Co(1)-C(3)	28.4(7)	C(3)-C(2)-K(1)	112.4(7)
C(3')-Co(1)-C(1')	72.6(3)	Co(1)-C(2)-K(1)	149.6(5)
C(2)-Co(1)-C(1')	57.5(3)	C(1)-C(2)-H(2A)	121.6
C(2')-Co(1)-C(1')	38.6(3)	C(3)-C(2)-H(2A)	121.6
C(6)-Co(1)-C(1')	111.2(2)	Co(1)-C(2)-H(2A)	121.6
C(5)-Co(1)-C(1')	146.0(3)	K(1)-C(2)-H(2A)	82.5
C(9)-Co(1)-C(1')	90.1(2)	C(4)-C(3)-C(2)	115.7(5)
C(10)-Co(1)-C(1')	122.8(2)	C(4)-C(3)-Co(1)	76.8(14)
C(1)-Co(1)-C(1')	17.4(2)	C(2)-C(3)-Co(1)	64.4(5)
C(4')-Co(1)-C(1')	79.6(7)	C(4)-C(3)-H(3A)	121.9
C(3)-Co(1)-C(1')	85.2(4)	C(2)-C(3)-H(3A)	121.9
C(3')-Co(1)-C(4)	48.1(8)	Co(1)-C(3)-H(3A)	121.9
C(2)-Co(1)-C(4)	69.9(7)	C(3)-C(4)-Co(1)	66.7(11)
C(2')-Co(1)-C(4)	80.3(8)	C(3)-C(4)-H(4A)	117.0
C(6)-Co(1)-C(4)	158.5(4)	Co(1)-C(4)-H(4A)	117.0
C(5)-Co(1)-C(4)	119.7(5)	C(3)-C(4)-H(4B)	117.0
C(9)-Co(1)-C(4)	112.8(5)	Co(1)-C(4)-H(4B)	117.0
C(10)-Co(1)-C(4)	91.7(7)	H(4A)-C(4)-H(4B)	114.1
C(1)-Co(1)-C(4)	78.9(7)	C(2')-C(1')-Co(1)	62.9(4)
C(4')-Co(1)-C(4)	8.5(11)	C(2')-C(1')-K(1)	56.8(5)
C(3)-Co(1)-C(4)	36.4(4)	Co(1)-C(1')-K(1)	115.6(3)
C(1')-Co(1)-C(4)	81.4(7)	C(2')-C(1')-H(1C)	117.5
C(2)-C(1)-Co(1)	68.0(4)	Co(1)-C(1')-H(1C)	117.5
C(2)-C(1)-K(1)	73.7(5)	K(1)-C(1')-H(1C)	108.8
Co(1)-C(1)-K(1)	140.3(4)	C(2')-C(1')-H(1D)	117.5
C(2)-C(1)-H(1A)	116.9	Co(1)-C(1')-H(1D)	117.5
Co(1)-C(1)-H(1A)	116.9	K(1)-C(1')-H(1D)	75.6

H(1C)-C(1')-H(1D)	114.5	C(5)-C(6)-H(6A)	114.5
C(1')-C(2')-C(3')	116.7(5)	C(7)-C(6)-H(6A)	114.5
C(1')-C(2')-Co(1)	78.5(5)	Co(1)-C(6)-H(6A)	114.5
C(3')-C(2')-Co(1)	66.4(5)	C(6)-C(7)-C(8)	111.12(19)
C(1')-C(2')-K(1)	99.8(6)	C(6)-C(7)-H(7A)	109.4
C(3')-C(2')-K(1)	94.5(6)	C(8)-C(7)-H(7A)	109.4
Co(1)-C(2')-K(1)	156.5(4)	C(6)-C(7)-H(7B)	109.4
C(1')-C(2')-H(2B)	121.6	C(8)-C(7)-H(7B)	109.4
C(3')-C(2')-H(2B)	121.6	H(7A)-C(7)-H(7B)	108.0
Co(1)-C(2')-H(2B)	121.6	C(9)-C(8)-C(7)	112.4(2)
K(1)-C(2')-H(2B)	79.5	C(9)-C(8)-H(8A)	109.1
C(4')-C(3')-C(2')	116.0(5)	C(7)-C(8)-H(8A)	109.1
C(4')-C(3')-Co(1)	74.4(15)	C(9)-C(8)-H(8B)	109.1
C(2')-C(3')-Co(1)	69.0(5)	C(7)-C(8)-H(8B)	109.1
C(4')-C(3')-K(1)	116.1(16)	H(8A)-C(8)-H(8B)	107.9
C(2')-C(3')-K(1)	59.5(5)	C(10)-C(9)-C(8)	123.5(2)
Co(1)-C(3')-K(1)	126.7(4)	C(10)-C(9)-Co(1)	69.46(14)
C(4')-C(3')-H(3B)	121.9	C(8)-C(9)-Co(1)	111.33(17)
C(2')-C(3')-H(3B)	121.9	C(10)-C(9)-H(9A)	114.7
Co(1)-C(3')-H(3B)	121.9	C(8)-C(9)-H(9A)	114.7
K(1)-C(3')-H(3B)	97.3	Co(1)-C(9)-H(9A)	114.7
C(3')-C(4')-Co(1)	66.0(11)	C(9)-C(10)-C(11)	121.5(2)
C(3')-C(4')-H(4C)	117.1	C(9)-C(10)-Co(1)	69.40(14)
Co(1)-C(4')-H(4C)	117.1	C(11)-C(10)-Co(1)	112.78(17)
C(3')-C(4')-H(4D)	117.1	C(9)-C(10)-H(10A)	115.0
Co(1)-C(4')-H(4D)	117.1	C(11)-C(10)-H(10A)	115.0
H(4C)-C(4')-H(4D)	114.1	Co(1)-C(10)-H(10A)	115.0
C(6)-C(5)-C(12)	122.9(2)	C(10)-C(11)-C(12)	112.1(2)
C(6)-C(5)-Co(1)	69.32(14)	C(10)-C(11)-K(1)#1	143.90(17)
C(12)-C(5)-Co(1)	112.19(17)	C(12)-C(11)-K(1)#1	102.97(15)
C(6)-C(5)-H(5A)	114.7	C(10)-C(11)-H(11A)	109.2
C(12)-C(5)-H(5A)	114.7	C(12)-C(11)-H(11A)	109.2
Co(1)-C(5)-H(5A)	114.7	K(1)#1-C(11)-H(11A)	48.4
C(5)-C(6)-C(7)	122.5(2)	C(10)-C(11)-H(11B)	109.2
C(5)-C(6)-Co(1)	69.47(14)	C(12)-C(11)-H(11B)	109.2
C(7)-C(6)-Co(1)	113.45(16)	K(1)#1-C(11)-H(11B)	64.9

H(11A)-C(11)-H(11B)	107.9	O(1)-K(1)-C(1)	85.85(19)
C(5)-C(12)-C(11)	111.4(2)	O(2)-K(1)-C(1)	85.23(16)
C(5)-C(12)-H(12A)	109.3	O(4)-K(1)-C(1)	105.89(19)
C(11)-C(12)-H(12A)	109.3	O(3)-K(1)-C(1)	83.17(17)
C(5)-C(12)-H(12B)	109.3	O(6)-K(1)-C(1)	105.32(17)
C(11)-C(12)-H(12B)	109.3	C(2')-K(1)-C(1)	13.90(19)
H(12A)-C(12)-H(12B)	108.0	C(2)-K(1)-C(1)	26.29(16)
O(5)-K(1)-O(1)	120.72(5)	O(5)-K(1)-C(11)#2	90.34(6)
O(5)-K(1)-O(2)	169.77(5)	O(1)-K(1)-C(11)#2	77.63(6)
O(1)-K(1)-O(2)	61.24(5)	O(2)-K(1)-C(11)#2	80.22(6)
O(5)-K(1)-O(4)	60.12(5)	O(4)-K(1)-C(11)#2	90.30(6)
O(1)-K(1)-O(4)	167.83(5)	O(3)-K(1)-C(11)#2	98.55(6)
O(2)-K(1)-O(4)	115.60(5)	O(6)-K(1)-C(11)#2	73.01(6)
O(5)-K(1)-O(3)	118.83(5)	C(2')-K(1)-C(11)#2	175.7(2)
O(1)-K(1)-O(3)	120.31(5)	C(2)-K(1)-C(11)#2	169.3(2)
O(2)-K(1)-O(3)	59.47(5)	C(1)-K(1)-C(11)#2	161.81(19)
O(4)-K(1)-O(3)	59.45(5)	O(5)-K(1)-C(3')	70.69(16)
O(5)-K(1)-O(6)	60.76(5)	O(1)-K(1)-C(3')	99.5(2)
O(1)-K(1)-O(6)	60.19(5)	O(2)-K(1)-C(3')	119.44(16)
O(2)-K(1)-O(6)	119.20(5)	O(4)-K(1)-C(3')	92.15(19)
O(4)-K(1)-O(6)	117.99(5)	O(3)-K(1)-C(3')	103.0(2)
O(3)-K(1)-O(6)	171.43(5)	O(6)-K(1)-C(3')	85.1(2)
O(5)-K(1)-C(2')	93.6(2)	C(2')-K(1)-C(3')	26.0(2)
O(1)-K(1)-C(2')	98.72(16)	C(2)-K(1)-C(3')	14.0(2)
O(2)-K(1)-C(2')	96.0(2)	C(1)-K(1)-C(3')	34.3(2)
O(4)-K(1)-C(2')	93.27(16)	C(11)#2-K(1)-C(3')	156.30(19)
O(3)-K(1)-C(2')	81.19(18)	O(5)-K(1)-C(1')	112.68(14)
O(6)-K(1)-C(2')	107.34(18)	O(1)-K(1)-C(1')	77.38(16)
O(5)-K(1)-C(2)	79.5(2)	O(2)-K(1)-C(1')	77.48(14)
O(1)-K(1)-C(2)	104.85(16)	O(4)-K(1)-C(1')	114.05(16)
O(2)-K(1)-C(2)	110.2(2)	O(3)-K(1)-C(1')	84.03(15)
O(4)-K(1)-C(2)	87.30(16)	O(6)-K(1)-C(1')	104.14(15)
O(3)-K(1)-C(2)	89.17(18)	C(2')-K(1)-C(1')	23.36(17)
O(6)-K(1)-C(2)	99.00(18)	C(2)-K(1)-C(1')	35.5(2)
C(2')-K(1)-C(2)	14.18(13)	C(1)-K(1)-C(1')	9.48(19)
O(5)-K(1)-C(1)	104.78(16)	C(11)#2-K(1)-C(1')	152.33(15)

C(3')-K(1)-C(1')	42.01(16)	H(15A)-C(15)-H(15B)	108.3
C(13)-O(1)-C(24)	112.24(19)	O(3)-C(16)-C(15)	108.9(2)
C(13)-O(1)-K(1)	114.53(14)	O(3)-C(16)-H(16A)	109.9
C(24)-O(1)-K(1)	116.82(14)	C(15)-C(16)-H(16A)	109.9
C(14)-O(2)-C(15)	112.34(18)	O(3)-C(16)-H(16B)	109.9
C(14)-O(2)-K(1)	111.57(13)	C(15)-C(16)-H(16B)	109.9
C(15)-O(2)-K(1)	114.19(13)	H(16A)-C(16)-H(16B)	108.3
C(17)-O(3)-C(16)	112.51(19)	O(3)-C(17)-C(18)	108.8(2)
C(17)-O(3)-K(1)	116.16(13)	O(3)-C(17)-H(17A)	109.9
C(16)-O(3)-K(1)	115.95(13)	C(18)-C(17)-H(17A)	109.9
C(19)-O(4)-C(18)	111.96(19)	O(3)-C(17)-H(17B)	109.9
C(19)-O(4)-K(1)	112.99(14)	C(18)-C(17)-H(17B)	109.9
C(18)-O(4)-K(1)	113.04(14)	H(17A)-C(17)-H(17B)	108.3
C(20)-O(5)-C(21)	113.02(19)	O(4)-C(18)-C(17)	108.9(2)
C(20)-O(5)-K(1)	117.44(14)	O(4)-C(18)-H(18A)	109.9
C(21)-O(5)-K(1)	117.32(14)	C(17)-C(18)-H(18A)	109.9
C(22)-O(6)-C(23)	112.44(19)	O(4)-C(18)-H(18B)	109.9
C(22)-O(6)-K(1)	107.24(13)	C(17)-C(18)-H(18B)	109.9
C(23)-O(6)-K(1)	110.99(13)	H(18A)-C(18)-H(18B)	108.3
O(1)-C(13)-C(14)	108.0(2)	O(4)-C(19)-C(20)	109.1(2)
O(1)-C(13)-H(13A)	110.1	O(4)-C(19)-H(19A)	109.9
C(14)-C(13)-H(13A)	110.1	C(20)-C(19)-H(19A)	109.9
O(1)-C(13)-H(13B)	110.1	O(4)-C(19)-H(19B)	109.9
C(14)-C(13)-H(13B)	110.1	C(20)-C(19)-H(19B)	109.9
H(13A)-C(13)-H(13B)	108.4	H(19A)-C(19)-H(19B)	108.3
O(2)-C(14)-C(13)	108.5(2)	O(5)-C(20)-C(19)	108.7(2)
O(2)-C(14)-H(14A)	110.0	O(5)-C(20)-H(20A)	109.9
C(13)-C(14)-H(14A)	110.0	C(19)-C(20)-H(20A)	109.9
O(2)-C(14)-H(14B)	110.0	O(5)-C(20)-H(20B)	109.9
C(13)-C(14)-H(14B)	110.0	C(19)-C(20)-H(20B)	109.9
H(14A)-C(14)-H(14B)	108.4	H(20A)-C(20)-H(20B)	108.3
O(2)-C(15)-C(16)	108.63(19)	O(5)-C(21)-C(22)	108.7(2)
O(2)-C(15)-H(15A)	110.0	O(5)-C(21)-H(21A)	110.0
C(16)-C(15)-H(15A)	110.0	C(22)-C(21)-H(21A)	110.0
O(2)-C(15)-H(15B)	110.0	O(5)-C(21)-H(21B)	110.0
C(16)-C(15)-H(15B)	110.0	C(22)-C(21)-H(21B)	110.0

H(21A)-C(21)-H(21B)	108.3	O(6)-C(23)-H(23B)	110.0
O(6)-C(22)-C(21)	108.3(2)	C(24)-C(23)-H(23B)	110.0
O(6)-C(22)-H(22A)	110.0	H(23A)-C(23)-H(23B)	108.4
C(21)-C(22)-H(22A)	110.0	O(1)-C(24)-C(23)	107.8(2)
O(6)-C(22)-H(22B)	110.0	O(1)-C(24)-H(24A)	110.2
C(21)-C(22)-H(22B)	110.0	C(23)-C(24)-H(24A)	110.2
H(22A)-C(22)-H(22B)	108.4	O(1)-C(24)-H(24B)	110.2
O(6)-C(23)-C(24)	108.5(2)	C(23)-C(24)-H(24B)	110.2
O(6)-C(23)-H(23A)	110.0	H(24A)-C(24)-H(24B)	108.5
C(24)-C(23)-H(23A)	110.0		

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 x,y+1,z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 320. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	30(1)	20(1)	37(1)	2(1)	1(1)	16(1)
C1	33(2)	22(2)	62(6)	7(4)	7(4)	14(2)
C2	60(6)	38(4)	64(5)	-10(3)	3(3)	40(4)
C3	70(7)	77(8)	41(2)	18(4)	21(5)	62(6)
C4	41(4)	50(7)	61(6)	7(5)	5(4)	29(3)
C1'	33(2)	22(2)	62(6)	7(4)	7(4)	14(2)
C2'	60(6)	38(4)	64(5)	-10(3)	3(3)	40(4)
C3'	70(7)	77(8)	41(2)	18(4)	21(5)	62(6)
C4'	41(4)	50(7)	61(6)	7(5)	5(4)	29(3)
C5	29(1)	33(1)	29(1)	-1(1)	1(1)	16(1)
C6	32(1)	22(1)	28(1)	-2(1)	-2(1)	10(1)
C7	21(1)	26(1)	29(1)	4(1)	1(1)	7(1)
C8	30(1)	30(1)	29(1)	3(1)	5(1)	12(1)
C9	38(1)	35(1)	26(1)	7(1)	4(1)	22(1)
C10	30(1)	28(1)	35(1)	-6(1)	-6(1)	16(1)
C11	25(1)	19(1)	49(2)	-2(1)	0(1)	6(1)
C12	22(1)	27(1)	39(1)	10(1)	2(1)	8(1)
K1	20(1)	20(1)	27(1)	3(1)	3(1)	10(1)
O1	24(1)	36(1)	30(1)	5(1)	-1(1)	9(1)
O2	22(1)	31(1)	26(1)	-1(1)	3(1)	11(1)
O3	23(1)	31(1)	26(1)	-1(1)	0(1)	9(1)
O4	27(1)	37(1)	25(1)	5(1)	2(1)	12(1)
O5	22(1)	35(1)	33(1)	2(1)	6(1)	12(1)
O6	23(1)	25(1)	34(1)	1(1)	0(1)	6(1)
C13	36(1)	44(2)	26(1)	8(1)	0(1)	7(1)
C14	34(1)	40(2)	23(1)	1(1)	7(1)	8(1)
C15	21(1)	36(1)	37(1)	6(1)	10(1)	14(1)
C16	18(1)	34(1)	40(1)	3(1)	2(1)	7(1)
C17	25(1)	40(1)	31(1)	-8(1)	-5(1)	13(1)
C18	34(1)	46(2)	27(1)	-2(1)	-6(1)	18(1)
C19	40(2)	42(2)	26(1)	9(1)	6(1)	11(1)

C20	34(1)	39(2)	33(1)	4(1)	14(1)	11(1)
C21	22(1)	39(1)	47(2)	13(1)	12(1)	14(1)
C22	18(1)	30(1)	50(2)	10(1)	2(1)	4(1)
C23	24(1)	34(1)	40(1)	-9(1)	-6(1)	10(1)
C24	29(1)	44(2)	30(1)	-2(1)	-7(1)	16(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 320.

	x	y	z	U(eq)
H1A	4152	5511	2139	45
H1B	2330	5147	1548	45
H2A	2689	5102	3452	58
H3A	-261	3295	3328	62
H4A	-250	3704	1471	56
H4B	-1224	2242	1908	56
H1C	4322	5232	1528	45
H1D	2349	4998	1205	45
H2B	3690	5507	3025	58
H3B	742	4083	3436	62
H4C	-108	3709	1568	56
H4D	-1008	2586	2311	56
H5A	2193	2480	4066	35
H6A	4727	3704	3592	33
H7A	4869	1366	2969	31
H7B	6338	2805	2925	31
H8A	5672	2992	1482	35
H8B	4934	1408	1479	35
H9A	2967	2435	814	37
H10A	580	962	1318	36
H11A	2603	-37	2310	38
H11B	593	-641	2261	38
H12A	512	298	3577	36
H12B	2314	224	3760	36
H13A	2533	9227	405	46
H13B	2170	8143	-403	46
H14A	4042	7320	417	41
H14B	4984	8793	83	41
H15A	7113	9290	1247	36
H15B	6264	7841	1636	36

H16A	7939	9440	2773	38
H16B	6721	10222	2625	38
H17A	5934	9852	4143	39
H17B	7180	9095	4297	39
H18A	4818	7130	4568	42
H18B	5119	8300	5303	42
H19A	2246	7481	5612	45
H19B	1925	6236	4938	45
H20A	-583	6608	5090	43
H20B	297	8041	4684	43
H21A	-2048	7159	3507	41
H21B	-2670	5703	3894	41
H22A	-1913	4944	2527	41
H22B	-3433	5427	2366	41
H23A	-2755	6092	854	40
H23B	-1408	5423	980	40
H24A	-708	7081	-131	41
H24B	-465	8170	657	41

Table 6. Torsion angles [°] for 320.

C3'-Co1-C1-C2	24.8(6)	C4-Co1-C2-C1	-96.6(6)
C2'-Co1-C1-C2	-19.7(8)	C3'-Co1-C2-C3	2.1(12)
C6-Co1-C1-C2	-86.9(5)	C2'-Co1-C2-C3	146.4(11)
C5-Co1-C1-C2	-48.7(6)	C6-Co1-C2-C3	-129.3(5)
C9-Co1-C1-C2	-177.5(4)	C5-Co1-C2-C3	-87.2(6)
C10-Co1-C1-C2	151.4(4)	C9-Co1-C2-C3	131.3(7)
C4'-Co1-C1-C2	64.3(7)	C10-Co1-C2-C3	25.8(14)
C3-Co1-C1-C2	34.8(4)	C1-Co1-C2-C3	126.8(6)
C1'-Co1-C1-C2	168.5(17)	C4'-Co1-C2-C3	27.1(9)
C4-Co1-C1-C2	71.9(5)	C1'-Co1-C2-C3	122.7(7)
C3'-Co1-C1-K1	8.2(6)	C4-Co1-C2-C3	30.2(6)
C2-Co1-C1-K1	-16.6(5)	C3'-Co1-C2-K1	-102.9(13)
C2'-Co1-C1-K1	-36.3(6)	C2'-Co1-C2-K1	41.3(9)
C6-Co1-C1-K1	-103.5(6)	C6-Co1-C2-K1	125.7(8)
C5-Co1-C1-K1	-65.3(7)	C5-Co1-C2-K1	167.8(8)
C9-Co1-C1-K1	165.9(6)	C9-Co1-C2-K1	26.3(12)
C10-Co1-C1-K1	134.8(5)	C10-Co1-C2-K1	-79.2(16)
C4'-Co1-C1-K1	47.7(8)	C1-Co1-C2-K1	21.7(7)
C3-Co1-C1-K1	18.2(6)	C4'-Co1-C2-K1	-77.9(10)
C1'-Co1-C1-K1	152(2)	C3-Co1-C2-K1	-105.0(9)
C4-Co1-C1-K1	55.3(6)	C1'-Co1-C2-K1	17.7(7)
Co1-C1-C2-C3	-58.9(8)	C4-Co1-C2-K1	-74.9(9)
K1-C1-C2-C3	110.2(9)	C1-C2-C3-C4	-1(2)
K1-C1-C2-Co1	169.0(3)	Co1-C2-C3-C4	-59(2)
Co1-C1-C2-K1	-169.0(3)	K1-C2-C3-C4	89(2)
C3'-Co1-C2-C1	-124.7(11)	C1-C2-C3-Co1	58.3(8)
C2'-Co1-C2-C1	19.6(9)	K1-C2-C3-Co1	148.1(5)
C6-Co1-C2-C1	103.9(5)	C3'-Co1-C3-C4	124(2)
C5-Co1-C2-C1	146.1(5)	C2-Co1-C3-C4	127.4(13)
C9-Co1-C2-C1	4.5(8)	C2'-Co1-C3-C4	114.1(12)
C10-Co1-C2-C1	-100.9(12)	C6-Co1-C3-C4	-165.5(12)
C4'-Co1-C2-C1	-99.7(9)	C5-Co1-C3-C4	-132.1(12)
C3-Co1-C2-C1	-126.8(7)	C9-Co1-C3-C4	-0.2(15)
C1'-Co1-C2-C1	-4.1(6)	C10-Co1-C3-C4	-43.5(13)

C1-Co1-C3-C4	94.5(12)	C2'-Co1-C1'-K1	-22.1(4)
C4'-Co1-C3-C4	5(3)	C6-Co1-C1'-K1	-98.8(3)
C1'-Co1-C3-C4	82.0(12)	C5-Co1-C1'-K1	-69.1(5)
C3'-Co1-C3-C2	-3.1(18)	C9-Co1-C1'-K1	176.1(3)
C2'-Co1-C3-C2	-13.3(4)	C10-Co1-C1'-K1	149.56(19)
C6-Co1-C3-C2	67.1(6)	C1-Co1-C1'-K1	-17.3(12)
C5-Co1-C3-C2	100.5(5)	C4'-Co1-C1'-K1	54.6(5)
C9-Co1-C3-C2	-127.6(7)	C3-Co1-C1'-K1	26.6(5)
C10-Co1-C3-C2	-170.8(4)	C4-Co1-C1'-K1	63.1(6)
C1-Co1-C3-C2	-32.9(4)	Co1-C1'-C2'-C3'	-56.0(8)
C4'-Co1-C3-C2	-122.2(18)	K1-C1'-C2'-C3'	100.1(9)
C1'-Co1-C3-C2	-45.4(6)	K1-C1'-C2'-Co1	156.1(4)
C4-Co1-C3-C2	-127.4(13)	Co1-C1'-C2'-K1	-156.1(4)
C2-C3-C4-Co1	52.7(14)	C3'-Co1-C2'-C1'	-126.1(6)
C3'-Co1-C4-C3	-19.3(8)	C2-Co1-C2'-C1'	-147.1(12)
C2-Co1-C4-C3	-35.2(9)	C6-Co1-C2'-C1'	113.4(5)
C2'-Co1-C4-C3	-54.6(10)	C5-Co1-C2'-C1'	153.4(4)
C6-Co1-C4-C3	34(3)	C9-Co1-C2'-C1'	22.8(6)
C5-Co1-C4-C3	57.9(14)	C10-Co1-C2'-C1'	-21.4(12)
C9-Co1-C4-C3	179.9(8)	C1-Co1-C2'-C1'	-3.9(10)
C10-Co1-C4-C3	143.4(10)	C4'-Co1-C2'-C1'	-93.8(5)
C1-Co1-C4-C3	-76.1(11)	C3-Co1-C2'-C1'	-121.8(8)
C4'-Co1-C4-C3	-17(8)	C4-Co1-C2'-C1'	-88.4(8)
C1'-Co1-C4-C3	-93.6(11)	C2-Co1-C2'-C3'	-21.1(10)
C3'-Co1-C1'-C2'	36.5(4)	C6-Co1-C2'-C3'	-120.5(5)
C2-Co1-C1'-C2'	13.6(5)	C5-Co1-C2'-C3'	-80.6(5)
C6-Co1-C1'-C2'	-76.7(5)	C9-Co1-C2'-C3'	148.9(5)
C5-Co1-C1'-C2'	-47.0(7)	C10-Co1-C2'-C3'	104.7(11)
C9-Co1-C1'-C2'	-161.8(5)	C1-Co1-C2'-C3'	122.1(11)
C10-Co1-C1'-C2'	171.6(5)	C4'-Co1-C2'-C3'	32.2(5)
C1-Co1-C1'-C2'	4.7(13)	C3-Co1-C2'-C3'	4.3(8)
C4'-Co1-C1'-C2'	76.7(5)	C1'-Co1-C2'-C3'	126.1(6)
C3-Co1-C1'-C2'	48.6(7)	C4-Co1-C2'-C3'	37.7(8)
C4-Co1-C1'-C2'	85.1(8)	C3'-Co1-C2'-K1	-37.8(11)
C3'-Co1-C1'-K1	14.5(4)	C2-Co1-C2'-K1	-58.9(13)
C2-Co1-C1'-K1	-8.5(3)	C6-Co1-C2'-K1	-158.3(12)

C5-Co1-C2'-K1	-118.4(11)	C2'-Co1-C3'-K1	15.3(4)
C9-Co1-C2'-K1	111.0(12)	C6-Co1-C3'-K1	88.8(5)
C10-Co1-C2'-K1	66.9(19)	C5-Co1-C3'-K1	129.0(5)
C1-Co1-C2'-K1	84.3(13)	C9-Co1-C3'-K1	-64.8(11)
C4'-Co1-C2'-K1	-5.6(12)	C10-Co1-C3'-K1	-136.3(4)
C3-Co1-C2'-K1	-33.5(11)	C1-Co1-C3'-K1	-5.9(4)
C1'-Co1-C2'-K1	88.2(12)	C4'-Co1-C3'-K1	-111.3(11)
C4-Co1-C2'-K1	-0.1(12)	C3-Co1-C3'-K1	-152(3)
C1'-C2'-C3'-C4'	3(2)	C1'-Co1-C3'-K1	-16.6(4)
Co1-C2'-C3'-C4'	-59(2)	C4-Co1-C3'-K1	-110.6(12)
K1-C2'-C3'-C4'	106(2)	C2'-C3'-C4'-Co1	56.6(13)
C1'-C2'-C3'-Co1	62.4(8)	K1-C3'-C4'-Co1	123.6(7)
K1-C2'-C3'-Co1	165.8(4)	C2-Co1-C4'-C3'	-16.7(6)
C1'-C2'-C3'-K1	-103.4(8)	C2'-Co1-C4'-C3'	-36.0(8)
Co1-C2'-C3'-K1	-165.8(4)	C6-Co1-C4'-C3'	41(2)
C2-Co1-C3'-C4'	144.2(13)	C5-Co1-C4'-C3'	73.3(11)
C2'-Co1-C3'-C4'	126.5(11)	C9-Co1-C4'-C3'	-159.1(6)
C6-Co1-C3'-C4'	-160.0(10)	C10-Co1-C4'-C3'	162.9(8)
C5-Co1-C3'-C4'	-119.7(10)	C1-Co1-C4'-C3'	-58.1(8)
C9-Co1-C3'-C4'	46.5(14)	C3-Co1-C4'-C3'	24.1(11)
C10-Co1-C3'-C4'	-25.1(11)	C1'-Co1-C4'-C3'	-75.3(8)
C1-Co1-C3'-C4'	105.4(11)	C4-Co1-C4'-C3'	-177(9)
C3-Co1-C3'-C4'	-41(2)	C3'-Co1-C5-C6	-119.4(4)
C1'-Co1-C3'-C4'	94.7(10)	C2-Co1-C5-C6	-93.3(3)
C4-Co1-C3'-C4'	0.6(18)	C2'-Co1-C5-C6	-74.5(4)
C2-Co1-C3'-C2'	17.6(8)	C9-Co1-C5-C6	66.54(16)
C6-Co1-C3'-C2'	73.5(5)	C10-Co1-C5-C6	103.71(15)
C5-Co1-C3'-C2'	113.7(4)	C1-Co1-C5-C6	-63.4(4)
C9-Co1-C3'-C2'	-80.1(10)	C4'-Co1-C5-C6	-157.8(7)
C10-Co1-C3'-C2'	-151.6(4)	C3-Co1-C5-C6	-136.5(4)
C1-Co1-C3'-C2'	-21.2(5)	C1'-Co1-C5-C6	-44.5(4)
C4'-Co1-C3'-C2'	-126.5(11)	C4-Co1-C5-C6	-167.0(8)
C3-Co1-C3'-C2'	-167(2)	C3'-Co1-C5-C12	122.3(4)
C1'-Co1-C3'-C2'	-31.9(4)	C2-Co1-C5-C12	148.5(3)
C4-Co1-C3'-C2'	-125.9(11)	C2'-Co1-C5-C12	167.2(4)
C2-Co1-C3'-K1	32.9(6)	C6-Co1-C5-C12	-118.3(2)

C9-Co1-C5-C12	-51.73(19)	C3'-Co1-C9-C10	-99.8(8)
C10-Co1-C5-C12	-14.57(18)	C2-Co1-C9-C10	-152.4(4)
C1-Co1-C5-C12	178.3(4)	C2'-Co1-C9-C10	-159.2(3)
C4'-Co1-C5-C12	83.9(7)	C6-Co1-C9-C10	103.56(15)
C3-Co1-C5-C12	105.2(4)	C5-Co1-C9-C10	66.23(15)
C1'-Co1-C5-C12	-162.8(4)	C1-Co1-C9-C10	-149.4(3)
C4-Co1-C5-C12	74.7(8)	C4'-Co1-C9-C10	-67.3(8)
C12-C5-C6-C7	-1.7(4)	C3-Co1-C9-C10	-64.3(7)
Co1-C5-C6-C7	-105.4(2)	C1'-Co1-C9-C10	-145.2(3)
C12-C5-C6-Co1	103.7(2)	C4-Co1-C9-C10	-64.5(8)
C3'-Co1-C6-C5	74.4(4)	C3'-Co1-C9-C8	141.1(8)
C2-Co1-C6-C5	95.8(4)	C2-Co1-C9-C8	88.5(5)
C2'-Co1-C6-C5	117.3(4)	C2'-Co1-C9-C8	81.8(3)
C9-Co1-C6-C5	-116.48(15)	C6-Co1-C9-C8	-15.51(18)
C10-Co1-C6-C5	-76.52(15)	C5-Co1-C9-C8	-52.83(19)
C1-Co1-C6-C5	137.1(3)	C10-Co1-C9-C8	-119.1(2)
C4'-Co1-C6-C5	46.4(15)	C1-Co1-C9-C8	91.6(3)
C3-Co1-C6-C5	56.0(4)	C4'-Co1-C9-C8	173.6(8)
C1'-Co1-C6-C5	155.2(3)	C3-Co1-C9-C8	176.6(6)
C4-Co1-C6-C5	32(2)	C1'-Co1-C9-C8	95.7(3)
C3'-Co1-C6-C7	-168.0(4)	C4-Co1-C9-C8	176.5(8)
C2-Co1-C6-C7	-146.6(4)	C8-C9-C10-C11	-2.2(4)
C2'-Co1-C6-C7	-125.0(4)	Co1-C9-C10-C11	-104.8(2)
C5-Co1-C6-C7	117.6(2)	C8-C9-C10-Co1	102.6(2)
C9-Co1-C6-C7	1.15(17)	C3'-Co1-C10-C9	142.5(5)
C10-Co1-C6-C7	41.12(18)	C2-Co1-C10-C9	127.7(10)
C1-Co1-C6-C7	-105.3(3)	C2'-Co1-C10-C9	58.5(9)
C4'-Co1-C6-C7	164.1(15)	C6-Co1-C10-C9	-76.72(15)
C3-Co1-C6-C7	173.6(4)	C5-Co1-C10-C9	-116.73(15)
C1'-Co1-C6-C7	-87.2(3)	C1-Co1-C10-C9	48.8(4)
C4-Co1-C6-C7	150(2)	C4'-Co1-C10-C9	126.6(6)
C5-C6-C7-C8	93.0(3)	C3-Co1-C10-C9	147.8(4)
Co1-C6-C7-C8	13.2(2)	C1'-Co1-C10-C9	42.8(3)
C6-C7-C8-C9	-25.9(3)	C4-Co1-C10-C9	123.7(5)
C7-C8-C9-C10	-52.0(3)	C3'-Co1-C10-C11	-100.9(5)
C7-C8-C9-Co1	26.8(3)	C2-Co1-C10-C11	-115.7(10)

C2'-Co1-C10-C11	175.1(9)	C3'-C2'-K1-C2	23.0(10)
C6-Co1-C10-C11	39.87(19)	Co1-C2'-K1-C2	57.3(13)
C5-Co1-C10-C11	-0.14(18)	C1'-C2'-K1-C1	1.8(10)
C9-Co1-C10-C11	116.6(2)	C3'-C2'-K1-C1	-116.2(11)
C1-Co1-C10-C11	165.4(4)	Co1-C2'-K1-C1	-81.9(12)
C4'-Co1-C10-C11	-116.8(6)	C1'-C2'-K1-C11#2	-8(3)
C3-Co1-C10-C11	-95.6(4)	C3'-C2'-K1-C11#2	-126(3)
C1'-Co1-C10-C11	159.4(3)	Co1-C2'-K1-C11#2	-92(3)
C4-Co1-C10-C11	-119.8(5)	C1'-C2'-K1-C3'	118.1(6)
C9-C10-C11-C12	93.7(3)	Co1-C2'-K1-C3'	34.3(10)
Co1-C10-C11-C12	14.7(3)	C3'-C2'-K1-C1'	-118.1(6)
C9-C10-C11-K1#1	-71.7(4)	Co1-C2'-K1-C1'	-83.7(11)
Co1-C10-C11-K1#1	-150.75(18)	C1-C2-K1-O5	164.3(5)
C6-C5-C12-C11	-52.8(3)	C3-C2-K1-O5	49.4(7)
Co1-C5-C12-C11	26.2(2)	Co1-C2-K1-O5	143.4(9)
C10-C11-C12-C5	-26.3(3)	C1-C2-K1-O1	45.1(5)
K1#1-C11-C12-C5	144.96(16)	C3-C2-K1-O1	-69.8(7)
C1'-C2'-K1-O5	146.0(6)	Co1-C2-K1-O1	24.2(9)
C3'-C2'-K1-O5	28.0(5)	C1-C2-K1-O2	-19.3(5)
Co1-C2'-K1-O5	62.3(12)	C3-C2-K1-O2	-134.1(7)
C1'-C2'-K1-O1	24.2(6)	Co1-C2-K1-O2	-40.2(9)
C3'-C2'-K1-O1	-93.9(5)	C1-C2-K1-O4	-135.6(5)
Co1-C2'-K1-O1	-59.6(13)	C3-C2-K1-O4	109.5(7)
C1'-C2'-K1-O2	-37.6(6)	Co1-C2-K1-O4	-156.5(9)
C3'-C2'-K1-O2	-155.6(5)	C1-C2-K1-O3	-76.1(5)
Co1-C2'-K1-O2	-121.3(12)	C3-C2-K1-O3	169.0(7)
C1'-C2'-K1-O4	-153.7(6)	Co1-C2-K1-O3	-97.1(9)
C3'-C2'-K1-O4	88.2(5)	C1-C2-K1-O6	106.5(5)
Co1-C2'-K1-O4	122.5(12)	C3-C2-K1-O6	-8.4(7)
C1'-C2'-K1-O3	-95.3(6)	Co1-C2-K1-O6	85.6(9)
C3'-C2'-K1-O3	146.6(5)	C1-C2-K1-C2'	-20.7(9)
Co1-C2'-K1-O3	-179.1(13)	C3-C2-K1-C2'	-135.6(11)
C1'-C2'-K1-O6	85.6(6)	Co1-C2-K1-C2'	-41.7(9)
C3'-C2'-K1-O6	-32.5(5)	C3-C2-K1-C1	-114.9(6)
Co1-C2'-K1-O6	1.8(13)	Co1-C2-K1-C1	-20.9(6)
C1'-C2'-K1-C2	141.0(12)	C1-C2-K1-C11#2	147.2(9)

C3-C2-K1-C11#2	32.4(12)	C2'-C3'-K1-O2	28.1(6)
Co1-C2-K1-C11#2	126.3(10)	Co1-C3'-K1-O2	11.5(7)
C1-C2-K1-C3'	114.3(12)	C4'-C3'-K1-O4	160.8(10)
C3-C2-K1-C3'	-0.6(12)	C2'-C3'-K1-O4	-93.1(5)
Co1-C2-K1-C3'	93.4(13)	Co1-C3'-K1-O4	-109.7(6)
C1-C2-K1-C1'	4.7(6)	C4'-C3'-K1-O3	-140.1(10)
C3-C2-K1-C1'	-110.2(8)	C2'-C3'-K1-O3	-33.9(5)
Co1-C2-K1-C1'	-16.2(7)	Co1-C3'-K1-O3	-50.5(6)
C2-C1-K1-O5	-16.0(5)	C4'-C3'-K1-O6	42.9(10)
Co1-C1-K1-O5	0.1(7)	C2'-C3'-K1-O6	149.0(5)
C2-C1-K1-O1	-136.7(5)	Co1-C3'-K1-O6	132.4(6)
Co1-C1-K1-O1	-120.6(7)	C4'-C3'-K1-C2'	-106.2(10)
C2-C1-K1-O2	161.9(5)	Co1-C3'-K1-C2'	-16.6(4)
Co1-C1-K1-O2	177.9(7)	C4'-C3'-K1-C2	-129.4(13)
C2-C1-K1-O4	46.6(5)	C2'-C3'-K1-C2	-23.2(8)
Co1-C1-K1-O4	62.6(7)	Co1-C3'-K1-C2	-39.8(7)
C2-C1-K1-O3	102.1(5)	C4'-C3'-K1-C1	-83.7(10)
Co1-C1-K1-O3	118.1(7)	C2'-C3'-K1-C1	22.4(5)
C2-C1-K1-O6	-79.1(5)	Co1-C3'-K1-C1	5.8(4)
Co1-C1-K1-O6	-63.1(7)	C4'-C3'-K1-C11#2	65.1(10)
C2-C1-K1-C2'	21.2(8)	C2'-C3'-K1-C11#2	171.3(4)
Co1-C1-K1-C2'	37.2(7)	Co1-C3'-K1-C11#2	154.7(3)
Co1-C1-K1-C2	16.0(5)	C4'-C3'-K1-C1'	-74.6(9)
C2-C1-K1-C11#2	-161.3(5)	C2'-C3'-K1-C1'	31.5(3)
Co1-C1-K1-C11#2	-145.3(4)	Co1-C3'-K1-C1'	14.9(4)
C2-C1-K1-C3'	-23.1(5)	C2'-C1'-K1-O5	-37.2(6)
Co1-C1-K1-C3'	-7.1(5)	Co1-C1'-K1-O5	-13.6(4)
C2-C1-K1-C1'	-163.2(19)	C2'-C1'-K1-O1	-155.5(6)
Co1-C1-K1-C1'	-147(2)	Co1-C1'-K1-O1	-131.9(4)
C4'-C3'-K1-O5	103.6(11)	C2'-C1'-K1-O2	141.6(6)
C2'-C3'-K1-O5	-150.3(5)	Co1-C1'-K1-O2	165.2(4)
Co1-C3'-K1-O5	-166.9(7)	C2'-C1'-K1-O4	28.9(6)
C4'-C3'-K1-O1	-15.8(10)	Co1-C1'-K1-O4	52.5(4)
C2'-C3'-K1-O1	90.4(5)	C2'-C1'-K1-O3	81.6(6)
Co1-C3'-K1-O1	73.8(6)	Co1-C1'-K1-O3	105.2(3)
C4'-C3'-K1-O2	-78.0(11)	C2'-C1'-K1-O6	-101.1(6)

Co1-C1'-K1-O6	-77.5(4)	O6-K1-O2-C14	-37.65(16)
Co1-C1'-K1-C2'	23.6(5)	C2'-K1-O2-C14	76.0(2)
C2'-C1'-K1-C2	-15.4(5)	C2-K1-O2-C14	75.7(2)
Co1-C1'-K1-C2	8.2(3)	C1-K1-O2-C14	67.2(2)
C2'-C1'-K1-C1	-2.7(15)	C11#2-K1-O2-C14	-101.81(16)
Co1-C1'-K1-C1	20.9(14)	C3'-K1-O2-C14	64.0(3)
C2'-C1'-K1-C11#2	178.6(5)	C1'-K1-O2-C14	61.7(2)
Co1-C1'-K1-C11#2	-157.80(16)	O5-K1-O2-C15	106.7(3)
C2'-C1'-K1-C3'	-35.4(4)	O1-K1-O2-C15	-149.35(16)
Co1-C1'-K1-C3'	-11.8(3)	O4-K1-O2-C15	43.87(16)
O5-K1-O1-C13	153.14(16)	O3-K1-O2-C15	23.39(14)
O2-K1-O1-C13	-15.29(16)	O6-K1-O2-C15	-166.37(14)
O4-K1-O1-C13	62.8(3)	C2'-K1-O2-C15	-52.7(2)
O3-K1-O1-C13	-22.53(19)	C2-K1-O2-C15	-53.0(2)
O6-K1-O1-C13	147.57(18)	C1-K1-O2-C15	-61.5(2)
C2'-K1-O1-C13	-107.4(3)	C11#2-K1-O2-C15	129.47(15)
C2-K1-O1-C13	-120.4(3)	C3'-K1-O2-C15	-64.7(3)
C1-K1-O1-C13	-102.1(2)	C1'-K1-O2-C15	-67.0(2)
C11#2-K1-O1-C13	70.23(17)	O5-K1-O3-C17	-21.84(17)
C3'-K1-O1-C13	-133.7(2)	O1-K1-O3-C17	153.92(15)
C1'-K1-O1-C13	-97.8(2)	O2-K1-O3-C17	146.55(17)
O5-K1-O1-C24	18.96(18)	O4-K1-O3-C17	-11.96(15)
O2-K1-O1-C24	-149.48(18)	O6-K1-O3-C17	63.0(4)
O4-K1-O1-C24	-71.4(3)	C2'-K1-O3-C17	-111.1(3)
O3-K1-O1-C24	-156.72(15)	C2-K1-O3-C17	-99.3(2)
O6-K1-O1-C24	13.39(15)	C1-K1-O3-C17	-125.0(2)
C2'-K1-O1-C24	118.4(3)	C11#2-K1-O3-C17	73.30(16)
C2-K1-O1-C24	105.4(3)	C3'-K1-O3-C17	-96.7(2)
C1-K1-O1-C24	123.7(2)	C1'-K1-O3-C17	-134.5(2)
C11#2-K1-O1-C24	-63.96(16)	O5-K1-O3-C16	-157.36(15)
C3'-K1-O1-C24	92.1(2)	O1-K1-O3-C16	18.39(17)
C1'-K1-O1-C24	128.0(2)	O2-K1-O3-C16	11.03(14)
O5-K1-O2-C14	-124.5(3)	O4-K1-O3-C16	-147.49(17)
O1-K1-O2-C14	-20.63(15)	O6-K1-O3-C16	-72.5(4)
O4-K1-O2-C14	172.59(15)	C2'-K1-O3-C16	113.4(3)
O3-K1-O2-C14	152.12(17)	C2-K1-O3-C16	125.2(2)

C1-K1-O3-C16	99.5(2)	C1'-K1-O5-C20	121.0(2)
C11#2-K1-O3-C16	-62.22(16)	O1-K1-O5-C21	-10.68(18)
C3'-K1-O3-C16	127.7(2)	O2-K1-O5-C21	87.5(3)
C1'-K1-O3-C16	90.0(2)	O4-K1-O5-C21	155.25(18)
O5-K1-O4-C19	18.95(15)	O3-K1-O5-C21	165.06(15)
O1-K1-O4-C19	116.5(3)	O6-K1-O5-C21	-5.14(15)
O2-K1-O4-C19	-171.54(15)	C2'-K1-O5-C21	-113.0(2)
O3-K1-O4-C19	-151.07(17)	C2-K1-O5-C21	-111.8(2)
O6-K1-O4-C19	38.32(17)	C1-K1-O5-C21	-104.7(2)
C2'-K1-O4-C19	-73.3(3)	C11#2-K1-O5-C21	65.10(17)
C2-K1-O4-C19	-60.4(3)	C3'-K1-O5-C21	-100.4(3)
C1-K1-O4-C19	-79.2(2)	C1'-K1-O5-C21	-99.1(2)
C11#2-K1-O4-C19	109.17(16)	O5-K1-O6-C22	-29.18(14)
C3'-K1-O4-C19	-47.3(2)	O1-K1-O6-C22	145.34(16)
C1'-K1-O4-C19	-84.4(2)	O2-K1-O6-C22	162.54(14)
O5-K1-O4-C18	147.40(17)	O4-K1-O6-C22	-48.41(16)
O1-K1-O4-C18	-115.1(3)	O3-K1-O6-C22	-118.8(3)
O2-K1-O4-C18	-43.09(17)	C2'-K1-O6-C22	55.1(3)
O3-K1-O4-C18	-22.62(15)	C2-K1-O6-C22	43.3(2)
O6-K1-O4-C18	166.77(15)	C1-K1-O6-C22	69.4(2)
C2'-K1-O4-C18	55.2(3)	C11#2-K1-O6-C22	-129.43(16)
C2-K1-O4-C18	68.0(3)	C3'-K1-O6-C22	41.4(2)
C1-K1-O4-C18	49.2(2)	C1'-K1-O6-C22	79.2(2)
C11#2-K1-O4-C18	-122.38(16)	O5-K1-O6-C23	-152.35(16)
C3'-K1-O4-C18	81.2(2)	O1-K1-O6-C23	22.16(14)
C1'-K1-O4-C18	44.1(2)	O2-K1-O6-C23	39.37(16)
O1-K1-O5-C20	-150.50(16)	O4-K1-O6-C23	-171.59(14)
O2-K1-O5-C20	-52.3(4)	O3-K1-O6-C23	118.0(3)
O4-K1-O5-C20	15.43(16)	C2'-K1-O6-C23	-68.1(3)
O3-K1-O5-C20	25.24(18)	C2-K1-O6-C23	-79.9(2)
O6-K1-O5-C20	-144.97(18)	C1-K1-O6-C23	-53.7(2)
C2'-K1-O5-C20	107.2(2)	C11#2-K1-O6-C23	107.39(15)
C2-K1-O5-C20	108.4(2)	C3'-K1-O6-C23	-81.8(2)
C1-K1-O5-C20	115.5(2)	C1'-K1-O6-C23	-44.0(2)
C11#2-K1-O5-C20	-74.73(17)	C24-O1-C13-C14	-175.8(2)
C3'-K1-O5-C20	119.7(3)	K1-O1-C13-C14	47.9(2)

C15-O2-C14-C13	-176.7(2)	K1-O4-C19-C20	-49.9(2)
K1-O2-C14-C13	53.6(2)	C21-O5-C20-C19	171.9(2)
O1-C13-C14-O2	-68.9(3)	K1-O5-C20-C19	-46.6(2)
C14-O2-C15-C16	176.5(2)	O4-C19-C20-O5	64.1(3)
K1-O2-C15-C16	-55.2(2)	C20-O5-C21-C22	179.1(2)
C17-O3-C16-C15	-179.37(19)	K1-O5-C21-C22	37.5(2)
K1-O3-C16-C15	-42.3(2)	C23-O6-C22-C21	-176.09(19)
O2-C15-C16-O3	64.6(3)	K1-O6-C22-C21	61.6(2)
C16-O3-C17-C18	-179.3(2)	O5-C21-C22-O6	-68.3(3)
K1-O3-C17-C18	43.6(2)	C22-O6-C23-C24	-175.1(2)
C19-O4-C18-C17	-176.2(2)	K1-O6-C23-C24	-55.0(2)
K1-O4-C18-C17	54.8(2)	C13-O1-C24-C23	178.8(2)
O3-C17-C18-O4	-65.9(3)	K1-O1-C24-C23	-46.0(2)
C18-O4-C19-C20	-178.9(2)	O6-C23-C24-O1	67.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 x,y+1,z

REFERENCE NUMBER: 04313 [14]

CRYSTAL STRUCTURE REPORT

$C_{26} H_{46} Co K O_6$

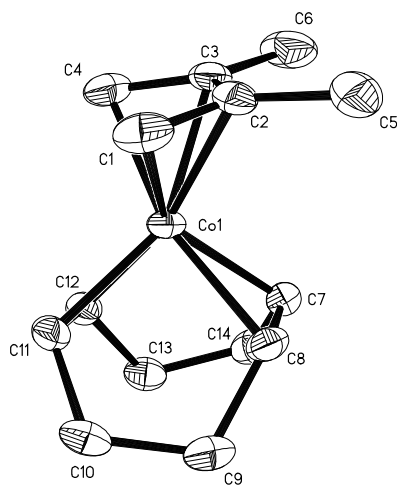
or

[K(18-crown-6)][Co(1,5-COD)(2,3-dimethyl-1,3-butadiene)]

Report prepared for:

W. Brennessel, Prof. J. Ellis

November 09, 2004



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Data collection

A crystal (approximate dimensions $0.32 \times 0.14 \times 0.10 \text{ mm}^3$) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Siemens SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 65 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 25 seconds and a detector distance of 4.91 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 3701 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ 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 hydrogen atoms of the cation and the methyl hydrogen atoms of the anion were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. All remaining hydrogen atoms were found from the difference Fourier map and refined with relative isotropic displacement parameters. One relatively large peak of electron density (1.4 electrons per Å³) lies within the van der Waals surface of a CH₂ group of the 18-crown-6 complexant, and therefore, could not be modeled. The final full matrix least squares refinement converged to $R1 = 0.0398$ and $wR2 = 0.1024$ (F^2 , all data).

Structure description

The structure is the one suggested. All atoms lie on general positions. One C3 and C4 of the butadiene ligand and one CH₂ group (C9) of the cyclooctadiene ligand on the anion are weakly coordinated to neighboring potassium cations, thereby completing the potassium coordination spheres. The net result is a pseudo polymeric structure in one dimension along the *b* axis. The cell constants of this structure are extremely close to those of [K(18-crown-6)][Co(COD)₂] (local code 04077).

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-

- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
- ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
- ³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
- ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
- ⁵ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

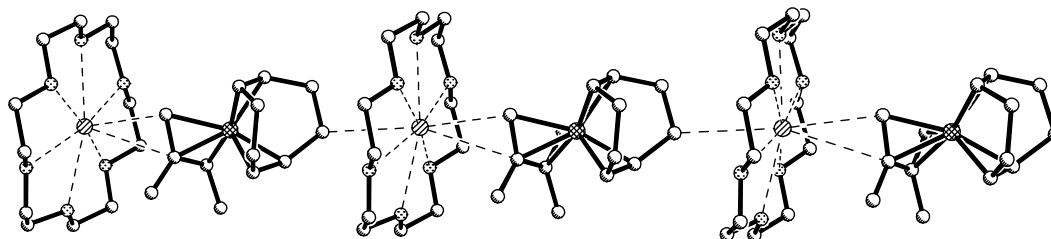
$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

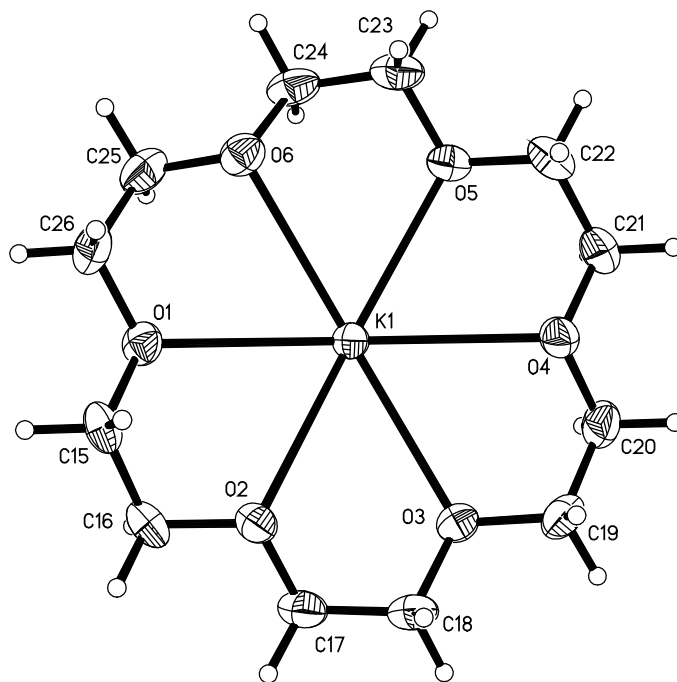
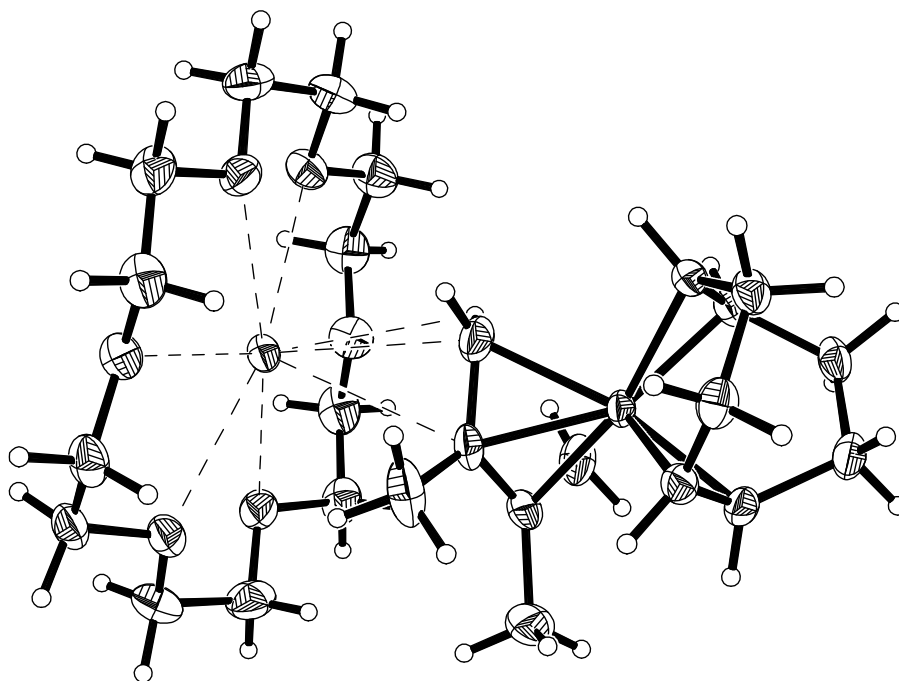
$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2 (F_o^2) + (a^*P)^2 + b^*P + d + e^* \sin(\theta)]$$

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





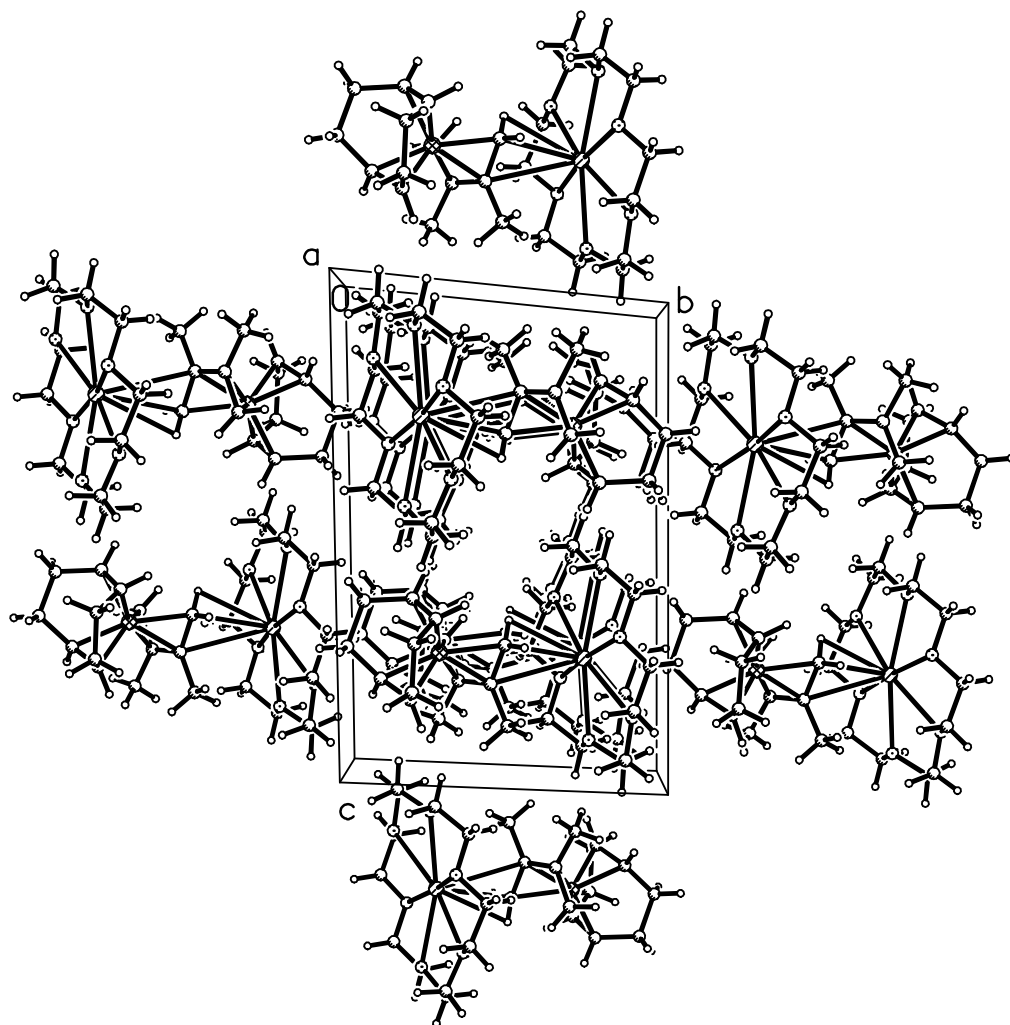


Table 1. Crystal data and structure refinement for 04313.

Identification code	04313	
Empirical formula	C ₂₆ H ₄₆ Co K O ₆	
Formula weight	552.66	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 8.764(1) Å	α = 81.571(2)°
	<i>b</i> = 11.2048(13) Å	β = 79.646(2)°
	<i>c</i> = 15.863(2) Å	γ = 67.214(2)°
Volume	1407.7(3) Å ³	
<i>Z</i>	2	
Density (calculated)	1.304 Mg/m ³	
Absorption coefficient	0.793 mm ⁻¹	
<i>F</i> (000)	592	
Crystal color, morphology	orange, block	
Crystal size	0.32 x 0.14 x 0.10 mm ³	
Theta range for data collection	1.31 to 27.49°	
Index ranges	-11 ≤ <i>h</i> ≤ 11, -14 ≤ <i>k</i> ≤ 14, -20 ≤ <i>l</i> ≤ 20	
Reflections collected	15563	
Independent reflections	6375 [<i>R</i> (int) = 0.0310]	
Observed reflections	4894	
Completeness to theta = 27.49°	98.2%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9249 and 0.7854	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	6375 / 0 / 357	
Goodness-of-fit on <i>F</i> ²	1.028	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0398, <i>wR</i> 2 = 0.0936	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0620, <i>wR</i> 2 = 0.1024	
Largest diff. peak and hole	1.400 and -0.517 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04313. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	8050(1)	7047(1)	2633(1)	21(1)
C1	5661(3)	6944(2)	2834(2)	35(1)
C2	6593(3)	6508(2)	2036(1)	29(1)
C3	8218(3)	5500(2)	2059(1)	28(1)
C4	8713(3)	5049(2)	2884(2)	33(1)
C5	5958(4)	7145(3)	1196(2)	51(1)
C6	9368(4)	4992(3)	1252(2)	48(1)
C7	9223(3)	7910(2)	1692(1)	27(1)
C8	7663(3)	8835(2)	2031(2)	27(1)
C9	7519(3)	9821(2)	2643(2)	31(1)
C10	7240(3)	9310(2)	3586(2)	31(1)
C11	8016(3)	7831(2)	3701(1)	25(1)
C12	9675(3)	7107(2)	3354(1)	24(1)
C13	10905(3)	7714(2)	2871(2)	28(1)
C14	10897(3)	7810(2)	1897(2)	29(1)
K1	8127(1)	2607(1)	2689(1)	24(1)
O1	7888(2)	2460(2)	977(1)	32(1)
C15	9180(3)	1373(2)	591(1)	33(1)
C16	10836(3)	1369(2)	720(2)	34(1)
O2	10956(2)	1166(2)	1614(1)	31(1)
C17	12498(3)	1147(2)	1802(2)	37(1)
C18	12645(3)	664(2)	2726(2)	37(1)
O3	11318(2)	1548(2)	3249(1)	31(1)
C19	11319(3)	1100(2)	4139(2)	38(1)
C20	9893(3)	2063(3)	4652(2)	39(1)
O4	8361(2)	2083(2)	4446(1)	33(1)
C21	6958(3)	2904(3)	4971(2)	41(1)
C22	5384(3)	2930(3)	4711(2)	41(1)
O5	5272(2)	3499(2)	3854(1)	36(1)
C23	3710(3)	3738(3)	3586(2)	42(1)
C24	3744(3)	4298(2)	2669(2)	41(1)

O6	4908(2)	3311(2)	2146(1)	35(1)
C25	5003(3)	3725(3)	1264(2)	43(1)
C26	6289(3)	2644(3)	775(2)	42(1)

Table 3. Bond lengths [Å] and angles [°] for 04313.

Co(1)-C(7)	2.004(2)	C(10)-C(11)	1.525(3)
Co(1)-C(12)	2.006(2)	C(10)-H(10A)	1.00(3)
Co(1)-C(11)	2.010(2)	C(10)-H(10B)	0.98(3)
Co(1)-C(8)	2.017(2)	C(11)-C(12)	1.416(3)
Co(1)-C(3)	2.019(2)	C(11)-H(11A)	1.00(2)
Co(1)-C(2)	2.023(2)	C(12)-C(13)	1.527(3)
Co(1)-C(4)	2.080(2)	C(12)-H(12A)	1.01(2)
Co(1)-C(1)	2.106(2)	C(13)-C(14)	1.533(3)
C(1)-C(2)	1.418(4)	C(13)-H(13A)	1.01(3)
C(1)-H(1A)	0.92(3)	C(13)-H(13B)	1.00(2)
C(1)-H(1B)	1.04(3)	C(14)-H(14A)	1.02(3)
C(2)-C(3)	1.437(3)	C(14)-H(14B)	1.01(2)
C(2)-C(5)	1.509(3)	K(1)-O(5)	2.7611(17)
C(3)-C(4)	1.414(3)	K(1)-O(4)	2.7915(16)
C(3)-C(6)	1.511(3)	K(1)-O(1)	2.7941(16)
C(3)-K(1)	3.276(2)	K(1)-O(2)	2.8015(16)
C(4)-K(1)	3.040(2)	K(1)-O(3)	2.8345(16)
C(4)-H(4A)	1.01(3)	K(1)-O(6)	2.8762(17)
C(4)-H(4B)	0.99(3)	K(1)-C(9)#2	3.376(2)
C(5)-H(5A)	0.9800	K(1)-H(4B)	2.88(2)
C(5)-H(5B)	0.9800	O(1)-C(26)	1.424(3)
C(5)-H(5C)	0.9800	O(1)-C(15)	1.429(3)
C(6)-H(6A)	0.9800	C(15)-C(16)	1.500(3)
C(6)-H(6B)	0.9800	C(15)-H(15A)	0.9900
C(6)-H(6C)	0.9800	C(15)-H(15B)	0.9900
C(7)-C(8)	1.427(3)	C(16)-O(2)	1.419(3)
C(7)-C(14)	1.518(3)	C(16)-H(16A)	0.9900
C(7)-H(7A)	1.01(2)	C(16)-H(16B)	0.9900
C(8)-C(9)	1.531(3)	O(2)-C(17)	1.427(3)
C(8)-H(8A)	1.01(2)	C(17)-C(18)	1.497(4)
C(9)-C(10)	1.532(3)	C(17)-H(17A)	0.9900
C(9)-K(1)#1	3.376(2)	C(17)-H(17B)	0.9900
C(9)-H(9A)	0.93(3)	C(18)-O(3)	1.422(3)
C(9)-H(9B)	1.01(3)	C(18)-H(18A)	0.9900

C(18)-H(18B)	0.9900	C(11)-Co(1)-C(3)	149.61(9)
O(3)-C(19)	1.427(3)	C(8)-Co(1)-C(3)	124.47(9)
C(19)-C(20)	1.495(4)	C(7)-Co(1)-C(2)	104.80(9)
C(19)-H(19A)	0.9900	C(12)-Co(1)-C(2)	165.25(9)
C(19)-H(19B)	0.9900	C(11)-Co(1)-C(2)	141.49(10)
C(20)-O(4)	1.429(3)	C(8)-Co(1)-C(2)	99.89(9)
C(20)-H(20A)	0.9900	C(3)-Co(1)-C(2)	41.65(9)
C(20)-H(20B)	0.9900	C(7)-Co(1)-C(4)	124.67(10)
O(4)-C(21)	1.426(3)	C(12)-Co(1)-C(4)	93.25(9)
C(21)-C(22)	1.497(4)	C(11)-Co(1)-C(4)	109.82(10)
C(21)-H(21A)	0.9900	C(8)-Co(1)-C(4)	163.00(10)
C(21)-H(21B)	0.9900	C(3)-Co(1)-C(4)	40.33(9)
C(22)-O(5)	1.418(3)	C(2)-Co(1)-C(4)	72.12(9)
C(22)-H(22A)	0.9900	C(7)-Co(1)-C(1)	133.03(10)
C(22)-H(22B)	0.9900	C(12)-Co(1)-C(1)	137.39(10)
O(5)-C(23)	1.420(3)	C(11)-Co(1)-C(1)	101.43(10)
C(23)-C(24)	1.498(4)	C(8)-Co(1)-C(1)	103.42(10)
C(23)-H(23A)	0.9900	C(3)-Co(1)-C(1)	72.38(9)
C(23)-H(23B)	0.9900	C(2)-Co(1)-C(1)	40.10(10)
C(24)-O(6)	1.429(3)	C(4)-Co(1)-C(1)	80.39(10)
C(24)-H(24A)	0.9900	C(2)-C(1)-Co(1)	66.78(13)
C(24)-H(24B)	0.9900	C(2)-C(1)-H(1A)	120.6(17)
O(6)-C(25)	1.407(3)	Co(1)-C(1)-H(1A)	108.3(17)
C(25)-C(26)	1.498(4)	C(2)-C(1)-H(1B)	111.6(14)
C(25)-H(25A)	0.9900	Co(1)-C(1)-H(1B)	120.0(15)
C(25)-H(25B)	0.9900	H(1A)-C(1)-H(1B)	119(2)
C(26)-H(26A)	0.9900	C(1)-C(2)-C(3)	117.2(2)
C(26)-H(26B)	0.9900	C(1)-C(2)-C(5)	121.2(2)
C(7)-Co(1)-C(12)	84.88(9)	C(3)-C(2)-C(5)	121.4(2)
C(7)-Co(1)-C(11)	104.40(9)	C(1)-C(2)-Co(1)	73.12(13)
C(12)-Co(1)-C(11)	41.29(9)	C(3)-C(2)-Co(1)	69.05(12)
C(7)-Co(1)-C(8)	41.56(9)	C(5)-C(2)-Co(1)	124.72(16)
C(12)-Co(1)-C(8)	94.72(9)	C(4)-C(3)-C(2)	115.8(2)
C(11)-Co(1)-C(8)	85.89(9)	C(4)-C(3)-C(6)	121.7(2)
C(7)-Co(1)-C(3)	100.77(9)	C(2)-C(3)-C(6)	122.5(2)
C(12)-Co(1)-C(3)	126.40(9)	C(4)-C(3)-Co(1)	72.13(13)

C(2)-C(3)-Co(1)	69.31(12)	C(9)-C(8)-Co(1)	112.46(15)
C(6)-C(3)-Co(1)	126.03(16)	C(7)-C(8)-H(8A)	116.8(14)
C(4)-C(3)-K(1)	67.85(12)	C(9)-C(8)-H(8A)	114.7(13)
C(2)-C(3)-K(1)	113.86(14)	Co(1)-C(8)-H(8A)	111.5(13)
C(6)-C(3)-K(1)	90.47(13)	C(8)-C(9)-C(10)	111.41(18)
Co(1)-C(3)-K(1)	136.32(10)	C(8)-C(9)-K(1)#1	142.06(15)
C(3)-C(4)-Co(1)	67.54(12)	C(10)-C(9)-K(1)#1	105.77(13)
C(3)-C(4)-K(1)	86.63(13)	C(8)-C(9)-H(9A)	109.6(16)
Co(1)-C(4)-K(1)	148.82(11)	C(10)-C(9)-H(9A)	108.4(16)
C(3)-C(4)-H(4A)	114.6(14)	K(1)#1-C(9)-H(9A)	49.3(15)
Co(1)-C(4)-H(4A)	121.3(15)	C(8)-C(9)-H(9B)	112.5(14)
K(1)-C(4)-H(4A)	84.5(15)	C(10)-C(9)-H(9B)	108.0(14)
C(3)-C(4)-H(4B)	119.8(15)	K(1)#1-C(9)-H(9B)	60.6(14)
Co(1)-C(4)-H(4B)	106.1(15)	H(9A)-C(9)-H(9B)	107(2)
K(1)-C(4)-H(4B)	71.1(15)	C(11)-C(10)-C(9)	111.56(18)
H(4A)-C(4)-H(4B)	118(2)	C(11)-C(10)-H(10A)	112.5(14)
C(2)-C(5)-H(5A)	109.5	C(9)-C(10)-H(10A)	109.8(14)
C(2)-C(5)-H(5B)	109.5	C(11)-C(10)-H(10B)	106.3(15)
H(5A)-C(5)-H(5B)	109.5	C(9)-C(10)-H(10B)	108.5(14)
C(2)-C(5)-H(5C)	109.5	H(10A)-C(10)-H(10B)	108.0(19)
H(5A)-C(5)-H(5C)	109.5	C(12)-C(11)-C(10)	123.1(2)
H(5B)-C(5)-H(5C)	109.5	C(12)-C(11)-Co(1)	69.20(12)
C(3)-C(6)-H(6A)	109.5	C(10)-C(11)-Co(1)	110.98(15)
C(3)-C(6)-H(6B)	109.5	C(12)-C(11)-H(11A)	118.0(14)
H(6A)-C(6)-H(6B)	109.5	C(10)-C(11)-H(11A)	113.1(13)
C(3)-C(6)-H(6C)	109.5	Co(1)-C(11)-H(11A)	113.7(13)
H(6A)-C(6)-H(6C)	109.5	C(11)-C(12)-C(13)	124.03(19)
H(6B)-C(6)-H(6C)	109.5	C(11)-C(12)-Co(1)	69.51(12)
C(8)-C(7)-C(14)	123.5(2)	C(13)-C(12)-Co(1)	113.86(15)
C(8)-C(7)-Co(1)	69.71(12)	C(11)-C(12)-H(12A)	114.1(13)
C(14)-C(7)-Co(1)	112.36(15)	C(13)-C(12)-H(12A)	115.6(13)
C(8)-C(7)-H(7A)	116.5(14)	Co(1)-C(12)-H(12A)	110.1(13)
C(14)-C(7)-H(7A)	114.7(14)	C(12)-C(13)-C(14)	110.74(18)
Co(1)-C(7)-H(7A)	110.1(13)	C(12)-C(13)-H(13A)	110.5(14)
C(7)-C(8)-C(9)	123.0(2)	C(14)-C(13)-H(13A)	110.1(14)
C(7)-C(8)-Co(1)	68.72(12)	C(12)-C(13)-H(13B)	110.9(14)

C(14)-C(13)-H(13B)	111.8(13)	O(5)-K(1)-C(9)#2	90.63(6)
H(13A)-C(13)-H(13B)	102.6(19)	O(4)-K(1)-C(9)#2	90.88(5)
C(7)-C(14)-C(13)	111.17(18)	O(1)-K(1)-C(9)#2	73.92(5)
C(7)-C(14)-H(14A)	113.6(14)	O(2)-K(1)-C(9)#2	77.14(6)
C(13)-C(14)-H(14A)	111.6(14)	O(3)-K(1)-C(9)#2	99.04(5)
C(7)-C(14)-H(14B)	111.9(14)	O(6)-K(1)-C(9)#2	72.91(5)
C(13)-C(14)-H(14B)	106.4(14)	C(4)-K(1)-C(9)#2	175.28(6)
H(14A)-C(14)-H(14B)	101.6(19)	C(3)-K(1)-C(9)#2	159.12(6)
O(5)-K(1)-O(4)	60.73(5)	O(5)-K(1)-H(4B)	69.1(5)
O(5)-K(1)-O(1)	120.13(5)	O(4)-K(1)-H(4B)	70.9(5)
O(4)-K(1)-O(1)	164.66(5)	O(1)-K(1)-H(4B)	124.3(5)
O(5)-K(1)-O(2)	167.25(5)	O(2)-K(1)-H(4B)	122.2(5)
O(4)-K(1)-O(2)	115.15(5)	O(3)-K(1)-H(4B)	83.8(5)
O(1)-K(1)-O(2)	60.24(5)	O(6)-K(1)-H(4B)	103.4(5)
O(5)-K(1)-O(3)	120.48(5)	C(4)-K(1)-H(4B)	19.1(5)
O(4)-K(1)-O(3)	60.54(5)	C(3)-K(1)-H(4B)	39.1(5)
O(1)-K(1)-O(3)	118.97(5)	C(9)#2-K(1)-H(4B)	157.5(5)
O(2)-K(1)-O(3)	59.16(5)	C(26)-O(1)-C(15)	111.98(18)
O(5)-K(1)-O(6)	60.27(5)	C(26)-O(1)-K(1)	117.32(14)
O(4)-K(1)-O(6)	118.13(5)	C(15)-O(1)-K(1)	113.99(13)
O(1)-K(1)-O(6)	59.89(5)	O(1)-C(15)-C(16)	108.56(18)
O(2)-K(1)-O(6)	118.08(5)	O(1)-C(15)-H(15A)	110.0
O(3)-K(1)-O(6)	171.93(5)	C(16)-C(15)-H(15A)	110.0
O(5)-K(1)-C(4)	87.34(6)	O(1)-C(15)-H(15B)	110.0
O(4)-K(1)-C(4)	84.42(6)	C(16)-C(15)-H(15B)	110.0
O(1)-K(1)-C(4)	110.77(6)	H(15A)-C(15)-H(15B)	108.4
O(2)-K(1)-C(4)	104.58(6)	O(2)-C(16)-C(15)	108.73(18)
O(3)-K(1)-C(4)	78.39(6)	O(2)-C(16)-H(16A)	109.9
O(6)-K(1)-C(4)	109.62(6)	C(15)-C(16)-H(16A)	109.9
O(5)-K(1)-C(3)	94.50(5)	O(2)-C(16)-H(16B)	109.9
O(4)-K(1)-C(3)	109.28(5)	C(15)-C(16)-H(16B)	109.9
O(1)-K(1)-C(3)	86.05(5)	H(16A)-C(16)-H(16B)	108.3
O(2)-K(1)-C(3)	98.22(5)	C(16)-O(2)-C(17)	112.84(18)
O(3)-K(1)-C(3)	95.75(5)	C(16)-O(2)-K(1)	116.13(13)
O(6)-K(1)-C(3)	92.15(5)	C(17)-O(2)-K(1)	114.60(13)
C(4)-K(1)-C(3)	25.52(6)	O(2)-C(17)-C(18)	108.4(2)

O(2)-C(17)-H(17A)	110.0	O(5)-C(22)-H(22A)	110.0
C(18)-C(17)-H(17A)	110.0	C(21)-C(22)-H(22A)	110.0
O(2)-C(17)-H(17B)	110.0	O(5)-C(22)-H(22B)	110.0
C(18)-C(17)-H(17B)	110.0	C(21)-C(22)-H(22B)	110.0
H(17A)-C(17)-H(17B)	108.4	H(22A)-C(22)-H(22B)	108.4
O(3)-C(18)-C(17)	108.76(19)	C(22)-O(5)-C(23)	112.93(19)
O(3)-C(18)-H(18A)	109.9	C(22)-O(5)-K(1)	116.28(14)
C(17)-C(18)-H(18A)	109.9	C(23)-O(5)-K(1)	118.37(14)
O(3)-C(18)-H(18B)	109.9	O(5)-C(23)-C(24)	108.5(2)
C(17)-C(18)-H(18B)	109.9	O(5)-C(23)-H(23A)	110.0
H(18A)-C(18)-H(18B)	108.3	C(24)-C(23)-H(23A)	110.0
C(18)-O(3)-C(19)	111.65(18)	O(5)-C(23)-H(23B)	110.0
C(18)-O(3)-K(1)	117.55(13)	C(24)-C(23)-H(23B)	110.0
C(19)-O(3)-K(1)	114.95(13)	H(23A)-C(23)-H(23B)	108.4
O(3)-C(19)-C(20)	109.04(19)	O(6)-C(24)-C(23)	108.1(2)
O(3)-C(19)-H(19A)	109.9	O(6)-C(24)-H(24A)	110.1
C(20)-C(19)-H(19A)	109.9	C(23)-C(24)-H(24A)	110.1
O(3)-C(19)-H(19B)	109.9	O(6)-C(24)-H(24B)	110.1
C(20)-C(19)-H(19B)	109.9	C(23)-C(24)-H(24B)	110.1
H(19A)-C(19)-H(19B)	108.3	H(24A)-C(24)-H(24B)	108.4
O(4)-C(20)-C(19)	108.9(2)	C(25)-O(6)-C(24)	112.86(19)
O(4)-C(20)-H(20A)	109.9	C(25)-O(6)-K(1)	109.21(14)
C(19)-C(20)-H(20A)	109.9	C(24)-O(6)-K(1)	107.14(13)
O(4)-C(20)-H(20B)	109.9	O(6)-C(25)-C(26)	108.9(2)
C(19)-C(20)-H(20B)	109.9	O(6)-C(25)-H(25A)	109.9
H(20A)-C(20)-H(20B)	108.3	C(26)-C(25)-H(25A)	109.9
C(21)-O(4)-C(20)	111.35(18)	O(6)-C(25)-H(25B)	109.9
C(21)-O(4)-K(1)	113.72(13)	C(26)-C(25)-H(25B)	109.9
C(20)-O(4)-K(1)	112.68(13)	H(25A)-C(25)-H(25B)	108.3
O(4)-C(21)-C(22)	109.4(2)	O(1)-C(26)-C(25)	108.3(2)
O(4)-C(21)-H(21A)	109.8	O(1)-C(26)-H(26A)	110.0
C(22)-C(21)-H(21A)	109.8	C(25)-C(26)-H(26A)	110.0
O(4)-C(21)-H(21B)	109.8	O(1)-C(26)-H(26B)	110.0
C(22)-C(21)-H(21B)	109.8	C(25)-C(26)-H(26B)	110.0
H(21A)-C(21)-H(21B)	108.3	H(26A)-C(26)-H(26B)	108.4
O(5)-C(22)-C(21)	108.5(2)		

Symmetry transformations used to generate equivalent atoms:

#1 $x, y+1, z$ #2 $x, y-1, z$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04313. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	23(1)	16(1)	26(1)	-3(1)	-5(1)	-9(1)
C1	28(1)	28(1)	53(2)	-8(1)	-1(1)	-14(1)
C2	34(1)	29(1)	33(1)	-3(1)	-11(1)	-19(1)
C3	35(1)	22(1)	31(1)	-8(1)	0(1)	-16(1)
C4	36(1)	21(1)	45(2)	-1(1)	-9(1)	-14(1)
C5	71(2)	48(2)	52(2)	8(1)	-36(2)	-35(2)
C6	60(2)	40(2)	51(2)	-25(1)	14(1)	-28(1)
C7	37(1)	26(1)	23(1)	0(1)	-4(1)	-17(1)
C8	32(1)	21(1)	34(1)	3(1)	-11(1)	-14(1)
C9	31(1)	19(1)	45(1)	-3(1)	-9(1)	-10(1)
C10	28(1)	24(1)	40(1)	-14(1)	-5(1)	-6(1)
C11	29(1)	28(1)	24(1)	-5(1)	-4(1)	-15(1)
C12	27(1)	24(1)	26(1)	-2(1)	-8(1)	-12(1)
C13	24(1)	27(1)	36(1)	-7(1)	-6(1)	-11(1)
C14	28(1)	27(1)	34(1)	-2(1)	3(1)	-14(1)
K1	25(1)	24(1)	27(1)	-6(1)	-3(1)	-10(1)
O1	35(1)	31(1)	32(1)	-8(1)	-7(1)	-14(1)
C15	47(2)	31(1)	24(1)	-9(1)	1(1)	-18(1)
C16	41(1)	33(1)	28(1)	-10(1)	8(1)	-16(1)
O2	29(1)	34(1)	30(1)	-7(1)	1(1)	-13(1)
C17	26(1)	39(1)	45(2)	-12(1)	1(1)	-11(1)
C18	23(1)	34(1)	48(2)	-9(1)	-4(1)	-4(1)
O3	29(1)	27(1)	35(1)	-1(1)	-7(1)	-7(1)
C19	35(1)	41(1)	40(1)	6(1)	-16(1)	-12(1)
C20	43(2)	50(2)	30(1)	-4(1)	-12(1)	-20(1)
O4	31(1)	40(1)	28(1)	-8(1)	-2(1)	-14(1)
C21	43(2)	50(2)	27(1)	-10(1)	3(1)	-15(1)
C22	37(2)	47(2)	35(1)	-8(1)	9(1)	-16(1)
O5	26(1)	43(1)	37(1)	-5(1)	0(1)	-14(1)
C23	25(1)	45(2)	55(2)	-16(1)	2(1)	-10(1)
C24	24(1)	34(1)	59(2)	-12(1)	-9(1)	-3(1)

O6	32(1)	30(1)	40(1)	-4(1)	-9(1)	-7(1)
C25	37(2)	44(2)	47(2)	5(1)	-20(1)	-12(1)
C26	45(2)	55(2)	33(1)	-4(1)	-15(1)	-21(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04313.

	x	y	z	U(eq)
H1A	5610(30)	6360(30)	3303(17)	42
H1B	4610(30)	7780(30)	2749(16)	42
H4A	9920(30)	4450(20)	2882(16)	39
H4B	7890(30)	4920(20)	3374(16)	39
H5A	5672	6540	926	76
H5B	6827	7378	812	76
H5C	4963	7930	1304	76
H6A	9041	4357	1042	72
H6B	10520	4574	1380	72
H6C	9289	5715	810	72
H7A	9270(30)	7590(20)	1120(15)	32
H8A	6730(30)	9120(20)	1672(15)	33
H9A	8490(30)	9990(20)	2553(16)	37
H9B	6570(30)	10680(30)	2546(15)	37
H10A	7660(30)	9730(20)	3956(16)	37
H10B	6040(30)	9550(20)	3763(15)	37
H11A	7510(30)	7460(20)	4239(15)	30
H12A	10190(30)	6230(20)	3676(15)	29
H13A	12070(30)	7190(20)	3017(15)	33
H13B	10660(30)	8580(20)	3079(15)	33
H14A	11280(30)	8530(20)	1585(15)	35
H14B	11830(30)	7010(20)	1680(15)	35
H15A	9110	1438	-32	40
H15B	9051	556	859	40
H16A	11752	669	414	41
H16B	10933	2210	486	41
H17A	12525	2032	1696	44
H17B	13443	568	1427	44
H18A	12582	-209	2836	44
H18B	13733	599	2865	44

H19A	12386	999	4323	46
H19B	11204	244	4235	46
H20A	9955	1818	5274	47
H20B	9951	2937	4516	47
H21A	6965	3795	4902	49
H21B	7017	2575	5583	49
H22A	5400	2036	4750	49
H22B	4405	3444	5101	49
H23A	2797	4354	3954	51
H23B	3511	2917	3639	51
H24A	2618	4593	2493	49
H24B	4088	5054	2602	49
H25A	5314	4499	1159	51
H25B	3903	3963	1069	51
H26A	6062	1835	937	51
H26B	6256	2867	149	51

Table 6. Torsion angles [°] for 04313.

C7-Co1-C1-C2	55.54(19)	C5-C2-C3-Co1	118.7(2)
C12-Co1-C1-C2	-157.92(14)	C1-C2-C3-K1	75.9(2)
C11-Co1-C1-C2	177.94(14)	C5-C2-C3-K1	-108.6(2)
C8-Co1-C1-C2	89.48(15)	Co1-C2-C3-K1	132.71(11)
C3-Co1-C1-C2	-32.85(14)	C7-Co1-C3-C4	132.12(15)
C4-Co1-C1-C2	-73.60(15)	C12-Co1-C3-C4	40.56(18)
Co1-C1-C2-C3	54.79(17)	C11-Co1-C3-C4	-13.4(3)
Co1-C1-C2-C5	-120.8(2)	C8-Co1-C3-C4	169.63(15)
C7-Co1-C2-C1	-141.43(15)	C2-Co1-C3-C4	-127.7(2)
C12-Co1-C2-C1	88.7(4)	C1-Co1-C3-C4	-95.94(16)
C11-Co1-C2-C1	-3.3(2)	C7-Co1-C3-C2	-100.22(14)
C8-Co1-C2-C1	-99.12(16)	C12-Co1-C3-C2	168.21(13)
C3-Co1-C2-C1	128.9(2)	C11-Co1-C3-C2	114.2(2)
C4-Co1-C2-C1	96.36(16)	C8-Co1-C3-C2	-62.71(16)
C7-Co1-C2-C3	89.64(14)	C4-Co1-C3-C2	127.7(2)
C12-Co1-C2-C3	-40.2(4)	C1-Co1-C3-C2	31.72(14)
C11-Co1-C2-C3	-132.18(16)	C7-Co1-C3-C6	15.5(2)
C8-Co1-C2-C3	131.95(13)	C12-Co1-C3-C6	-76.0(2)
C4-Co1-C2-C3	-32.57(13)	C11-Co1-C3-C6	-130.0(2)
C1-Co1-C2-C3	-128.9(2)	C8-Co1-C3-C6	53.0(3)
C7-Co1-C2-C5	-24.8(2)	C2-Co1-C3-C6	115.8(3)
C12-Co1-C2-C5	-154.7(3)	C4-Co1-C3-C6	-116.6(3)
C11-Co1-C2-C5	113.4(2)	C1-Co1-C3-C6	147.5(3)
C8-Co1-C2-C5	17.5(2)	C7-Co1-C3-K1	156.45(13)
C3-Co1-C2-C5	-114.4(3)	C12-Co1-C3-K1	64.88(17)
C4-Co1-C2-C5	-147.0(2)	C11-Co1-C3-K1	10.9(3)
C1-Co1-C2-C5	116.7(3)	C8-Co1-C3-K1	-166.04(12)
C1-C2-C3-C4	0.0(3)	C2-Co1-C3-K1	-103.33(19)
C5-C2-C3-C4	175.6(2)	C4-Co1-C3-K1	24.32(14)
Co1-C2-C3-C4	56.83(17)	C1-Co1-C3-K1	-71.61(15)
C1-C2-C3-C6	-177.2(2)	C2-C3-C4-Co1	-55.36(16)
C5-C2-C3-C6	-1.6(3)	C6-C3-C4-Co1	121.8(2)
Co1-C2-C3-C6	-120.3(2)	K1-C3-C4-Co1	-162.11(9)
C1-C2-C3-Co1	-56.85(18)	C2-C3-C4-K1	106.75(17)

C6-C3-C4-K1	-76.1(2)	C1-Co1-C8-C7	-142.03(14)
Co1-C3-C4-K1	162.11(9)	C7-Co1-C8-C9	-118.1(2)
C7-Co1-C4-C3	-62.37(17)	C12-Co1-C8-C9	-41.26(18)
C12-Co1-C4-C3	-148.39(15)	C11-Co1-C8-C9	-0.89(17)
C11-Co1-C4-C3	172.83(14)	C3-Co1-C8-C9	177.56(15)
C8-Co1-C4-C3	-30.5(4)	C2-Co1-C8-C9	140.73(17)
C2-Co1-C4-C3	33.56(14)	C4-Co1-C8-C9	-159.0(3)
C1-Co1-C4-C3	74.05(15)	C1-Co1-C8-C9	99.90(18)
C7-Co1-C4-K1	-98.7(2)	C7-C8-C9-C10	-93.6(3)
C12-Co1-C4-K1	175.3(2)	Co1-C8-C9-C10	-15.1(3)
C11-Co1-C4-K1	136.5(2)	C7-C8-C9-K1#1	74.4(3)
C8-Co1-C4-K1	-66.8(5)	Co1-C8-C9-K1#1	152.85(17)
C3-Co1-C4-K1	-36.31(19)	C8-C9-C10-C11	28.7(3)
C2-Co1-C4-K1	-2.7(2)	K1#1-C9-C10-C11	-143.63(15)
C1-Co1-C4-K1	37.7(2)	C9-C10-C11-C12	48.9(3)
C12-Co1-C7-C8	-103.04(14)	C9-C10-C11-Co1	-29.3(2)
C11-Co1-C7-C8	-66.35(14)	C7-Co1-C11-C12	-64.40(14)
C3-Co1-C7-C8	130.84(13)	C8-Co1-C11-C12	-101.94(14)
C2-Co1-C7-C8	88.27(14)	C3-Co1-C11-C12	80.6(2)
C4-Co1-C7-C8	166.55(13)	C2-Co1-C11-C12	157.32(14)
C1-Co1-C7-C8	54.95(18)	C4-Co1-C11-C12	71.39(15)
C12-Co1-C7-C14	15.95(16)	C1-Co1-C11-C12	155.19(14)
C11-Co1-C7-C14	52.64(18)	C7-Co1-C11-C10	54.28(18)
C8-Co1-C7-C14	119.0(2)	C12-Co1-C11-C10	118.7(2)
C3-Co1-C7-C14	-110.17(16)	C8-Co1-C11-C10	16.75(17)
C2-Co1-C7-C14	-152.74(16)	C3-Co1-C11-C10	-160.73(18)
C4-Co1-C7-C14	-74.46(19)	C2-Co1-C11-C10	-84.0(2)
C1-Co1-C7-C14	173.94(15)	C4-Co1-C11-C10	-169.92(16)
C14-C7-C8-C9	-0.3(3)	C1-Co1-C11-C10	-86.13(18)
Co1-C7-C8-C9	103.7(2)	C10-C11-C12-C13	3.5(3)
C14-C7-C8-Co1	-104.0(2)	Co1-C11-C12-C13	105.6(2)
C12-Co1-C8-C7	76.81(14)	C10-C11-C12-Co1	-102.1(2)
C11-Co1-C8-C7	117.19(14)	C7-Co1-C12-C11	118.71(14)
C3-Co1-C8-C7	-64.36(16)	C8-Co1-C12-C11	78.28(14)
C2-Co1-C8-C7	-101.20(14)	C3-Co1-C12-C11	-141.67(13)
C4-Co1-C8-C7	-40.9(4)	C2-Co1-C12-C11	-109.4(4)

C4-Co1-C12-C11	-116.74(14)	Co1-C3-K1-O4	-11.40(16)
C1-Co1-C12-C11	-37.42(19)	C4-C3-K1-O1	-165.88(15)
C7-Co1-C12-C13	-0.49(16)	C2-C3-K1-O1	84.61(15)
C11-Co1-C12-C13	-119.2(2)	C6-C3-K1-O1	-41.58(16)
C8-Co1-C12-C13	-40.92(17)	Co1-C3-K1-O1	169.08(15)
C3-Co1-C12-C13	99.12(17)	C4-C3-K1-O2	-106.72(15)
C2-Co1-C12-C13	131.4(3)	C2-C3-K1-O2	143.76(15)
C4-Co1-C12-C13	124.05(17)	C6-C3-K1-O2	17.57(16)
C1-Co1-C12-C13	-156.62(15)	Co1-C3-K1-O2	-131.77(14)
C11-C12-C13-C14	-95.3(2)	C4-C3-K1-O3	-47.12(15)
Co1-C12-C13-C14	-14.7(2)	C2-C3-K1-O3	-156.64(15)
C8-C7-C14-C13	51.7(3)	C6-C3-K1-O3	77.17(16)
Co1-C7-C14-C13	-28.0(2)	Co1-C3-K1-O3	-72.16(14)
C12-C13-C14-C7	27.2(3)	C4-C3-K1-O6	134.50(15)
C3-C4-K1-O5	-106.24(15)	C2-C3-K1-O6	24.99(15)
Co1-C4-K1-O5	-73.0(2)	C6-C3-K1-O6	-101.20(16)
C3-C4-K1-O4	-167.08(15)	Co1-C3-K1-O6	109.46(14)
Co1-C4-K1-O4	-133.8(2)	C2-C3-K1-C4	-109.5(2)
C3-C4-K1-O1	15.09(16)	C6-C3-K1-C4	124.3(2)
Co1-C4-K1-O1	48.3(3)	Co1-C3-K1-C4	-25.04(14)
C3-C4-K1-O2	78.35(15)	C4-C3-K1-C9#2	177.89(18)
Co1-C4-K1-O2	111.6(2)	C2-C3-K1-C9#2	68.4(2)
C3-C4-K1-O3	131.90(15)	C6-C3-K1-C9#2	-57.8(3)
Co1-C4-K1-O3	165.1(2)	Co1-C3-K1-C9#2	152.85(14)
C3-C4-K1-O6	-49.17(16)	O5-K1-O1-C26	-10.50(17)
Co1-C4-K1-O6	-15.9(3)	O4-K1-O1-C26	78.3(2)
Co1-C4-K1-C3	33.24(18)	O2-K1-O1-C26	154.78(17)
C3-C4-K1-C9#2	-170.8(8)	O3-K1-O1-C26	162.19(15)
Co1-C4-K1-C9#2	-137.6(7)	O6-K1-O1-C26	-8.62(15)
C4-C3-K1-O5	74.17(15)	C4-K1-O1-C26	-109.87(16)
C2-C3-K1-O5	-35.35(15)	C3-K1-O1-C26	-103.41(16)
C6-C3-K1-O5	-161.54(15)	C9#2-K1-O1-C26	70.63(16)
Co1-C3-K1-O5	49.12(15)	O5-K1-O1-C15	-144.21(13)
C4-C3-K1-O4	13.64(16)	O4-K1-O1-C15	-55.4(2)
C2-C3-K1-O4	-95.88(15)	O2-K1-O1-C15	21.07(13)
C6-C3-K1-O4	137.94(15)	O3-K1-O1-C15	28.48(15)

O6-K1-O1-C15	-142.33(15)	C3-K1-O3-C18	-105.70(15)
C4-K1-O1-C15	116.42(14)	C9#2-K1-O3-C18	59.51(16)
C3-K1-O1-C15	122.87(14)	O5-K1-O3-C19	21.06(16)
C9#2-K1-O1-C15	-63.08(14)	O4-K1-O3-C19	10.81(14)
C26-O1-C15-C16	171.44(19)	O1-K1-O3-C19	-151.61(14)
K1-O1-C15-C16	-52.4(2)	O2-K1-O3-C19	-144.11(16)
O1-C15-C16-O2	64.5(2)	O6-K1-O3-C19	-71.9(4)
C15-C16-O2-C17	-179.97(18)	C4-K1-O3-C19	100.93(16)
C15-C16-O2-K1	-44.8(2)	C3-K1-O3-C19	119.73(15)
O5-K1-O2-C16	108.9(2)	C9#2-K1-O3-C19	-75.06(15)
O4-K1-O2-C16	177.02(13)	C18-O3-C19-C20	-179.6(2)
O1-K1-O2-C16	13.52(13)	K1-O3-C19-C20	-42.4(2)
O3-K1-O2-C16	-158.93(15)	O3-C19-C20-O4	66.1(3)
O6-K1-O2-C16	29.79(15)	C19-C20-O4-C21	175.0(2)
C4-K1-O2-C16	-92.35(15)	C19-C20-O4-K1	-55.8(2)
C3-K1-O2-C16	-67.11(14)	O5-K1-O4-C21	-18.35(15)
C9#2-K1-O2-C16	92.17(14)	O1-K1-O4-C21	-116.0(2)
O5-K1-O2-C17	-116.7(2)	O2-K1-O4-C21	175.23(15)
O4-K1-O2-C17	-48.54(16)	O3-K1-O4-C21	151.53(16)
O1-K1-O2-C17	147.96(16)	O6-K1-O4-C21	-37.55(16)
O3-K1-O2-C17	-24.49(14)	C4-K1-O4-C21	71.73(16)
O6-K1-O2-C17	164.23(14)	C3-K1-O4-C21	65.87(16)
C4-K1-O2-C17	42.09(16)	C9#2-K1-O4-C21	-108.58(16)
C3-K1-O2-C17	67.33(15)	O5-K1-O4-C20	-146.27(16)
C9#2-K1-O2-C17	-133.39(15)	O1-K1-O4-C20	116.1(2)
C16-O2-C17-C18	-168.69(19)	O2-K1-O4-C20	47.31(16)
K1-O2-C17-C18	55.4(2)	O3-K1-O4-C20	23.61(14)
O2-C17-C18-O3	-62.5(2)	O6-K1-O4-C20	-165.48(14)
C17-C18-O3-C19	176.10(19)	C4-K1-O4-C20	-56.19(15)
C17-C18-O3-K1	40.1(2)	C3-K1-O4-C20	-62.05(15)
O5-K1-O3-C18	155.62(14)	C9#2-K1-O4-C20	123.50(15)
O4-K1-O3-C18	145.38(16)	C20-O4-C21-C22	178.0(2)
O1-K1-O3-C18	-17.04(16)	K1-O4-C21-C22	49.4(2)
O2-K1-O3-C18	-9.55(14)	O4-C21-C22-O5	-63.9(3)
O6-K1-O3-C18	62.6(4)	C21-C22-O5-C23	-171.7(2)
C4-K1-O3-C18	-124.51(16)	C21-C22-O5-K1	46.7(2)

O4-K1-O5-C22	-15.89(15)	O5-K1-O6-C25	151.76(16)
O1-K1-O5-C22	146.46(15)	O4-K1-O6-C25	171.06(14)
O2-K1-O5-C22	58.5(3)	O1-K1-O6-C25	-26.37(14)
O3-K1-O5-C22	-26.12(17)	O2-K1-O6-C25	-42.69(16)
O6-K1-O5-C22	144.59(17)	O3-K1-O6-C25	-110.6(4)
C4-K1-O5-C22	-100.98(16)	C4-K1-O6-C25	76.85(16)
C3-K1-O5-C22	-125.50(16)	C3-K1-O6-C25	57.81(15)
C9#2-K1-O5-C22	74.76(16)	C9#2-K1-O6-C25	-107.35(15)
O4-K1-O5-C23	-155.40(18)	O5-K1-O6-C24	29.22(14)
O1-K1-O5-C23	6.95(18)	O4-K1-O6-C24	48.51(15)
O2-K1-O5-C23	-81.0(3)	O1-K1-O6-C24	-148.91(15)
O3-K1-O5-C23	-165.63(16)	O2-K1-O6-C24	-165.24(14)
O6-K1-O5-C23	5.08(16)	O3-K1-O6-C24	126.9(3)
C4-K1-O5-C23	119.51(17)	C4-K1-O6-C24	-45.70(16)
C3-K1-O5-C23	94.99(17)	C3-K1-O6-C24	-64.74(15)
C9#2-K1-O5-C23	-64.75(17)	C9#2-K1-O6-C24	130.10(15)
C22-O5-C23-C24	-178.3(2)	C24-O6-C25-C26	178.1(2)
K1-O5-C23-C24	-37.5(2)	K1-O6-C25-C26	59.1(2)
O5-C23-C24-O6	68.0(3)	C15-O1-C26-C25	175.24(19)
C23-C24-O6-C25	178.3(2)	K1-O1-C26-C25	40.7(2)
C23-C24-O6-K1	-61.5(2)	O6-C25-C26-O1	-68.1(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 x,y-1,z

REFERENCE NUMBER: 05346 [15]

CRYSTAL STRUCTURE REPORT

$C_{30} H_{44} Co K N_2 O_6$

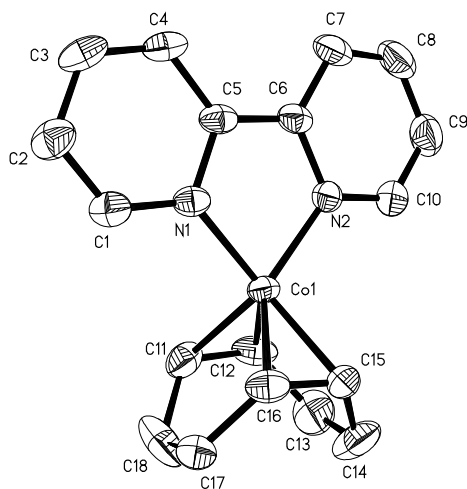
or

$[K(18\text{-crown-}6)][Co(1,5\text{-COD})(bipy)]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

December 07, 2005



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Data collection

A crystal (approximate dimensions 0.45 x 0.24 x 0.12 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Siemens SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 135 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 15 seconds and a detector distance of 4.91 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.77 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 3335 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ 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. The COD ligand ethylene hydrogen atoms were found from the difference map and refined with individual isotropic displacement parameters. All remaining 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 $R1 = 0.0473$ and $wR2 = 0.0873$ (F^2 , all data).

Structure description

The structure is the one suggested. All atoms lie on general positions. The axial positions of the potassium atom are coordinated by close contacts with COD ligands. The twist angle is 89.1 degrees: the anion is tetrahedral.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
 - ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
 - ³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
 - ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Casciarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
 - ⁵ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

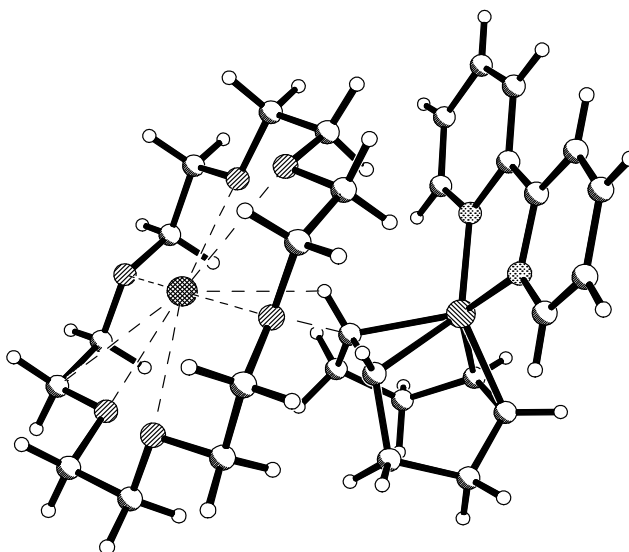
$$R_{\text{int}} = \Sigma |F_o|^2 - \langle F_o^2 \rangle / \Sigma |F_o|^2$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2(F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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



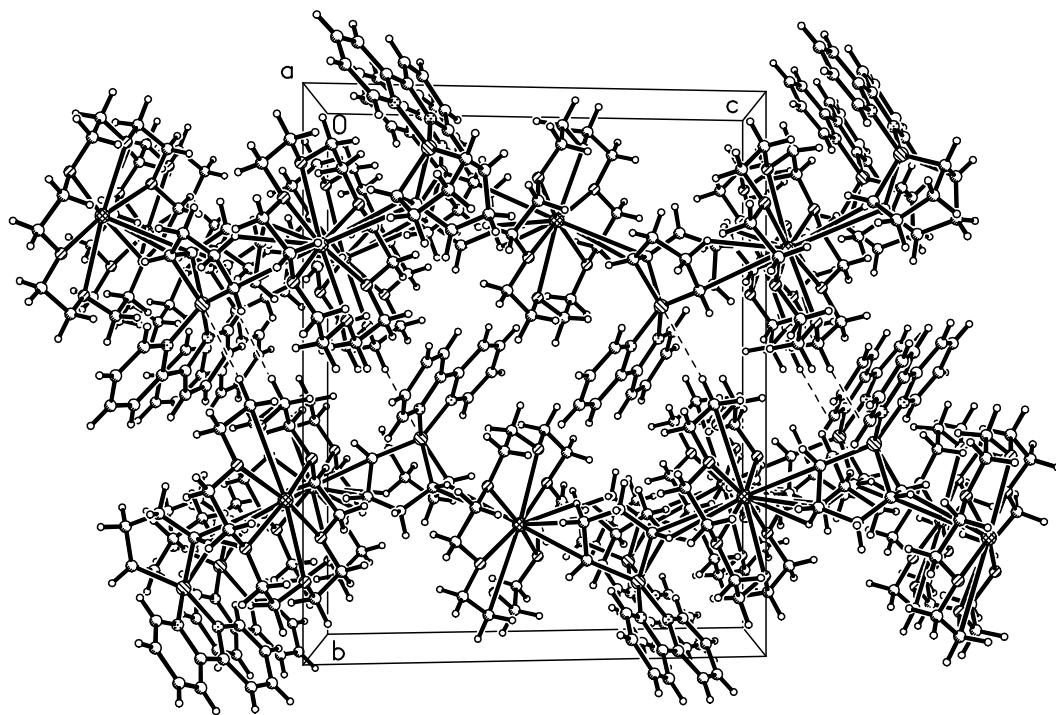
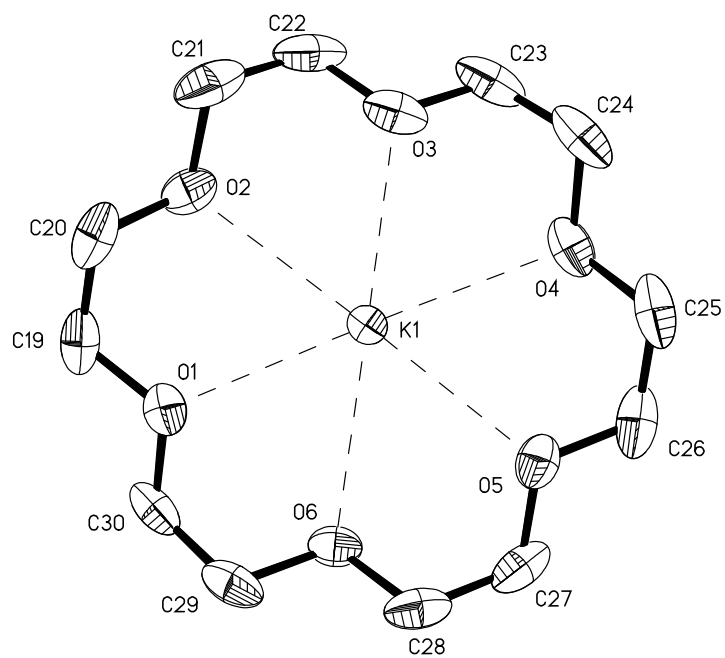


Table 1. Crystal data and structure refinement for 05346.

Identification code	05346	
Empirical formula	C ₃₀ H ₄₄ Co K N ₂ O ₆	
Formula weight	626.70	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	$a = 9.776(1)$ Å	$\alpha = 90^\circ$
	$b = 19.690(2)$ Å	$\beta = 99.094(2)^\circ$
	$c = 16.0969(16)$ Å	$\gamma = 90^\circ$
Volume	3059.7(5) Å ³	
Z	4	
Density (calculated)	1.360 Mg/m ³	
Absorption coefficient	0.741 mm ⁻¹	
$F(000)$	1328	
Crystal color, morphology	red-violet, plate	
Crystal size	0.45 x 0.24 x 0.12 mm ³	
Theta range for data collection	1.65 to 27.51°	
Index ranges	$-12 \leq h \leq 12$, $-25 \leq k \leq 25$, $-20 \leq l \leq 20$	
Reflections collected	32445	
Independent reflections	7011 [$R(\text{int}) = 0.0475$]	
Observed reflections	5339	
Completeness to $\theta = 27.51^\circ$	99.7%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9164 and 0.7316	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7011 / 0 / 377	
Goodness-of-fit on F^2	1.034	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0473$, $wR2 = 0.0805$	
R indices (all data)	$R1 = 0.0734$, $wR2 = 0.0873$	
Largest diff. peak and hole	0.353 and -0.344 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05346. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	3045(1)	1217(1)	2745(1)	25(1)
N1	3555(2)	499(1)	2049(1)	28(1)
C1	4717(2)	462(1)	1674(2)	35(1)
C2	4952(3)	-29(1)	1120(2)	42(1)
C3	3948(3)	-544(1)	909(2)	42(1)
C4	2792(3)	-539(1)	1279(2)	35(1)
C5	2584(2)	-21(1)	1856(1)	29(1)
C6	1396(2)	59(1)	2244(1)	29(1)
C7	226(3)	-373(1)	2144(2)	40(1)
C8	-905(3)	-216(2)	2499(2)	51(1)
C9	-884(3)	385(2)	2983(2)	50(1)
C10	269(3)	783(1)	3075(2)	39(1)
N2	1425(2)	651(1)	2730(1)	29(1)
C11	3454(3)	2051(1)	2106(2)	41(1)
C12	2236(3)	2133(1)	2447(2)	39(1)
C13	2128(3)	2563(2)	3191(2)	61(1)
C14	3002(3)	2319(2)	3978(2)	60(1)
C15	3553(3)	1604(1)	3899(2)	38(1)
C16	4747(2)	1469(1)	3534(2)	35(1)
C17	5591(3)	2009(2)	3198(2)	51(1)
C18	4796(3)	2401(2)	2490(2)	62(1)
K1	1029(1)	2808(1)	429(1)	33(1)
O1	3081(2)	2081(1)	-211(1)	39(1)
C19	4080(3)	2456(2)	-565(2)	48(1)
C20	4532(3)	3039(2)	1(2)	49(1)
O2	3398(2)	3484(1)	7(1)	43(1)
C21	3763(3)	4072(2)	513(2)	61(1)
C22	2492(4)	4472(1)	548(2)	60(1)
O3	1618(2)	4095(1)	1004(1)	49(1)
C23	425(4)	4458(1)	1131(2)	59(1)
C24	-331(3)	4071(2)	1704(2)	62(1)

O4	-859(2)	3454(1)	1304(1)	47(1)
C25	-1497(3)	3034(2)	1843(2)	56(1)
C26	-2012(3)	2399(2)	1387(2)	56(1)
O5	-891(2)	2045(1)	1134(1)	39(1)
C27	-1270(3)	1403(1)	760(2)	49(1)
C28	-4(3)	1043(1)	603(2)	47(1)
O6	630(2)	1396(1)	-7(1)	37(1)
C29	1861(3)	1057(1)	-152(2)	46(1)
C30	2616(3)	1493(1)	-682(2)	45(1)

Table 3. Bond lengths [Å] and angles [°] for 05346.

Co(1)-N(1)	1.9191(18)	C(13)-H(13A)	0.9900
Co(1)-N(2)	1.9337(18)	C(13)-H(13B)	0.9900
Co(1)-C(16)	1.989(2)	C(14)-C(15)	1.520(4)
Co(1)-C(15)	1.995(2)	C(14)-K(1)#1	3.477(3)
Co(1)-C(12)	1.996(2)	C(14)-H(14A)	0.9900
Co(1)-C(11)	2.011(3)	C(14)-H(14B)	0.9900
N(1)-C(1)	1.370(3)	C(15)-C(16)	1.413(4)
N(1)-C(5)	1.398(3)	C(15)-K(1)#1	3.374(2)
C(1)-C(2)	1.359(3)	C(15)-H(15)	0.91(3)
C(1)-H(1)	0.9500	C(16)-C(17)	1.498(4)
C(2)-C(3)	1.414(4)	C(16)-K(1)#1	3.420(2)
C(2)-H(2)	0.9500	C(16)-H(16)	0.96(3)
C(3)-C(4)	1.358(4)	C(17)-C(18)	1.489(4)
C(3)-H(3)	0.9500	C(17)-H(17A)	0.9900
C(4)-C(5)	1.415(3)	C(17)-H(17B)	0.9900
C(4)-H(4)	0.9500	C(18)-H(18A)	0.9900
C(5)-C(6)	1.412(3)	C(18)-H(18B)	0.9900
C(6)-N(2)	1.402(3)	K(1)-O(3)	2.7281(18)
C(6)-C(7)	1.413(3)	K(1)-O(5)	2.7823(17)
C(7)-C(8)	1.357(4)	K(1)-O(1)	2.7902(17)
C(7)-H(7)	0.9500	K(1)-O(4)	2.7993(18)
C(8)-C(9)	1.414(4)	K(1)-O(2)	2.8454(18)
C(8)-H(8)	0.9500	K(1)-O(6)	2.8780(16)
C(9)-C(10)	1.362(4)	K(1)-C(15)#2	3.374(2)
C(9)-H(9)	0.9500	K(1)-C(16)#2	3.420(2)
C(10)-N(2)	1.361(3)	K(1)-C(14)#2	3.477(3)
C(10)-H(10)	0.9500	K(1)-C(23)	3.522(3)
C(11)-C(12)	1.397(4)	K(1)-H(12)	3.03(3)
C(11)-C(18)	1.524(4)	O(1)-C(19)	1.415(3)
C(11)-H(11)	0.88(3)	O(1)-C(30)	1.419(3)
C(12)-C(13)	1.485(4)	C(19)-C(20)	1.489(4)
C(12)-K(1)	3.535(3)	C(19)-H(19A)	0.9900
C(12)-H(12)	0.91(3)	C(19)-H(19B)	0.9900
C(13)-C(14)	1.491(4)	C(20)-O(2)	1.414(3)

C(20)-H(20A)	0.9900	N(1)-Co(1)-N(2)	81.68(8)
C(20)-H(20B)	0.9900	N(1)-Co(1)-C(16)	106.74(9)
O(2)-C(21)	1.427(3)	N(2)-Co(1)-C(16)	138.82(9)
C(21)-C(22)	1.481(4)	N(1)-Co(1)-C(15)	140.82(10)
C(21)-H(21A)	0.9900	N(2)-Co(1)-C(15)	108.34(9)
C(21)-H(21B)	0.9900	C(16)-Co(1)-C(15)	41.53(10)
C(22)-O(3)	1.421(3)	N(1)-Co(1)-C(12)	130.90(10)
C(22)-H(22A)	0.9900	N(2)-Co(1)-C(12)	103.00(9)
C(22)-H(22B)	0.9900	C(16)-Co(1)-C(12)	100.83(10)
O(3)-C(23)	1.411(3)	C(15)-Co(1)-C(12)	84.86(11)
C(23)-C(24)	1.481(4)	N(1)-Co(1)-C(11)	102.22(10)
C(23)-H(23A)	0.9900	N(2)-Co(1)-C(11)	133.84(10)
C(23)-H(23B)	0.9900	C(16)-Co(1)-C(11)	84.79(11)
C(24)-O(4)	1.432(3)	C(15)-Co(1)-C(11)	97.16(11)
C(24)-H(24A)	0.9900	C(12)-Co(1)-C(11)	40.81(11)
C(24)-H(24B)	0.9900	C(1)-N(1)-C(5)	116.38(19)
O(4)-C(25)	1.414(3)	C(1)-N(1)-Co(1)	127.35(15)
C(25)-C(26)	1.497(4)	C(5)-N(1)-Co(1)	116.10(15)
C(25)-H(25A)	0.9900	C(2)-C(1)-N(1)	124.4(2)
C(25)-H(25B)	0.9900	C(2)-C(1)-H(1)	117.8
C(26)-O(5)	1.412(3)	N(1)-C(1)-H(1)	117.8
C(26)-H(26A)	0.9900	C(1)-C(2)-C(3)	119.0(2)
C(26)-H(26B)	0.9900	C(1)-C(2)-H(2)	120.5
O(5)-C(27)	1.423(3)	C(3)-C(2)-H(2)	120.5
C(27)-C(28)	1.482(4)	C(4)-C(3)-C(2)	118.9(2)
C(27)-H(27A)	0.9900	C(4)-C(3)-H(3)	120.6
C(27)-H(27B)	0.9900	C(2)-C(3)-H(3)	120.6
C(28)-O(6)	1.423(3)	C(3)-C(4)-C(5)	120.6(2)
C(28)-H(28A)	0.9900	C(3)-C(4)-H(4)	119.7
C(28)-H(28B)	0.9900	C(5)-C(4)-H(4)	119.7
O(6)-C(29)	1.428(3)	N(1)-C(5)-C(6)	113.39(19)
C(29)-C(30)	1.487(4)	N(1)-C(5)-C(4)	120.7(2)
C(29)-H(29A)	0.9900	C(6)-C(5)-C(4)	125.8(2)
C(29)-H(29B)	0.9900	N(2)-C(6)-C(5)	113.19(19)
C(30)-H(30A)	0.9900	N(2)-C(6)-C(7)	120.5(2)
C(30)-H(30B)	0.9900	C(5)-C(6)-C(7)	126.2(2)

C(8)-C(7)-C(6)	120.9(2)	H(13A)-C(13)-H(13B)	107.7
C(8)-C(7)-H(7)	119.5	C(13)-C(14)-C(15)	113.0(2)
C(6)-C(7)-H(7)	119.5	C(13)-C(14)-K(1)#1	155.0(2)
C(7)-C(8)-C(9)	118.7(2)	C(15)-C(14)-K(1)#1	73.42(14)
C(7)-C(8)-H(8)	120.7	C(13)-C(14)-H(14A)	109.0
C(9)-C(8)-H(8)	120.7	C(15)-C(14)-H(14A)	109.0
C(10)-C(9)-C(8)	118.7(3)	K(1)#1-C(14)-H(14A)	90.3
C(10)-C(9)-H(9)	120.6	C(13)-C(14)-H(14B)	109.0
C(8)-C(9)-H(9)	120.6	C(15)-C(14)-H(14B)	109.0
N(2)-C(10)-C(9)	124.9(3)	K(1)#1-C(14)-H(14B)	48.1
N(2)-C(10)-H(10)	117.6	H(14A)-C(14)-H(14B)	107.8
C(9)-C(10)-H(10)	117.6	C(16)-C(15)-C(14)	122.4(2)
C(10)-N(2)-C(6)	116.2(2)	C(16)-C(15)-Co(1)	69.01(14)
C(10)-N(2)-Co(1)	128.02(16)	C(14)-C(15)-Co(1)	113.08(19)
C(6)-N(2)-Co(1)	115.57(15)	C(16)-C(15)-K(1)#1	79.82(14)
C(12)-C(11)-C(18)	121.4(3)	C(14)-C(15)-K(1)#1	81.00(14)
C(12)-C(11)-Co(1)	69.04(15)	Co(1)-C(15)-K(1)#1	148.69(12)
C(18)-C(11)-Co(1)	112.94(19)	C(16)-C(15)-H(15)	117.1(18)
C(12)-C(11)-H(11)	116(2)	C(14)-C(15)-H(15)	114.6(18)
C(18)-C(11)-H(11)	118(2)	Co(1)-C(15)-H(15)	111.3(18)
Co(1)-C(11)-H(11)	108(2)	K(1)#1-C(15)-H(15)	85.0(18)
C(11)-C(12)-C(13)	123.8(2)	C(15)-C(16)-C(17)	123.8(2)
C(11)-C(12)-Co(1)	70.15(14)	C(15)-C(16)-Co(1)	69.47(13)
C(13)-C(12)-Co(1)	113.40(19)	C(17)-C(16)-Co(1)	113.54(18)
C(11)-C(12)-K(1)	82.18(16)	C(15)-C(16)-K(1)#1	76.20(14)
C(13)-C(12)-K(1)	118.08(17)	C(17)-C(16)-K(1)#1	83.20(14)
Co(1)-C(12)-K(1)	128.51(11)	Co(1)-C(16)-K(1)#1	145.55(11)
C(11)-C(12)-H(12)	117.1(18)	C(15)-C(16)-H(16)	116.4(16)
C(13)-C(12)-H(12)	114.7(18)	C(17)-C(16)-H(16)	113.9(16)
Co(1)-C(12)-H(12)	107.0(18)	Co(1)-C(16)-H(16)	110.8(16)
K(1)-C(12)-H(12)	49.6(17)	K(1)#1-C(16)-H(16)	86.7(16)
C(12)-C(13)-C(14)	113.4(2)	C(18)-C(17)-C(16)	113.2(2)
C(12)-C(13)-H(13A)	108.9	C(18)-C(17)-H(17A)	108.9
C(14)-C(13)-H(13A)	108.9	C(16)-C(17)-H(17A)	108.9
C(12)-C(13)-H(13B)	108.9	C(18)-C(17)-H(17B)	108.9
C(14)-C(13)-H(13B)	108.9	C(16)-C(17)-H(17B)	108.9

H(17A)-C(17)-H(17B)	107.8	O(5)-K(1)-C(14)#2	71.20(6)
C(17)-C(18)-C(11)	112.8(2)	O(1)-K(1)-C(14)#2	107.51(7)
C(17)-C(18)-H(18A)	109.0	O(4)-K(1)-C(14)#2	79.15(7)
C(11)-C(18)-H(18A)	109.0	O(2)-K(1)-C(14)#2	120.78(6)
C(17)-C(18)-H(18B)	109.0	O(6)-K(1)-C(14)#2	72.48(6)
C(11)-C(18)-H(18B)	109.0	C(15)#2-K(1)-C(14)#2	25.58(7)
H(18A)-C(18)-H(18B)	107.8	C(16)#2-K(1)-C(14)#2	43.75(6)
O(3)-K(1)-O(5)	118.86(6)	O(3)-K(1)-C(23)	21.70(7)
O(3)-K(1)-O(1)	118.43(6)	O(5)-K(1)-C(23)	102.05(7)
O(5)-K(1)-O(1)	116.40(5)	O(1)-K(1)-C(23)	139.34(7)
O(3)-K(1)-O(4)	61.76(6)	O(4)-K(1)-C(23)	42.35(7)
O(5)-K(1)-O(4)	59.95(6)	O(2)-K(1)-C(23)	80.14(7)
O(1)-K(1)-O(4)	171.41(6)	O(6)-K(1)-C(23)	161.13(7)
O(3)-K(1)-O(2)	60.66(6)	C(15)#2-K(1)-C(23)	77.28(7)
O(5)-K(1)-O(2)	167.73(5)	C(16)#2-K(1)-C(23)	81.12(7)
O(1)-K(1)-O(2)	59.48(5)	C(14)#2-K(1)-C(23)	96.52(8)
O(4)-K(1)-O(2)	122.22(6)	O(3)-K(1)-C(12)	90.88(6)
O(3)-K(1)-O(6)	173.22(5)	O(5)-K(1)-C(12)	64.60(5)
O(5)-K(1)-O(6)	60.24(5)	O(1)-K(1)-C(12)	89.50(6)
O(1)-K(1)-O(6)	59.52(5)	O(4)-K(1)-C(12)	81.92(6)
O(4)-K(1)-O(6)	119.15(6)	O(2)-K(1)-C(12)	103.26(6)
O(2)-K(1)-O(6)	118.58(5)	O(6)-K(1)-C(12)	82.72(5)
O(3)-K(1)-C(15)#2	90.99(6)	C(15)#2-K(1)-C(12)	153.70(7)
O(5)-K(1)-C(15)#2	91.75(6)	C(16)#2-K(1)-C(12)	176.50(6)
O(1)-K(1)-C(15)#2	112.44(6)	C(14)#2-K(1)-C(12)	135.66(6)
O(4)-K(1)-C(15)#2	75.94(6)	C(23)-K(1)-C(12)	95.77(7)
O(2)-K(1)-C(15)#2	100.49(6)	O(3)-K(1)-H(12)	99.0(5)
O(6)-K(1)-C(15)#2	95.74(6)	O(5)-K(1)-H(12)	51.5(5)
O(3)-K(1)-C(16)#2	86.79(6)	O(1)-K(1)-H(12)	94.7(5)
O(5)-K(1)-C(16)#2	114.38(6)	O(4)-K(1)-H(12)	77.0(5)
O(1)-K(1)-C(16)#2	93.90(6)	O(2)-K(1)-H(12)	116.3(5)
O(4)-K(1)-C(16)#2	94.68(6)	O(6)-K(1)-H(12)	75.1(5)
O(2)-K(1)-C(16)#2	77.85(6)	C(15)#2-K(1)-H(12)	142.1(5)
O(6)-K(1)-C(16)#2	99.71(6)	C(16)#2-K(1)-H(12)	165.8(5)
C(15)#2-K(1)-C(16)#2	23.99(6)	C(14)#2-K(1)-H(12)	122.4(5)
O(3)-K(1)-C(14)#2	113.96(7)	C(23)-K(1)-H(12)	99.5(5)

C(12)-K(1)-H(12)	13.2(5)	C(24)-C(23)-K(1)	81.38(16)
C(19)-O(1)-C(30)	113.2(2)	O(3)-C(23)-H(23A)	109.8
C(19)-O(1)-K(1)	117.62(15)	C(24)-C(23)-H(23A)	109.8
C(30)-O(1)-K(1)	115.27(14)	K(1)-C(23)-H(23A)	87.4
O(1)-C(19)-C(20)	108.2(2)	O(3)-C(23)-H(23B)	109.8
O(1)-C(19)-H(19A)	110.1	C(24)-C(23)-H(23B)	109.8
C(20)-C(19)-H(19A)	110.1	K(1)-C(23)-H(23B)	155.1
O(1)-C(19)-H(19B)	110.1	H(23A)-C(23)-H(23B)	108.2
C(20)-C(19)-H(19B)	110.1	O(4)-C(24)-C(23)	109.7(2)
H(19A)-C(19)-H(19B)	108.4	O(4)-C(24)-H(24A)	109.7
O(2)-C(20)-C(19)	109.0(2)	C(23)-C(24)-H(24A)	109.7
O(2)-C(20)-H(20A)	109.9	O(4)-C(24)-H(24B)	109.7
C(19)-C(20)-H(20A)	109.9	C(23)-C(24)-H(24B)	109.7
O(2)-C(20)-H(20B)	109.9	H(24A)-C(24)-H(24B)	108.2
C(19)-C(20)-H(20B)	109.9	C(25)-O(4)-C(24)	112.5(2)
H(20A)-C(20)-H(20B)	108.3	C(25)-O(4)-K(1)	115.63(16)
C(20)-O(2)-C(21)	112.3(2)	C(24)-O(4)-K(1)	113.13(16)
C(20)-O(2)-K(1)	112.33(14)	O(4)-C(25)-C(26)	109.6(2)
C(21)-O(2)-K(1)	112.51(16)	O(4)-C(25)-H(25A)	109.8
O(2)-C(21)-C(22)	108.5(2)	C(26)-C(25)-H(25A)	109.8
O(2)-C(21)-H(21A)	110.0	O(4)-C(25)-H(25B)	109.8
C(22)-C(21)-H(21A)	110.0	C(26)-C(25)-H(25B)	109.8
O(2)-C(21)-H(21B)	110.0	H(25A)-C(25)-H(25B)	108.2
C(22)-C(21)-H(21B)	110.0	O(5)-C(26)-C(25)	109.7(2)
H(21A)-C(21)-H(21B)	108.4	O(5)-C(26)-H(26A)	109.7
O(3)-C(22)-C(21)	108.5(2)	C(25)-C(26)-H(26A)	109.7
O(3)-C(22)-H(22A)	110.0	O(5)-C(26)-H(26B)	109.7
C(21)-C(22)-H(22A)	110.0	C(25)-C(26)-H(26B)	109.7
O(3)-C(22)-H(22B)	110.0	H(26A)-C(26)-H(26B)	108.2
C(21)-C(22)-H(22B)	110.0	C(26)-O(5)-C(27)	113.4(2)
H(22A)-C(22)-H(22B)	108.4	C(26)-O(5)-K(1)	117.13(16)
C(23)-O(3)-C(22)	112.8(2)	C(27)-O(5)-K(1)	117.03(14)
C(23)-O(3)-K(1)	112.69(16)	O(5)-C(27)-C(28)	109.2(2)
C(22)-O(3)-K(1)	114.99(15)	O(5)-C(27)-H(27A)	109.8
O(3)-C(23)-C(24)	109.5(2)	C(28)-C(27)-H(27A)	109.8
O(3)-C(23)-K(1)	45.61(12)	O(5)-C(27)-H(27B)	109.8

C(28)-C(27)-H(27B)	109.8	O(6)-C(29)-H(29A)	109.8
H(27A)-C(27)-H(27B)	108.3	C(30)-C(29)-H(29A)	109.8
O(6)-C(28)-C(27)	110.5(2)	O(6)-C(29)-H(29B)	109.8
O(6)-C(28)-H(28A)	109.6	C(30)-C(29)-H(29B)	109.8
C(27)-C(28)-H(28A)	109.6	H(29A)-C(29)-H(29B)	108.3
O(6)-C(28)-H(28B)	109.6	O(1)-C(30)-C(29)	108.1(2)
C(27)-C(28)-H(28B)	109.6	O(1)-C(30)-H(30A)	110.1
H(28A)-C(28)-H(28B)	108.1	C(29)-C(30)-H(30A)	110.1
C(28)-O(6)-C(29)	110.79(19)	O(1)-C(30)-H(30B)	110.1
C(28)-O(6)-K(1)	111.19(14)	C(29)-C(30)-H(30B)	110.1
C(29)-O(6)-K(1)	113.98(14)	H(30A)-C(30)-H(30B)	108.4
O(6)-C(29)-C(30)	109.4(2)		

Symmetry transformations used to generate equivalent atoms:

#1 $x+1/2, -y+1/2, z+1/2$ #2 $x-1/2, -y+1/2, z-1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05346. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	28(1)	22(1)	24(1)	-2(1)	0(1)	-2(1)
N1	30(1)	22(1)	31(1)	0(1)	-1(1)	2(1)
C1	33(1)	31(1)	41(2)	-4(1)	1(1)	1(1)
C2	36(1)	39(1)	50(2)	-9(1)	5(1)	10(1)
C3	49(2)	30(1)	44(2)	-12(1)	-3(1)	13(1)
C4	42(1)	22(1)	36(1)	-5(1)	-7(1)	3(1)
C5	37(1)	20(1)	28(1)	3(1)	-4(1)	0(1)
C6	38(1)	24(1)	24(1)	6(1)	-4(1)	-4(1)
C7	49(2)	32(1)	37(2)	5(1)	-2(1)	-15(1)
C8	48(2)	52(2)	52(2)	7(1)	9(1)	-22(1)
C9	43(2)	65(2)	45(2)	1(1)	16(1)	-12(1)
C10	44(2)	43(2)	33(1)	-2(1)	10(1)	-6(1)
N2	34(1)	30(1)	23(1)	2(1)	3(1)	-4(1)
C11	69(2)	27(1)	27(1)	2(1)	9(1)	3(1)
C12	31(1)	27(1)	53(2)	0(1)	-12(1)	0(1)
C13	72(2)	42(2)	78(2)	-7(2)	36(2)	10(2)
C14	41(2)	80(2)	58(2)	-42(2)	8(1)	-2(2)
C15	46(2)	46(2)	22(1)	-4(1)	3(1)	-16(1)
C16	31(1)	32(1)	38(1)	-4(1)	-6(1)	-1(1)
C17	49(2)	63(2)	44(2)	-17(1)	12(1)	-28(1)
C18	45(2)	40(2)	107(3)	21(2)	35(2)	-1(1)
K1	35(1)	27(1)	39(1)	-5(1)	13(1)	-2(1)
O1	36(1)	44(1)	36(1)	-3(1)	9(1)	5(1)
C19	31(1)	70(2)	47(2)	9(2)	14(1)	10(1)
C20	27(1)	72(2)	48(2)	17(2)	6(1)	-5(1)
O2	40(1)	43(1)	44(1)	1(1)	-3(1)	-11(1)
C21	66(2)	57(2)	56(2)	-3(2)	-2(2)	-33(2)
C22	90(2)	31(2)	55(2)	-6(1)	2(2)	-20(2)
O3	69(1)	30(1)	46(1)	-6(1)	0(1)	4(1)
C23	91(2)	35(2)	49(2)	-12(1)	-1(2)	18(2)
C24	77(2)	61(2)	47(2)	-24(2)	8(2)	24(2)

O4	51(1)	59(1)	32(1)	-9(1)	9(1)	14(1)
C25	47(2)	88(2)	38(2)	-6(2)	17(1)	17(2)
C26	34(2)	94(2)	41(2)	4(2)	13(1)	0(2)
O5	30(1)	52(1)	35(1)	1(1)	5(1)	-5(1)
C27	54(2)	53(2)	37(2)	8(1)	2(1)	-27(1)
C28	68(2)	30(1)	39(2)	7(1)	-4(1)	-11(1)
O6	45(1)	27(1)	36(1)	5(1)	-2(1)	2(1)
C29	53(2)	32(1)	49(2)	-5(1)	-9(1)	15(1)
C30	47(2)	42(2)	45(2)	-11(1)	2(1)	20(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05346.

	x	y	z	U(eq)
H1	5404	802	1809	42
H2	5777	-27	878	50
H3	4081	-888	516	50
H4	2117	-885	1148	42
H7	231	-778	1825	48
H8	-1695	-504	2423	61
H9	-1660	508	3239	60
H10	266	1183	3405	47
H11	3350(30)	1944(16)	1570(20)	70(10)
H12	1420(30)	2065(14)	2096(17)	54(8)
H13A	1148	2575	3279	74
H13B	2406	3033	3075	74
H14A	2447	2329	4441	72
H14B	3793	2633	4127	72
H15	3360(30)	1310(14)	4295(18)	57(9)
H16	5270(30)	1072(14)	3732(17)	53(8)
H17A	5945	2326	3659	62
H17B	6399	1794	3002	62
H18A	5382	2466	2048	74
H18B	4576	2855	2696	74
H19A	3675	2623	-1131	58
H19B	4884	2164	-623	58
H20A	4863	2873	578	59
H20B	5302	3283	-200	59
H21A	4443	4349	267	73
H21B	4189	3934	1087	73
H22A	2735	4912	830	72
H22B	2007	4564	-29	72
H23A	-183	4530	585	71
H23B	695	4908	1379	71

H24A	302	3964	2231	74
H24B	-1105	4348	1848	74
H25A	-2280	3278	2029	68
H25B	-821	2917	2348	68
H26A	-2474	2107	1760	67
H26B	-2699	2515	887	67
H27A	-1906	1468	223	58
H27B	-1755	1130	1140	58
H28A	657	1007	1135	56
H28B	-249	577	401	56
H29A	1618	618	-440	55
H29B	2459	962	391	55
H30A	3415	1243	-840	54
H30B	1993	1624	-1204	54

Table 6. Torsion angles [°] for 05346.

N2-Co1-N1-C1	177.4(2)	C5-C6-N2-Co1	0.7(2)
C16-Co1-N1-C1	-44.0(2)	C7-C6-N2-Co1	-176.09(17)
C15-Co1-N1-C1	-73.7(2)	N1-Co1-N2-C10	-175.9(2)
C12-Co1-N1-C1	77.4(2)	C16-Co1-N2-C10	78.1(2)
C11-Co1-N1-C1	44.2(2)	C15-Co1-N2-C10	43.1(2)
N2-Co1-N1-C5	2.40(15)	C12-Co1-N2-C10	-45.8(2)
C16-Co1-N1-C5	141.02(16)	C11-Co1-N2-C10	-77.0(2)
C15-Co1-N1-C5	111.30(19)	N1-Co1-N2-C6	-1.66(15)
C12-Co1-N1-C5	-97.64(18)	C16-Co1-N2-C6	-107.62(18)
C11-Co1-N1-C5	-130.81(17)	C15-Co1-N2-C6	-142.63(16)
C5-N1-C1-C2	1.9(3)	C12-Co1-N2-C6	128.54(16)
Co1-N1-C1-C2	-173.13(19)	C11-Co1-N2-C6	97.33(19)
N1-C1-C2-C3	-0.3(4)	N1-Co1-C11-C12	140.74(15)
C1-C2-C3-C4	-1.2(4)	N2-Co1-C11-C12	50.6(2)
C2-C3-C4-C5	0.9(4)	C16-Co1-C11-C12	-113.24(17)
C1-N1-C5-C6	-178.27(19)	C15-Co1-C11-C12	-73.51(17)
Co1-N1-C5-C6	-2.7(2)	N1-Co1-C11-C18	-102.9(2)
C1-N1-C5-C4	-2.1(3)	N2-Co1-C11-C18	166.92(17)
Co1-N1-C5-C4	173.49(16)	C16-Co1-C11-C18	3.1(2)
C3-C4-C5-N1	0.8(3)	C15-Co1-C11-C18	42.8(2)
C3-C4-C5-C6	176.4(2)	C12-Co1-C11-C18	116.3(3)
N1-C5-C6-N2	1.3(3)	C18-C11-C12-C13	0.7(4)
C4-C5-C6-N2	-174.7(2)	Co1-C11-C12-C13	105.4(3)
N1-C5-C6-C7	177.8(2)	C18-C11-C12-Co1	-104.8(2)
C4-C5-C6-C7	1.9(4)	C18-C11-C12-K1	119.3(2)
N2-C6-C7-C8	1.5(4)	Co1-C11-C12-K1	-135.87(8)
C5-C6-C7-C8	-174.8(2)	N1-Co1-C12-C11	-54.9(2)
C6-C7-C8-C9	-1.0(4)	N2-Co1-C12-C11	-145.13(16)
C7-C8-C9-C10	0.0(4)	C16-Co1-C12-C11	68.70(17)
C8-C9-C10-N2	0.4(4)	C15-Co1-C12-C11	107.21(17)
C9-C10-N2-C6	0.2(4)	N1-Co1-C12-C13	-174.19(18)
C9-C10-N2-Co1	174.4(2)	N2-Co1-C12-C13	95.6(2)
C5-C6-N2-C10	175.6(2)	C16-Co1-C12-C13	-50.6(2)
C7-C6-N2-C10	-1.1(3)	C15-Co1-C12-C13	-12.1(2)

C11-Co1-C12-C13	-119.3(3)	Co1-C15-C16-K1#1	177.11(9)
N1-Co1-C12-K1	6.90(19)	N1-Co1-C16-C15	-151.81(15)
N2-Co1-C12-K1	-83.30(13)	N2-Co1-C16-C15	-55.2(2)
C16-Co1-C12-K1	130.53(13)	C12-Co1-C16-C15	69.28(17)
C15-Co1-C12-K1	169.03(14)	C11-Co1-C16-C15	106.97(17)
C11-Co1-C12-K1	61.82(17)	N1-Co1-C16-C17	89.2(2)
C11-C12-C13-C14	-64.0(4)	N2-Co1-C16-C17	-174.21(17)
Co1-C12-C13-C14	17.1(3)	C15-Co1-C16-C17	-119.0(3)
K1-C12-C13-C14	-163.9(2)	C12-Co1-C16-C17	-49.7(2)
C12-C13-C14-C15	-13.2(4)	C11-Co1-C16-C17	-12.0(2)
C12-C13-C14-K1#1	87.0(5)	N1-Co1-C16-K1#1	-156.78(18)
C13-C14-C15-C16	82.5(3)	N2-Co1-C16-K1#1	-60.2(3)
K1#1-C14-C15-C16	-71.8(2)	C15-Co1-C16-K1#1	-4.97(16)
C13-C14-C15-Co1	3.5(3)	C12-Co1-C16-K1#1	64.3(2)
K1#1-C14-C15-Co1	-150.79(16)	C11-Co1-C16-K1#1	102.0(2)
C13-C14-C15-K1#1	154.3(3)	C15-C16-C17-C18	-61.6(3)
N1-Co1-C15-C16	45.7(2)	Co1-C16-C17-C18	18.7(3)
N2-Co1-C15-C16	145.26(15)	K1#1-C16-C17-C18	-130.0(2)
C12-Co1-C15-C16	-112.73(17)	C16-C17-C18-C11	-15.9(4)
C11-Co1-C15-C16	-73.74(17)	C12-C11-C18-C17	85.0(3)
N1-Co1-C15-C14	163.14(17)	Co1-C11-C18-C17	6.3(3)
N2-Co1-C15-C14	-97.3(2)	C11-C12-K1-O3	-95.53(15)
C16-Co1-C15-C14	117.4(3)	C13-C12-K1-O3	28.8(2)
C12-Co1-C15-C14	4.7(2)	Co1-C12-K1-O3	-152.35(14)
C11-Co1-C15-C14	43.7(2)	C11-C12-K1-O5	142.66(16)
N1-Co1-C15-K1#1	51.2(3)	C13-C12-K1-O5	-93.0(2)
N2-Co1-C15-K1#1	150.7(2)	Co1-C12-K1-O5	85.84(13)
C16-Co1-C15-K1#1	5.48(18)	C11-C12-K1-O1	22.89(15)
C12-Co1-C15-K1#1	-107.2(2)	C13-C12-K1-O1	147.2(2)
C11-Co1-C15-K1#1	-68.3(2)	Co1-C12-K1-O1	-33.93(14)
C14-C15-C16-C17	0.5(4)	C11-C12-K1-O4	-156.84(16)
Co1-C15-C16-C17	105.2(2)	C13-C12-K1-O4	-32.5(2)
K1#1-C15-C16-C17	-71.9(2)	Co1-C12-K1-O4	146.34(14)
C14-C15-C16-Co1	-104.7(2)	C11-C12-K1-O2	-35.52(16)
K1#1-C15-C16-Co1	-177.11(9)	C13-C12-K1-O2	88.8(2)
C14-C15-C16-K1#1	72.4(2)	Co1-C12-K1-O2	-92.34(13)

C11-C12-K1-O6	82.22(15)	K1-O1-C19-C20	44.0(2)
C13-C12-K1-O6	-153.5(2)	O1-C19-C20-O2	-65.5(3)
Co1-C12-K1-O6	25.40(13)	C19-C20-O2-C21	-177.8(2)
C11-C12-K1-C15#2	170.45(16)	C19-C20-O2-K1	54.2(2)
C13-C12-K1-C15#2	-65.2(3)	O3-K1-O2-C20	142.55(17)
Co1-C12-K1-C15#2	113.63(17)	O5-K1-O2-C20	51.4(3)
C11-C12-K1-C16#2	-143.6(10)	O1-K1-O2-C20	-22.29(15)
C13-C12-K1-C16#2	-19.3(11)	O4-K1-O2-C20	147.84(15)
Co1-C12-K1-C16#2	159.5(9)	O6-K1-O2-C20	-29.74(17)
C11-C12-K1-C14#2	137.82(16)	C15#2-K1-O2-C20	-132.26(16)
C13-C12-K1-C14#2	-97.9(2)	C16#2-K1-O2-C20	-124.28(17)
Co1-C12-K1-C14#2	81.00(17)	C14#2-K1-O2-C20	-115.47(17)
C11-C12-K1-C23	-116.72(16)	C23-K1-O2-C20	152.78(17)
C13-C12-K1-C23	7.6(2)	C12-K1-O2-C20	59.12(17)
Co1-C12-K1-C23	-173.53(14)	O3-K1-O2-C21	14.61(17)
O3-K1-O1-C19	-27.53(18)	O5-K1-O2-C21	-76.6(3)
O5-K1-O1-C19	-179.36(16)	O1-K1-O2-C21	-150.24(19)
O4-K1-O1-C19	-116.5(4)	O4-K1-O2-C21	19.90(19)
O2-K1-O1-C19	-12.52(16)	O6-K1-O2-C21	-157.69(17)
O6-K1-O1-C19	159.89(18)	C15#2-K1-O2-C21	99.80(18)
C15#2-K1-O1-C19	76.64(17)	C16#2-K1-O2-C21	107.77(18)
C16#2-K1-O1-C19	60.92(17)	C14#2-K1-O2-C21	116.58(18)
C14#2-K1-O1-C19	103.39(17)	C23-K1-O2-C21	24.83(18)
C23-K1-O1-C19	-20.0(2)	C12-K1-O2-C21	-68.83(18)
C12-K1-O1-C19	-118.26(17)	C20-O2-C21-C22	-174.6(2)
O3-K1-O1-C30	-165.15(15)	K1-O2-C21-C22	-46.7(3)
O5-K1-O1-C30	43.03(17)	O2-C21-C22-O3	67.3(3)
O4-K1-O1-C30	105.9(4)	C21-C22-O3-C23	175.2(2)
O2-K1-O1-C30	-150.13(17)	C21-C22-O3-K1	-53.7(3)
O6-K1-O1-C30	22.28(15)	O5-K1-O3-C23	-42.26(19)
C15#2-K1-O1-C30	-60.97(17)	O1-K1-O3-C23	166.61(17)
C16#2-K1-O1-C30	-76.69(16)	O4-K1-O3-C23	-23.15(17)
C14#2-K1-O1-C30	-34.23(17)	O2-K1-O3-C23	151.78(19)
C23-K1-O1-C30	-157.60(16)	O6-K1-O3-C23	-122.7(5)
C12-K1-O1-C30	104.13(16)	C15#2-K1-O3-C23	50.29(18)
C30-O1-C19-C20	-177.5(2)	C16#2-K1-O3-C23	73.91(18)

C14#2-K1-O3-C23	38.66(19)	C23-C24-O4-C25	175.2(2)
C12-K1-O3-C23	-103.48(18)	C23-C24-O4-K1	41.9(3)
O5-K1-O3-C22	-173.44(18)	O3-K1-O4-C25	-142.48(18)
O1-K1-O3-C22	35.4(2)	O5-K1-O4-C25	18.17(16)
O4-K1-O3-C22	-154.3(2)	O1-K1-O4-C25	-48.9(5)
O2-K1-O3-C22	20.59(18)	O2-K1-O4-C25	-147.71(17)
O6-K1-O3-C22	106.1(5)	O6-K1-O4-C25	29.86(19)
C15#2-K1-O3-C22	-80.90(19)	C15#2-K1-O4-C25	118.62(18)
C16#2-K1-O3-C22	-57.27(19)	C16#2-K1-O4-C25	133.71(17)
C14#2-K1-O3-C22	-92.52(19)	C14#2-K1-O4-C25	92.61(18)
C23-K1-O3-C22	-131.2(3)	C23-K1-O4-C25	-154.9(2)
C12-K1-O3-C22	125.34(19)	C12-K1-O4-C25	-47.10(17)
C22-O3-C23-C24	-172.4(2)	O3-K1-O4-C24	-10.65(17)
K1-O3-C23-C24	55.3(3)	O5-K1-O4-C24	150.00(19)
C22-O3-C23-K1	132.3(2)	O1-K1-O4-C24	83.0(4)
O5-K1-C23-O3	142.97(17)	O2-K1-O4-C24	-15.88(19)
O1-K1-C23-O3	-18.2(2)	O6-K1-O4-C24	161.69(17)
O4-K1-C23-O3	149.1(2)	C15#2-K1-O4-C24	-109.55(18)
O2-K1-C23-O3	-24.74(17)	C16#2-K1-O4-C24	-94.47(18)
O6-K1-C23-O3	162.12(16)	C14#2-K1-O4-C24	-135.56(18)
C15#2-K1-C23-O3	-127.96(18)	C23-K1-O4-C24	-23.11(17)
C16#2-K1-C23-O3	-103.84(18)	C12-K1-O4-C24	84.73(18)
C14#2-K1-C23-O3	-144.93(17)	C24-O4-C25-C26	-179.6(2)
C12-K1-C23-O3	77.76(18)	K1-O4-C25-C26	-47.4(3)
O3-K1-C23-C24	-128.4(3)	O4-C25-C26-O5	60.3(3)
O5-K1-C23-C24	14.58(19)	C25-C26-O5-C27	174.7(2)
O1-K1-C23-C24	-146.60(16)	C25-C26-O5-K1	-44.2(3)
O4-K1-C23-C24	20.67(16)	O3-K1-O5-C26	34.22(18)
O2-K1-C23-C24	-153.13(18)	O1-K1-O5-C26	-174.08(16)
O6-K1-C23-C24	33.7(3)	O4-K1-O5-C26	14.75(16)
C15#2-K1-C23-C24	103.65(18)	O2-K1-O5-C26	118.6(3)
C16#2-K1-C23-C24	127.77(18)	O6-K1-O5-C26	-153.49(18)
C14#2-K1-C23-C24	86.68(18)	C15#2-K1-O5-C26	-57.88(17)
C12-K1-C23-C24	-50.63(18)	C16#2-K1-O5-C26	-66.12(18)
O3-C23-C24-O4	-66.0(3)	C14#2-K1-O5-C26	-73.37(17)
K1-C23-C24-O4	-29.6(2)	C23-K1-O5-C26	19.49(18)

C12-K1-O5-C26	110.20(17)	C15#2-K1-O6-C28	-108.52(16)
O3-K1-O5-C27	173.96(16)	C16#2-K1-O6-C28	-132.40(15)
O1-K1-O5-C27	-34.34(17)	C14#2-K1-O6-C28	-97.74(16)
O4-K1-O5-C27	154.49(18)	C23-K1-O6-C28	-41.5(3)
O2-K1-O5-C27	-101.7(3)	C12-K1-O6-C28	45.05(15)
O6-K1-O5-C27	-13.75(15)	O3-K1-O6-C29	-61.6(6)
C15#2-K1-O5-C27	81.86(17)	O5-K1-O6-C29	-145.88(16)
C16#2-K1-O5-C27	73.62(17)	O1-K1-O6-C29	12.68(15)
C14#2-K1-O5-C27	66.37(17)	O4-K1-O6-C29	-157.53(15)
C23-K1-O5-C27	159.23(16)	O2-K1-O6-C29	20.13(17)
C12-K1-O5-C27	-110.06(17)	C15#2-K1-O6-C29	125.39(16)
C26-O5-C27-C28	-173.9(2)	C16#2-K1-O6-C29	101.51(16)
K1-O5-C27-C28	44.9(2)	C14#2-K1-O6-C29	136.17(16)
O5-C27-C28-O6	-65.2(3)	C23-K1-O6-C29	-167.6(2)
C27-C28-O6-C29	179.2(2)	C12-K1-O6-C29	-81.04(16)
C27-C28-O6-K1	51.3(2)	C28-O6-C29-C30	-170.9(2)
O3-K1-O6-C28	64.5(5)	K1-O6-C29-C30	-44.6(2)
O5-K1-O6-C28	-19.79(15)	C19-O1-C30-C29	166.0(2)
O1-K1-O6-C28	138.77(16)	K1-O1-C30-C29	-54.5(2)
O4-K1-O6-C28	-31.44(16)	O6-C29-C30-O1	66.0(3)
O2-K1-O6-C28	146.22(15)		

Symmetry transformations used to generate equivalent atoms:

#1 $x+1/2, -y+1/2, z+1/2$ #2 $x-1/2, -y+1/2, z-1/2$

REFERENCE NUMBER: 05150 [16]

[Revised September 21, 2011]

CRYSTAL STRUCTURE REPORT

$C_{44} H_{84} Co K N_4 O_9$

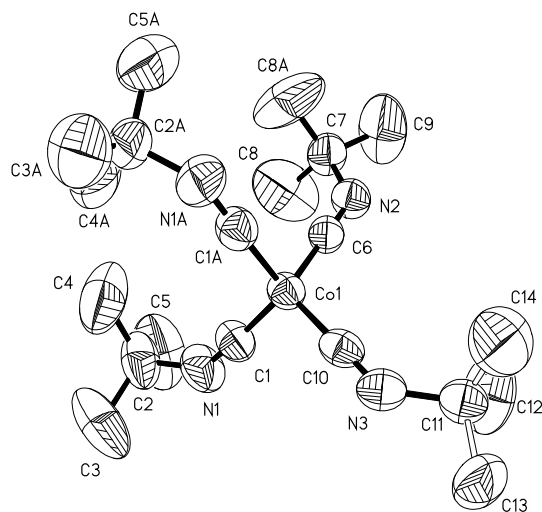
or

$[K(18\text{-crown-6})(THF)_2][Co(CNtBu)_4] \cdot THF$

Report prepared for:

W. Brennessel, Prof. J. Ellis

June 02, 2005



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Data collection

A crystal (approximate dimensions 0.45 x 0.45 x 0.40 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 223(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 134 reflections. At the normal operating temperature of 173 K, the unit cell was very close to orthorhombic; but refinement of the data led to no satisfactory result in crystal systems monoclinic (with a twin law) or orthorhombic. Data collected at 123 K provided slightly better, but unpublishable, results—very likely an even colder temperature would allow the crystal to settle fully into a twinned monoclinic setting. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 30 seconds and a detector distance of 4.97 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.84 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 3450 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ and refined using SHELXL-97.⁵ The space group *Pnmm* 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 uncoordinated THF solvent molecule (see below) was highly disordered over a mirror plane and the reflections contributing to it were removed using program PLATON, function SQUEEZE,⁶ which calculated a total solvent space of 599.6 Å³ containing 152 electrons per unit cell. This is equivalent to approximately four THF molecules, the expected number. The CheckCIF utility at the IUCR website shows some level A (serious) alerts for the refinement. The alerts for the carbon atoms whose thermal parameters are small relative to their methyl neighbors are known to appear incorrectly for terminal groups like the *tert*-butyl. The same alert for K2 is due to the high level of disorder in the axially coordinated THF solvent. The final full matrix least squares refinement converged to $R1 = 0.0541$ and $wR2 = 0.1516$ (F^2 , all data).

Structure description

The structure is the one suggested. The cobalt atom lies on a crystallographic mirror plane. The ligand containing atom N1 is modeled as disordered over a crystallographic mirror plane (50:50). The ligand containing N2 lies on the same plane such that methyl group C8 is across the mirror from its symmetry equivalent. The ligand containing

N3 also lies on the mirror plane, but the methyl groups are disordered over it (50:50). Due to the mirror plane, the symmetry equivalent of ligand N1 is the fourth ligand and the overall geometry is exactly tetrahedral. The charge is balanced by two independent potassium 18-crown-6 bis(THF) cations in which the potassium atoms lie on 2/m special positions (1/4 occupancy each). The axial THF solvent molecules are doubly disordered over a mirror plane and two general positions (50:50, 61:39 and 50:50, 63:37). The uncoordinated THF solvent molecule was highly disordered and could not be modeled satisfactorily; its reflection contributions were removed using program PLATON, function SQUEEZE⁶ (see above).

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

¹ SMART V5.629, Bruker Analytical X-ray Systems, Madison, WI (2003).

² SADABS V2.10, An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).

³ SAINT V7.06A, Bruker Analytical X-ray Systems, Madison, WI (2003).

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.

⁶ PLATON V300106, A multipurpose crystallographic tool, Utrecht University, Utrecht, The Netherlands, A. L. Spek (2006); A. L. Spek, *Acta. Cryst.* **A46**, C34 (1990).

Some equations of interest:

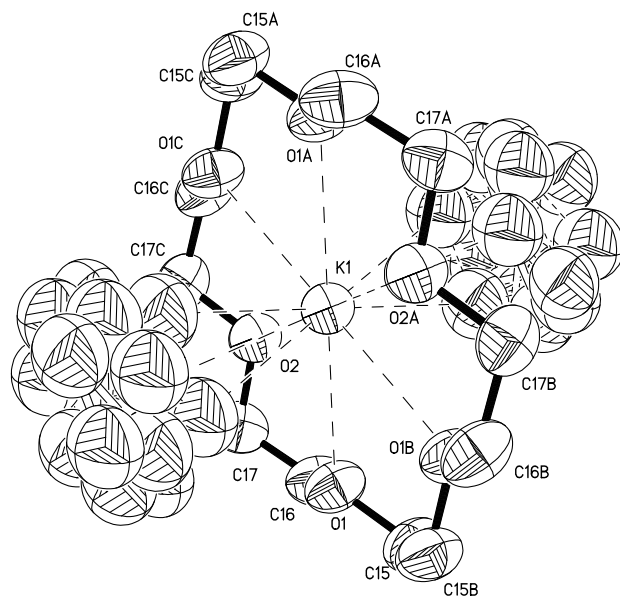
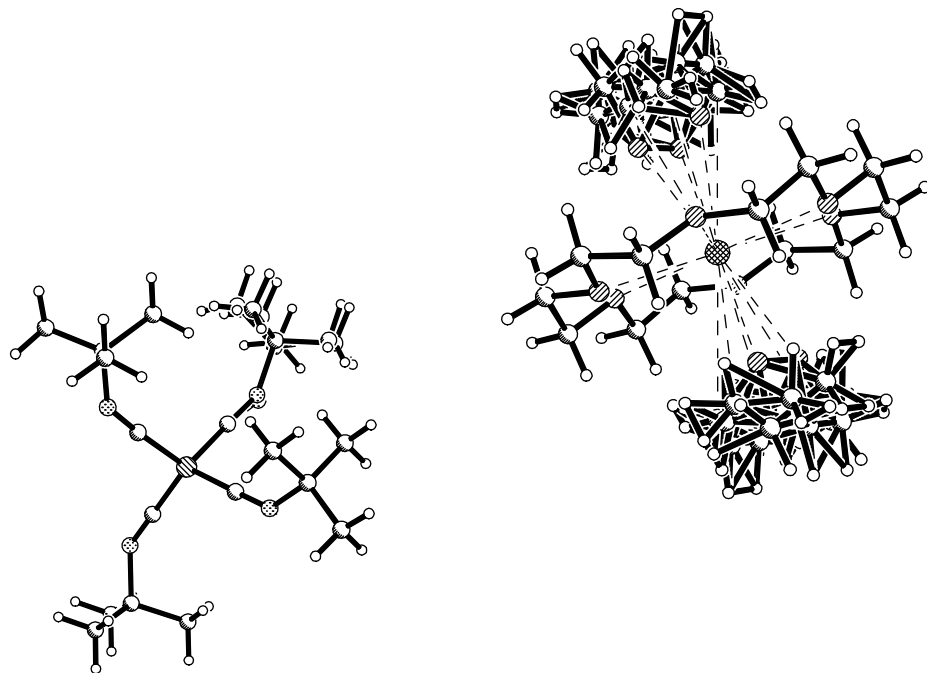
$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2(F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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



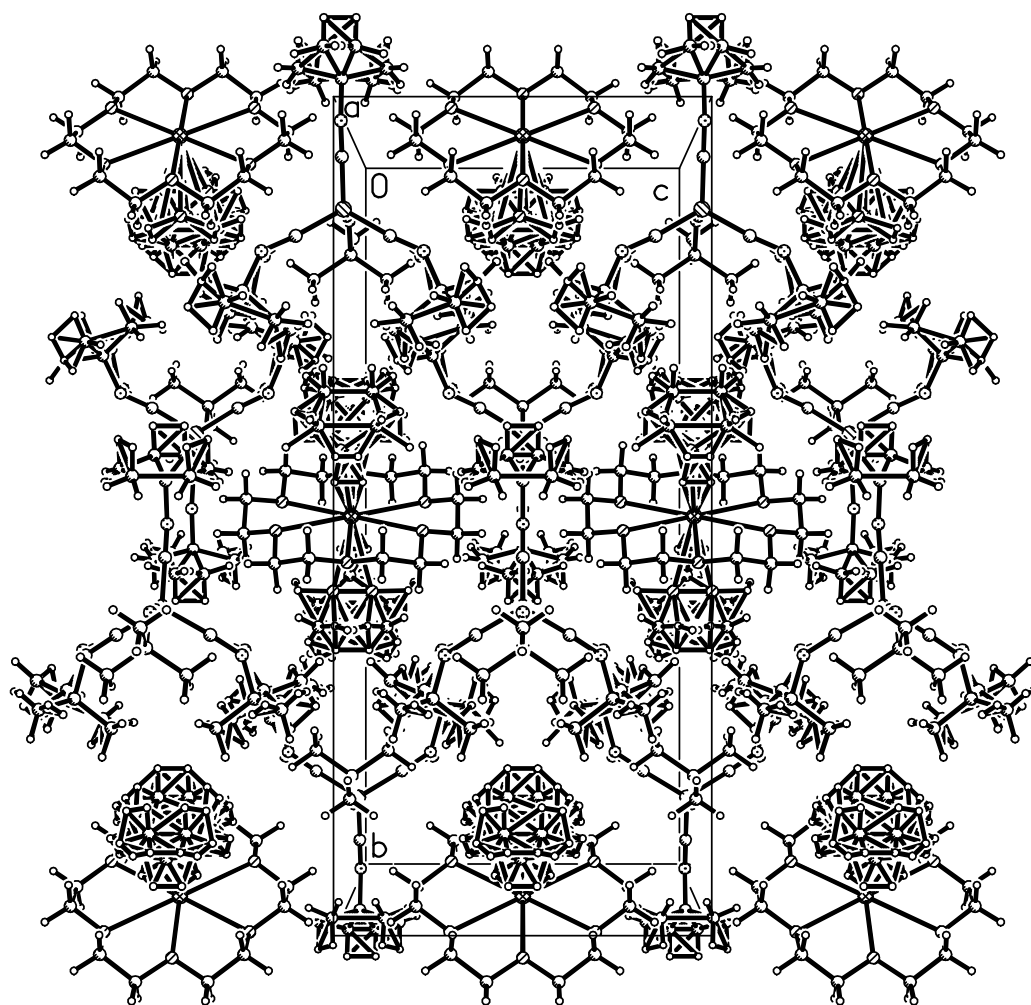


Table 1. Crystal data and structure refinement for 150.

Identification code	05150	
Empirical formula	C ₄₄ H ₈₄ Co K N ₄ O ₉	
Formula weight	911.18	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	<i>Pnnm</i>	
Unit cell dimensions	$a = 18.5263(14)$ Å	$\alpha = 90^\circ$
	$b = 25.4164(19)$ Å	$\beta = 90^\circ$
	$c = 11.4747(8)$ Å	$\gamma = 90^\circ$
Volume	5403.1(7) Å ³	
<i>Z</i>	4	
Density (calculated)	1.120 Mg/m ³	
Absorption coefficient	0.443 mm ⁻¹	
<i>F</i> (000)	1976	
Crystal color, morphology	orange, block	
Crystal size	0.45 x 0.45 x 0.40 mm ³	
Theta range for data collection	1.36 to 25.04°	
Index ranges	$-22 \leq h \leq 22$, $-30 \leq k \leq 30$, $-13 \leq l \leq 13$	
Reflections collected	51512	
Independent reflections	5041 [<i>R</i> (int) = 0.0273]	
Observed reflections	4134	
Completeness to theta = 25.04°	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8426 and 0.8254	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	5041 / 70 / 320	
Goodness-of-fit on <i>F</i> ²	1.065	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0541, <i>wR</i> 2 = 0.1453	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0636, <i>wR</i> 2 = 0.1516	
Largest diff. peak and hole	0.754 and -0.291 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 150. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	7338(1)	1140(1)	0	54(1)
C1	7535(1)	1489(1)	1308(3)	68(1)
N1	7634(13)	1754(3)	2165(4)	93(1)
C2	7663(7)	2310(3)	2479(8)	99(3)
C3	8367(9)	2408(6)	3091(14)	165(5)
C4	7546(10)	2665(3)	1413(14)	177(7)
C5	7043(10)	2404(9)	3294(17)	175(3)
C1'	7535(1)	1489(1)	1308(3)	68(1)
N1'	7604(13)	1692(3)	2251(4)	93(1)
C2'	7808(7)	2201(3)	2736(8)	99(3)
C3'	8382(10)	2108(6)	3640(14)	165(5)
C4'	8041(11)	2588(3)	1778(13)	177(7)
C5'	7142(9)	2422(9)	3293(18)	175(3)
C6	6376(2)	1153(1)	0	56(1)
N2	5726(2)	1167(1)	0	67(1)
C7	5180(2)	1576(2)	0	76(1)
C8	5279(3)	1905(2)	1056(5)	174(3)
C9	4458(3)	1315(3)	0	172(4)
C10	7786(2)	520(2)	0	59(1)
N3	8093(2)	100(1)	0	69(1)
C11	7850(2)	-450(2)	0	72(1)
C12	7211(5)	-496(5)	800(8)	148(5)
C13	8466(3)	-781(3)	433(7)	132(6)
C14	7648(6)	-605(6)	-1222(8)	179(8)
K1	0	5000	0	52(1)
C15	383(2)	4908(1)	3097(2)	73(1)
O1	494(1)	4583(1)	2103(2)	64(1)
C16	1209(1)	4367(1)	2055(2)	70(1)
C17	1257(1)	4019(1)	1031(2)	65(1)
O2	1205(1)	4323(1)	0	59(1)
O3	-632(4)	3992(3)	97(16)	107(2)

C18	-1140(8)	4035(8)	1082(14)	107(2)
C19	-1875(6)	4036(7)	522(12)	107(2)
C20	-1677(8)	4211(6)	-748(14)	107(2)
C21	-1024(8)	3860(8)	-962(15)	107(2)
O3'	-1106(7)	4360(5)	623(12)	107(2)
C18'	-851(14)	3823(8)	770(20)	107(2)
C19'	-966(11)	3627(7)	-442(16)	107(2)
C20'	-1600(15)	3957(9)	-970(20)	107(2)
C21'	-1766(9)	4355(7)	-50(30)	107(2)
K2	5000	5000	0	61(1)
C22	4750(2)	4772(2)	3102(3)	94(1)
O4	4291(1)	4809(1)	2111(2)	81(1)
C23	3785(2)	4391(2)	2075(3)	96(1)
C24	3316(2)	4464(2)	1038(3)	97(1)
O5	3727(1)	4408(1)	0	82(1)
O6	6111(7)	4152(6)	199(14)	137(3)
C25	5849(15)	3817(9)	1070(18)	137(3)
C26	5463(13)	3448(7)	559(16)	137(3)
C27	5843(11)	3389(7)	-692(16)	137(3)
C28	6167(14)	3836(8)	-832(18)	137(3)
O6'	5405(12)	4004(7)	-571(15)	137(3)
C25'	5170(14)	3530(8)	-70(30)	137(3)
C26'	5401(17)	3536(11)	1010(20)	137(3)
C27'	6080(19)	3906(16)	1040(30)	137(3)
C28'	5960(20)	4208(16)	130(30)	137(3)

Table 3. Bond lengths [Å] and angles [°] for 150.

Co(1)-C(1')#1	1.781(3)	C(7)-C(8)#1	1.484(5)
Co(1)-C(1)#1	1.781(3)	C(7)-C(8)	1.484(5)
Co(1)-C(1)	1.781(3)	C(7)-C(9)	1.494(7)
Co(1)-C(10)	1.781(4)	C(8)-H(8A)	0.9700
Co(1)-C(6)	1.784(4)	C(8)-H(8B)	0.9700
C(1)-N(1)	1.205(4)	C(8)-H(8C)	0.9700
N(1)-C(2)	1.459(5)	C(9)-H(9A)	0.9700
C(2)-C(5)	1.500(7)	C(9)-H(9B)	0.9700
C(2)-C(3)	1.503(8)	C(9)-H(9C)	0.9700
C(2)-C(4)	1.536(9)	C(10)-N(3)	1.211(5)
C(3)-H(3A)	0.9700	N(3)-C(11)	1.469(5)
C(3)-H(3B)	0.9700	C(11)-C(12)	1.502(5)
C(3)-H(3C)	0.9700	C(11)-C(12)#1	1.502(5)
C(4)-H(4A)	0.9700	C(11)-C(14)	1.503(5)
C(4)-H(4B)	0.9700	C(11)-C(14)#1	1.503(5)
C(4)-H(4C)	0.9700	C(11)-C(13)	1.503(5)
C(5)-H(5A)	0.9700	C(11)-C(13)#1	1.503(5)
C(5)-H(5B)	0.9700	C(12)-H(12A)	0.9700
C(5)-H(5C)	0.9700	C(12)-H(12B)	0.9700
N(1')-C(2')	1.459(5)	C(12)-H(12C)	0.9700
C(2')-C(5')	1.500(7)	C(13)-H(13A)	0.9700
C(2')-C(3')	1.503(8)	C(13)-H(13B)	0.9700
C(2')-C(4')	1.536(9)	C(13)-H(13C)	0.9700
C(3')-H(3D)	0.9700	C(14)-H(14A)	0.9700
C(3')-H(3E)	0.9700	C(14)-H(14B)	0.9700
C(3')-H(3F)	0.9700	C(14)-H(14C)	0.9700
C(4')-H(4D)	0.9700	K(1)-O(3')#1	2.711(14)
C(4')-H(4E)	0.9700	K(1)-O(3')#2	2.711(14)
C(4')-H(4F)	0.9700	K(1)-O(3')	2.711(14)
C(5')-H(5D)	0.9700	K(1)-O(3')#3	2.711(14)
C(5')-H(5E)	0.9700	K(1)-O(1)	2.7908(17)
C(5')-H(5F)	0.9700	K(1)-O(1)#3	2.7908(17)
C(6)-N(2)	1.203(5)	K(1)-O(1)#1	2.7908(17)
N(2)-C(7)	1.452(5)	K(1)-O(1)#2	2.7909(17)

K(1)-O(2)	2.819(2)	C(19')-H(19D)	0.9800
K(1)-O(2)#2	2.819(2)	C(20')-C(21')	1.489(18)
K(1)-O(3)#1	2.819(7)	C(20')-H(20C)	0.9800
K(1)-O(3)	2.819(7)	C(20')-H(20D)	0.9800
C(15)-O(1)	1.424(3)	C(21')-H(21C)	0.9800
C(15)-C(15)#3	1.494(6)	C(21')-H(21D)	0.9800
C(15)-H(15A)	0.9800	K(2)-C(28')#4	2.69(5)
C(15)-H(15B)	0.9800	K(2)-C(28')#5	2.69(5)
O(1)-C(16)	1.434(3)	K(2)-C(28')#1	2.69(5)
C(16)-C(17)	1.475(4)	K(2)-O(6')#5	2.719(18)
C(16)-H(16A)	0.9800	K(2)-O(6')#4	2.719(18)
C(16)-H(16B)	0.9800	K(2)-O(6')	2.719(18)
C(17)-O(2)	1.416(3)	K(2)-O(6')#1	2.719(18)
C(17)-H(17A)	0.9800	K(2)-O(5)#4	2.797(3)
C(17)-H(17B)	0.9800	K(2)-O(5)	2.798(3)
O(2)-C(17)#1	1.416(3)	K(2)-O(4)	2.7978(19)
O(3)-C(21)	1.454(13)	K(2)-O(4)#4	2.7978(19)
O(3)-C(18)	1.475(12)	K(2)-O(4)#5	2.7978(19)
C(18)-C(19)	1.505(14)	C(22)-O(4)	1.423(4)
C(18)-H(18A)	0.9800	C(22)-C(22)#5	1.485(7)
C(18)-H(18B)	0.9800	C(22)-H(22A)	0.9800
C(19)-C(20)	1.567(15)	C(22)-H(22B)	0.9800
C(19)-H(19A)	0.9800	O(4)-C(23)	1.418(4)
C(19)-H(19B)	0.9800	C(23)-C(24)	1.484(5)
C(20)-C(21)	1.522(15)	C(23)-H(23A)	0.9800
C(20)-H(20A)	0.9800	C(23)-H(23B)	0.9800
C(20)-H(20B)	0.9800	C(24)-O(5)	1.421(4)
C(21)-H(21A)	0.9800	C(24)-H(24A)	0.9800
C(21)-H(21B)	0.9800	C(24)-H(24B)	0.9800
O(3')-C(21')	1.448(16)	O(5)-C(24)#1	1.421(4)
O(3')-C(18')	1.453(15)	O(6)-C(25)	1.400(13)
C(18')-C(19')	1.488(17)	O(6)-C(28)	1.434(14)
C(18')-H(18C)	0.9800	C(25)-C(26)	1.317(18)
C(18')-H(18D)	0.9800	C(25)-H(25A)	0.9800
C(19')-C(20')	1.564(19)	C(25)-H(25B)	0.9800
C(19')-H(19C)	0.9800	C(26)-C(27)	1.606(17)

C(26)-H(26A)	0.9800	C(5)-C(2)-C(4)	107.2(6)
C(26)-H(26B)	0.9800	C(3)-C(2)-C(4)	113.3(6)
C(27)-C(28)	1.296(17)	C(2)-C(3)-H(3A)	109.5
C(27)-H(27A)	0.9800	C(2)-C(3)-H(3B)	109.5
C(27)-H(27B)	0.9800	H(3A)-C(3)-H(3B)	109.5
C(28)-H(28A)	0.9800	C(2)-C(3)-H(3C)	109.5
C(28)-H(28B)	0.9800	H(3A)-C(3)-H(3C)	109.5
O(6')-C(25')	1.405(17)	H(3B)-C(3)-H(3C)	109.5
O(6')-C(28')	1.410(17)	C(2)-C(4)-H(4A)	109.5
C(25')-C(26')	1.31(2)	C(2)-C(4)-H(4B)	109.5
C(25')-H(25C)	0.9800	H(4A)-C(4)-H(4B)	109.5
C(25')-H(25D)	0.9800	C(2)-C(4)-H(4C)	109.5
C(26')-C(27')	1.57(2)	H(4A)-C(4)-H(4C)	109.5
C(26')-H(26C)	0.9800	H(4B)-C(4)-H(4C)	109.5
C(26')-H(26D)	0.9800	C(2)-C(5)-H(5A)	109.5
C(27')-C(28')	1.31(2)	C(2)-C(5)-H(5B)	109.5
C(27')-H(27C)	0.9800	H(5A)-C(5)-H(5B)	109.5
C(27')-H(27D)	0.9800	C(2)-C(5)-H(5C)	109.5
C(28')-H(28C)	0.9800	H(5A)-C(5)-H(5C)	109.5
C(28')-H(28D)	0.9800	H(5B)-C(5)-H(5C)	109.5
C(1')#1-Co(1)-C(1)#1	0.0(2)	N(1')-C(2')-C(5')	106.3(4)
C(1')#1-Co(1)-C(1)	114.85(19)	N(1')-C(2')-C(3')	107.9(5)
C(1)#1-Co(1)-C(1)	114.85(19)	C(5')-C(2')-C(3')	110.3(6)
C(1')#1-Co(1)-C(10)	110.19(11)	N(1')-C(2')-C(4')	111.5(4)
C(1)#1-Co(1)-C(10)	110.19(11)	C(5')-C(2')-C(4')	107.2(6)
C(1)-Co(1)-C(10)	110.19(11)	C(3')-C(2')-C(4')	113.3(6)
C(1')#1-Co(1)-C(6)	101.32(10)	C(2')-C(3')-H(3D)	109.5
C(1)#1-Co(1)-C(6)	101.32(10)	C(2')-C(3')-H(3E)	109.5
C(1)-Co(1)-C(6)	101.32(10)	H(3D)-C(3')-H(3E)	109.5
C(10)-Co(1)-C(6)	118.75(16)	C(2')-C(3')-H(3F)	109.5
N(1)-C(1)-Co(1)	175.2(9)	H(3D)-C(3')-H(3F)	109.5
C(1)-N(1)-C(2)	138.4(5)	H(3E)-C(3')-H(3F)	109.5
N(1)-C(2)-C(5)	106.3(4)	C(2')-C(4')-H(4D)	109.5
N(1)-C(2)-C(3)	107.9(5)	C(2')-C(4')-H(4E)	109.5
C(5)-C(2)-C(3)	110.3(6)	H(4D)-C(4')-H(4E)	109.5
N(1)-C(2)-C(4)	111.5(4)	C(2')-C(4')-H(4F)	109.5

H(4D)-C(4')-H(4F)	109.5	N(3)-C(11)-C(13)	107.4(4)
H(4E)-C(4')-H(4F)	109.5	C(12)-C(11)-C(13)	110.7(3)
C(2')-C(5')-H(5D)	109.5	C(14)-C(11)-C(13)	110.5(3)
C(2')-C(5')-H(5E)	109.5	N(3)-C(11)-C(13)#1	107.4(4)
H(5D)-C(5')-H(5E)	109.5	C(12)#1-C(11)-C(13)#1	110.7(3)
C(2')-C(5')-H(5F)	109.5	C(14)#1-C(11)-C(13)#1	110.5(3)
H(5D)-C(5')-H(5F)	109.5	C(11)-C(12)-H(12A)	109.5
H(5E)-C(5')-H(5F)	109.5	C(11)-C(12)-H(12B)	109.5
N(2)-C(6)-Co(1)	179.3(3)	H(12A)-C(12)-H(12B)	109.5
C(6)-N(2)-C(7)	135.9(4)	C(11)-C(12)-H(12C)	109.5
N(2)-C(7)-C(8)#1	108.6(3)	H(12A)-C(12)-H(12C)	109.5
N(2)-C(7)-C(8)	108.6(3)	H(12B)-C(12)-H(12C)	109.5
C(8)#1-C(7)-C(8)	109.6(6)	C(11)-C(13)-H(13A)	109.5
N(2)-C(7)-C(9)	107.7(4)	C(11)-C(13)-H(13B)	109.5
C(8)#1-C(7)-C(9)	111.2(3)	H(13A)-C(13)-H(13B)	109.5
C(8)-C(7)-C(9)	111.2(3)	C(11)-C(13)-H(13C)	109.5
C(7)-C(8)-H(8A)	109.5	H(13A)-C(13)-H(13C)	109.5
C(7)-C(8)-H(8B)	109.5	H(13B)-C(13)-H(13C)	109.5
H(8A)-C(8)-H(8B)	109.5	C(11)-C(14)-H(14A)	109.5
C(7)-C(8)-H(8C)	109.5	C(11)-C(14)-H(14B)	109.5
H(8A)-C(8)-H(8C)	109.5	H(14A)-C(14)-H(14B)	109.5
H(8B)-C(8)-H(8C)	109.5	C(11)-C(14)-H(14C)	109.5
C(7)-C(9)-H(9A)	109.5	H(14A)-C(14)-H(14C)	109.5
C(7)-C(9)-H(9B)	109.5	H(14B)-C(14)-H(14C)	109.5
H(9A)-C(9)-H(9B)	109.5	O(3')#1-K(1)-O(3')#2	149.4(6)
C(7)-C(9)-H(9C)	109.5	O(3')#1-K(1)-O(3')	30.6(6)
H(9A)-C(9)-H(9C)	109.5	O(3')#2-K(1)-O(3')	179.999(1)
H(9B)-C(9)-H(9C)	109.5	O(3')#1-K(1)-O(3')#3	180.0(6)
N(3)-C(10)-Co(1)	179.7(3)	O(3')#2-K(1)-O(3')#3	30.6(6)
C(10)-N(3)-C(11)	134.1(3)	O(3')-K(1)-O(3')#3	149.4(6)
N(3)-C(11)-C(12)	108.4(6)	O(3')#1-K(1)-O(1)	104.4(3)
N(3)-C(11)-C(12)#1	108.4(6)	O(3')#2-K(1)-O(1)	102.0(3)
N(3)-C(11)-C(14)	109.0(7)	O(3')-K(1)-O(1)	78.0(3)
C(12)-C(11)-C(14)	110.7(3)	O(3')#3-K(1)-O(1)	75.6(3)
N(3)-C(11)-C(14)#1	109.0(7)	O(3')#1-K(1)-O(1)#3	102.0(3)
C(12)#1-C(11)-C(14)#1	110.7(3)	O(3')#2-K(1)-O(1)#3	104.4(3)

O(3')-K(1)-O(1)#3	75.6(3)	O(3')#3-K(1)-O(3)#1	150.4(4)
O(3')#3-K(1)-O(1)#3	78.0(3)	O(1)-K(1)-O(3)#1	79.9(4)
O(1)-K(1)-O(1)#3	60.27(7)	O(1)#3-K(1)-O(3)#1	104.1(3)
O(3')#1-K(1)-O(1)#1	78.0(3)	O(1)#1-K(1)-O(3)#1	75.9(3)
O(3')#2-K(1)-O(1)#1	75.6(3)	O(1)#2-K(1)-O(3)#1	100.1(4)
O(3')-K(1)-O(1)#1	104.4(3)	O(2)-K(1)-O(3)#1	76.97(15)
O(3')#3-K(1)-O(1)#1	102.0(3)	O(2)#2-K(1)-O(3)#1	103.03(15)
O(1)-K(1)-O(1)#1	119.73(7)	O(3')#1-K(1)-O(3)	32.0(3)
O(1)#3-K(1)-O(1)#1	180.0	O(3')#2-K(1)-O(3)	150.4(4)
O(3')#1-K(1)-O(1)#2	75.6(3)	O(3')-K(1)-O(3)	29.6(4)
O(3')#2-K(1)-O(1)#2	78.0(3)	O(3')#3-K(1)-O(3)	148.0(3)
O(3')-K(1)-O(1)#2	102.0(3)	O(1)-K(1)-O(3)	75.9(3)
O(3')#3-K(1)-O(1)#2	104.4(3)	O(1)#3-K(1)-O(3)	100.1(4)
O(1)-K(1)-O(1)#2	180.0	O(1)#1-K(1)-O(3)	79.9(4)
O(1)#3-K(1)-O(1)#2	119.73(7)	O(1)#2-K(1)-O(3)	104.1(3)
O(1)#1-K(1)-O(1)#2	60.27(7)	O(2)-K(1)-O(3)	76.97(15)
O(3')#1-K(1)-O(2)	103.5(3)	O(2)#2-K(1)-O(3)	103.03(15)
O(3')#2-K(1)-O(2)	76.6(3)	O(3)#1-K(1)-O(3)	4.5(8)
O(3')-K(1)-O(2)	103.4(3)	O(1)-C(15)-C(15)#3	108.6(2)
O(3')#3-K(1)-O(2)	76.6(3)	O(1)-C(15)-H(15A)	110.0
O(1)-K(1)-O(2)	60.54(3)	C(15)#3-C(15)-H(15A)	110.0
O(1)#3-K(1)-O(2)	119.46(3)	O(1)-C(15)-H(15B)	110.0
O(1)#1-K(1)-O(2)	60.54(3)	C(15)#3-C(15)-H(15B)	110.0
O(1)#2-K(1)-O(2)	119.46(3)	H(15A)-C(15)-H(15B)	108.4
O(3')#1-K(1)-O(2)#2	76.5(3)	C(15)-O(1)-C(16)	112.7(2)
O(3')#2-K(1)-O(2)#2	103.4(3)	C(15)-O(1)-K(1)	115.11(14)
O(3')-K(1)-O(2)#2	76.6(3)	C(16)-O(1)-K(1)	114.50(14)
O(3')#3-K(1)-O(2)#2	103.4(3)	O(1)-C(16)-C(17)	108.4(2)
O(1)-K(1)-O(2)#2	119.46(3)	O(1)-C(16)-H(16A)	110.0
O(1)#3-K(1)-O(2)#2	60.54(3)	C(17)-C(16)-H(16A)	110.0
O(1)#1-K(1)-O(2)#2	119.46(3)	O(1)-C(16)-H(16B)	110.0
O(1)#2-K(1)-O(2)#2	60.54(3)	C(17)-C(16)-H(16B)	110.0
O(2)-K(1)-O(2)#2	180.0	H(16A)-C(16)-H(16B)	108.4
O(3')#1-K(1)-O(3)#1	29.6(4)	O(2)-C(17)-C(16)	109.5(2)
O(3')#2-K(1)-O(3)#1	148.0(3)	O(2)-C(17)-H(17A)	109.8
O(3')-K(1)-O(3)#1	32.0(3)	C(16)-C(17)-H(17A)	109.8

O(2)-C(17)-H(17B)	109.8	O(3')-C(18')-C(19')	99.4(13)
C(16)-C(17)-H(17B)	109.8	O(3')-C(18')-K(1)	46.7(11)
H(17A)-C(17)-H(17B)	108.2	C(19')-C(18')-K(1)	96.8(13)
C(17)#1-O(2)-C(17)	113.2(3)	O(3')-C(18')-H(18C)	111.9
C(17)#1-O(2)-K(1)	112.77(14)	C(19')-C(18')-H(18C)	111.9
C(17)-O(2)-K(1)	112.77(14)	K(1)-C(18')-H(18C)	148.0
C(21)-O(3)-C(18)	109.8(8)	O(3')-C(18')-H(18D)	111.9
C(21)-O(3)-K(1)	112.6(11)	C(19')-C(18')-H(18D)	111.9
C(18)-O(3)-K(1)	103.2(9)	K(1)-C(18')-H(18D)	70.1
O(3)-C(18)-C(19)	104.5(9)	H(18C)-C(18')-H(18D)	109.6
O(3)-C(18)-H(18A)	110.9	C(18')-C(19')-C(20')	106.6(13)
C(19)-C(18)-H(18A)	110.9	C(18')-C(19')-H(19C)	110.4
O(3)-C(18)-H(18B)	110.9	C(20')-C(19')-H(19C)	110.4
C(19)-C(18)-H(18B)	110.9	C(18')-C(19')-H(19D)	110.4
H(18A)-C(18)-H(18B)	108.9	C(20')-C(19')-H(19D)	110.4
C(18)-C(19)-C(20)	100.7(10)	H(19C)-C(19')-H(19D)	108.6
C(18)-C(19)-H(19A)	111.6	C(21')-C(20')-C(19')	104.4(11)
C(20)-C(19)-H(19A)	111.6	C(21')-C(20')-H(20C)	110.9
C(18)-C(19)-H(19B)	111.6	C(19')-C(20')-H(20C)	110.9
C(20)-C(19)-H(19B)	111.6	C(21')-C(20')-H(20D)	110.9
H(19A)-C(19)-H(19B)	109.4	C(19')-C(20')-H(20D)	110.9
C(21)-C(20)-C(19)	99.8(12)	H(20C)-C(20')-H(20D)	108.9
C(21)-C(20)-H(20A)	111.8	O(3')-C(21')-C(20')	102.1(12)
C(19)-C(20)-H(20A)	111.8	O(3')-C(21')-H(21C)	111.3
C(21)-C(20)-H(20B)	111.8	C(20')-C(21')-H(21C)	111.3
C(19)-C(20)-H(20B)	111.8	O(3')-C(21')-H(21D)	111.3
H(20A)-C(20)-H(20B)	109.5	C(20')-C(21')-H(21D)	111.3
O(3)-C(21)-C(20)	97.3(9)	H(21C)-C(21')-H(21D)	109.2
O(3)-C(21)-H(21A)	112.3	C(28')#4-K(2)-C(28')#5	6.6(15)
C(20)-C(21)-H(21A)	112.3	C(28')#4-K(2)-C(28')#1	173.4(15)
O(3)-C(21)-H(21B)	112.3	C(28')#5-K(2)-C(28')#1	179.998(4)
C(20)-C(21)-H(21B)	112.3	C(28')#4-K(2)-O(6')#5	26.9(7)
H(21A)-C(21)-H(21B)	109.9	C(28')#5-K(2)-O(6')#5	30.2(4)
C(21')-O(3')-C(18')	109.0(13)	C(28')#1-K(2)-O(6')#5	149.8(4)
C(21')-O(3')-K(1)	120.2(13)	C(28')#4-K(2)-O(6')#4	30.2(4)
C(18')-O(3')-K(1)	110.3(14)	C(28')#5-K(2)-O(6')#4	26.9(7)

C(28')#1-K(2)-O(6')#4	153.1(7)	O(5)-K(2)-O(4)	60.72(5)
O(6')#5-K(2)-O(6')#4	27.9(7)	C(28')#4-K(2)-O(4)#4	97.5(8)
C(28')#4-K(2)-O(6')	149.8(4)	C(28')#5-K(2)-O(4)#4	103.3(6)
C(28')#5-K(2)-O(6')	153.1(7)	C(28')#1-K(2)-O(4)#4	76.7(6)
C(28')#1-K(2)-O(6')	26.9(7)	O(6')#5-K(2)-O(4)#4	76.1(4)
O(6')#5-K(2)-O(6')	152.1(7)	O(6')#4-K(2)-O(4)#4	100.2(4)
O(6')#4-K(2)-O(6')	180.0(3)	O(6')-K(2)-O(4)#4	79.8(4)
C(28')#4-K(2)-O(6')#1	153.1(7)	O(6')#1-K(2)-O(4)#4	103.9(4)
C(28')#5-K(2)-O(6')#1	149.8(4)	O(5)#4-K(2)-O(4)#4	60.72(5)
C(28')#1-K(2)-O(6')#1	30.2(4)	O(5)-K(2)-O(4)#4	119.28(5)
O(6')#5-K(2)-O(6')#1	179.999(2)	O(4)-K(2)-O(4)#4	180.00(9)
O(6')#4-K(2)-O(6')#1	152.1(7)	C(28')#4-K(2)-O(4)#5	103.3(6)
O(6')-K(2)-O(6')#1	27.9(7)	C(28')#5-K(2)-O(4)#5	97.5(8)
C(28')#4-K(2)-O(5)#4	98.9(6)	C(28')#1-K(2)-O(4)#5	82.5(8)
C(28')#5-K(2)-O(5)#4	98.9(6)	O(6')#5-K(2)-O(4)#5	100.2(4)
C(28')#1-K(2)-O(5)#4	81.1(6)	O(6')#4-K(2)-O(4)#5	76.1(4)
O(6')#5-K(2)-O(5)#4	74.4(4)	O(6')-K(2)-O(4)#5	103.9(4)
O(6')#4-K(2)-O(5)#4	74.4(4)	O(6')#1-K(2)-O(4)#5	79.8(4)
O(6')-K(2)-O(5)#4	105.6(4)	O(5)#4-K(2)-O(4)#5	60.72(5)
O(6')#1-K(2)-O(5)#4	105.6(4)	O(5)-K(2)-O(4)#5	119.28(5)
C(28')#4-K(2)-O(5)	81.1(6)	O(4)-K(2)-O(4)#5	60.06(9)
C(28')#5-K(2)-O(5)	81.1(6)	O(4)#4-K(2)-O(4)#5	119.94(9)
C(28')#1-K(2)-O(5)	98.9(6)	O(4)-C(22)-C(22)#5	108.7(3)
O(6')#5-K(2)-O(5)	105.6(4)	O(4)-C(22)-H(22A)	109.9
O(6')#4-K(2)-O(5)	105.6(4)	C(22)#5-C(22)-H(22A)	109.9
O(6')-K(2)-O(5)	74.4(4)	O(4)-C(22)-H(22B)	109.9
O(6')#1-K(2)-O(5)	74.4(4)	C(22)#5-C(22)-H(22B)	109.9
O(5)#4-K(2)-O(5)	180.0	H(22A)-C(22)-H(22B)	108.3
C(28')#4-K(2)-O(4)	82.5(8)	C(23)-O(4)-C(22)	111.6(3)
C(28')#5-K(2)-O(4)	76.7(6)	C(23)-O(4)-K(2)	114.56(18)
C(28')#1-K(2)-O(4)	103.3(6)	C(22)-O(4)-K(2)	115.05(17)
O(6')#5-K(2)-O(4)	103.9(4)	O(4)-C(23)-C(24)	108.5(3)
O(6')#4-K(2)-O(4)	79.8(4)	O(4)-C(23)-H(23A)	110.0
O(6')-K(2)-O(4)	100.2(4)	C(24)-C(23)-H(23A)	110.0
O(6')#1-K(2)-O(4)	76.1(4)	O(4)-C(23)-H(23B)	110.0
O(5)#4-K(2)-O(4)	119.28(5)	C(24)-C(23)-H(23B)	110.0

H(23A)-C(23)-H(23B)	108.4	C(27)-C(28)-H(28A)	109.5
O(5)-C(24)-C(23)	110.3(2)	O(6)-C(28)-H(28A)	109.5
O(5)-C(24)-H(24A)	109.6	C(27)-C(28)-H(28B)	109.5
C(23)-C(24)-H(24A)	109.6	O(6)-C(28)-H(28B)	109.5
O(5)-C(24)-H(24B)	109.6	H(28A)-C(28)-H(28B)	108.1
C(23)-C(24)-H(24B)	109.6	C(25')-O(6')-C(28')	108(2)
H(24A)-C(24)-H(24B)	108.1	C(25')-O(6')-K(2)	127.9(14)
C(24)#1-O(5)-C(24)	113.9(4)	C(28')-O(6')-K(2)	74(2)
C(24)#1-O(5)-K(2)	113.42(19)	C(26')-C(25')-O(6')	106.1(18)
C(24)-O(5)-K(2)	113.42(19)	C(26')-C(25')-H(25C)	110.5
C(25)-O(6)-C(28)	105.8(14)	O(6')-C(25')-H(25C)	110.5
C(25)-O(6)-K(2)	104.7(16)	C(26')-C(25')-H(25D)	110.5
C(28)-O(6)-K(2)	113.0(12)	O(6')-C(25')-H(25D)	110.5
C(26)-C(25)-O(6)	107.7(15)	H(25C)-C(25')-H(25D)	108.7
C(26)-C(25)-H(25A)	110.2	C(25')-C(26')-C(27')	106.8(14)
O(6)-C(25)-H(25A)	110.2	C(25')-C(26')-H(26C)	110.4
C(26)-C(25)-H(25B)	110.2	C(27')-C(26')-H(26C)	110.4
O(6)-C(25)-H(25B)	110.2	C(25')-C(26')-H(26D)	110.4
H(25A)-C(25)-H(25B)	108.5	C(27')-C(26')-H(26D)	110.4
C(25)-C(26)-C(27)	103.1(13)	H(26C)-C(26')-H(26D)	108.6
C(25)-C(26)-H(26A)	111.2	C(28')-C(27')-C(26')	101.4(16)
C(27)-C(26)-H(26A)	111.2	C(28')-C(27')-H(27C)	111.5
C(25)-C(26)-H(26B)	111.2	C(26')-C(27')-H(27C)	111.5
C(27)-C(26)-H(26B)	111.2	C(28')-C(27')-H(27D)	111.5
H(26A)-C(26)-H(26B)	109.1	C(26')-C(27')-H(27D)	111.5
C(28)-C(27)-C(26)	103.4(12)	H(27C)-C(27')-H(27D)	109.3
C(28)-C(27)-H(27A)	111.1	C(27')-C(28')-O(6')	111(2)
C(26)-C(27)-H(27A)	111.1	C(27')-C(28')-H(28C)	109.4
C(28)-C(27)-H(27B)	111.1	O(6')-C(28')-H(28C)	109.4
C(26)-C(27)-H(27B)	111.1	C(27')-C(28')-H(28D)	109.4
H(27A)-C(27)-H(27B)	109.0	O(6')-C(28')-H(28D)	109.4
C(27)-C(28)-O(6)	110.8(13)	H(28C)-C(28')-H(28D)	108.0

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z #2 -x,-y+1,-z #3 -x,-y+1,z #4 -x+1,-y+1,-z

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 150. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	54(1)	61(1)	47(1)	0	0	-5(1)
C1	63(2)	77(2)	64(2)	-2(2)	-2(1)	-12(1)
N1	111(3)	101(2)	68(2)	-19(2)	-9(2)	-23(2)
C2	126(5)	96(4)	76(4)	-21(4)	7(4)	-42(4)
C3	150(5)	171(14)	175(14)	-43(9)	-54(9)	-43(10)
C4	260(20)	102(5)	164(11)	3(5)	14(11)	-56(7)
C5	156(6)	157(5)	211(7)	-79(5)	52(5)	-22(5)
C1'	63(2)	77(2)	64(2)	-2(2)	-2(1)	-12(1)
N1'	111(3)	101(2)	68(2)	-19(2)	-9(2)	-23(2)
C2'	126(5)	96(4)	76(4)	-21(4)	7(4)	-42(4)
C3'	150(5)	171(14)	175(14)	-43(9)	-54(9)	-43(10)
C4'	260(20)	102(5)	164(11)	3(5)	14(11)	-56(7)
C5'	156(6)	157(5)	211(7)	-79(5)	52(5)	-22(5)
C6	67(2)	54(2)	47(2)	0	0	-8(2)
N2	52(2)	67(2)	82(2)	0	0	2(2)
C7	60(2)	64(2)	103(3)	0	0	8(2)
C8	147(4)	171(5)	205(6)	-94(5)	-20(4)	66(4)
C9	60(3)	113(5)	343(13)	0	0	5(3)
C10	49(2)	82(3)	47(2)	0	0	-3(2)
N3	54(2)	80(2)	72(2)	0	0	12(2)
C11	52(2)	80(3)	85(3)	0	0	5(2)
C12	137(9)	107(8)	199(13)	9(8)	86(9)	-26(7)
C13	91(4)	81(4)	225(19)	27(6)	-29(6)	12(3)
C14	290(20)	127(9)	117(9)	-38(7)	-62(12)	11(13)
K1	48(1)	57(1)	52(1)	0	0	4(1)
C15	85(2)	83(2)	52(2)	-1(1)	-10(1)	16(2)
O1	58(1)	81(1)	52(1)	-1(1)	-5(1)	15(1)
C16	57(2)	93(2)	60(2)	15(2)	-6(1)	19(1)
C17	54(1)	69(2)	72(2)	12(1)	-1(1)	18(1)
O2	56(1)	63(1)	57(1)	0	0	12(1)
O3	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)

C18	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
C19	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
C20	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
C21	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
O3'	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
C18'	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
C19'	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
C20'	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
C21'	101(3)	106(4)	114(4)	3(4)	-8(4)	-21(2)
K2	51(1)	79(1)	53(1)	0	0	1(1)
C22	103(3)	125(3)	53(2)	11(2)	12(2)	17(2)
O4	80(1)	102(2)	60(1)	10(1)	13(1)	-1(1)
C23	86(2)	113(3)	87(2)	7(2)	35(2)	-12(2)
C24	57(2)	119(3)	114(3)	0(2)	21(2)	-15(2)
O5	51(2)	109(2)	84(2)	0	0	-6(2)
O6	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C25	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C26	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C27	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C28	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
O6'	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C25'	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C26'	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C27'	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)
C28'	161(6)	118(4)	133(6)	-30(5)	44(5)	-19(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 150.

	x	y	z	U(eq)
H3A	8763	2351	2551	248
H3B	8414	2169	3745	248
H3C	8381	2768	3371	248
H4A	7941	2618	869	265
H4B	7528	3030	1660	265
H4C	7095	2572	1036	265
H5A	7096	2183	3978	262
H5B	6593	2319	2903	262
H5C	7038	2770	3529	262
H3D	8811	1967	3268	248
H3E	8206	1859	4214	248
H3F	8500	2438	4020	248
H4D	8468	2454	1390	265
H4E	8146	2927	2124	265
H4F	7653	2626	1215	265
H5D	6975	2185	3897	262
H5E	6768	2463	2708	262
H5F	7251	2762	3633	262
H8A	5223	1688	1746	261
H8B	4919	2183	1065	261
H8C	5757	2060	1049	261
H9A	4408	1102	-698	258
H9B	4082	1580	16	258
H9C	4416	1091	682	258
H12A	7360	-421	1593	222
H12B	7017	-850	758	222
H12C	6843	-246	565	222
H13A	8878	-738	-81	198
H13B	8322	-1148	444	198
H13C	8597	-671	1214	198

H14A	8065	-569	-1726	268
H14B	7263	-379	-1499	268
H14C	7485	-968	-1228	268
H15A	710	5211	3070	88
H15B	484	4709	3810	88
H16A	1310	4167	2767	84
H16B	1565	4651	1991	84
H17A	1717	3829	1041	78
H17B	866	3760	1053	78
H18A	-1059	4361	1519	129
H18B	-1088	3735	1612	129
H19A	-2200	4288	899	129
H19B	-2095	3685	534	129
H20A	-2068	4137	-1299	129
H20B	-1550	4585	-786	129
H21A	-1154	3487	-997	129
H21B	-759	3960	-1667	129
H18C	-1141	3628	1335	129
H18D	-341	3811	991	129
H19C	-1090	3252	-432	129
H19D	-527	3673	-907	129
H20C	-1453	4127	-1694	129
H20D	-2021	3733	-1120	129
H21C	-1864	4700	-397	129
H21D	-2179	4247	424	129
H22A	5025	4443	3074	112
H22B	4459	4773	3817	112
H23A	3491	4392	2786	115
H23B	4037	4053	2026	115
H24A	2928	4202	1049	116
H24B	3097	4814	1060	116
H25A	6251	3658	1499	165
H25B	5550	4015	1621	165
H26A	4958	3557	478	165
H26B	5483	3118	997	165
H27A	6189	3097	-693	165

H27B	5484	3330	-1306	165
H28A	5951	4024	-1491	165
H28B	6677	3774	-1013	165
H25C	4642	3506	-91	165
H25D	5372	3229	-490	165
H26C	5532	3180	1259	165
H26D	5024	3670	1529	165
H27C	6100	4111	1762	165
H27D	6529	3706	953	165
H28C	6405	4237	-326	165
H28D	5830	4561	401	165

Table 6. Torsion angles [°] for 150.

C1#1-Co1-C1-N1	58(10)	O1#1-K1-O1-C15	162.64(15)
C1#1-Co1-C1-N1	58(10)	O1#2-K1-O1-C15	39.5(13)
C10-Co1-C1-N1	-177(100)	O2-K1-O1-C15	149.3(2)
C6-Co1-C1-N1	-50(10)	O2#2-K1-O1-C15	-30.7(2)
Co1-C1-N1-C2	-33(12)	O3#1-K1-O1-C15	-130.1(3)
C1-N1-C2-C5	115(3)	O3-K1-O1-C15	-127.9(3)
C1-N1-C2-C3	-127(3)	O3'#1-K1-O1-C16	113.8(3)
C1-N1-C2-C4	-1(3)	O3'#2-K1-O1-C16	-50.6(3)
C1#1-Co1-C6-N2	-59.25(10)	O3'-K1-O1-C16	129.4(3)
C1#1-Co1-C6-N2	-59.25(10)	O3'#3-K1-O1-C16	-66.2(3)
C1-Co1-C6-N2	59.25(10)	O1#3-K1-O1-C16	-150.4(2)
C10-Co1-C6-N2	180.0	O1#1-K1-O1-C16	29.6(2)
Co1-C6-N2-C7	0.0	O1#2-K1-O1-C16	-93.5(13)
C6-N2-C7-C8#1	59.5(3)	O2-K1-O1-C16	16.26(18)
C6-N2-C7-C8	-59.5(3)	O2#2-K1-O1-C16	-163.74(18)
C6-N2-C7-C9	180.0	O3#1-K1-O1-C16	96.9(3)
C1#1-Co1-C10-N3	64(100)	O3-K1-O1-C16	99.1(3)
C1#1-Co1-C10-N3	64(100)	C15-O1-C16-C17	177.4(2)
C1-Co1-C10-N3	-64(100)	K1-O1-C16-C17	-48.5(3)
C6-Co1-C10-N3	180(100)	O1-C16-C17-O2	67.4(3)
Co1-C10-N3-C11	180(100)	C16-C17-O2-C17#1	179.15(17)
C10-N3-C11-C12	-40.1(4)	C16-C17-O2-K1	-51.3(2)
C10-N3-C11-C12#1	40.1(4)	O3'#1-K1-O2-C17#1	49.2(3)
C10-N3-C11-C14	80.5(4)	O3'#2-K1-O2-C17#1	-99.4(3)
C10-N3-C11-C14#1	-80.5(4)	O3'-K1-O2-C17#1	80.6(3)
C10-N3-C11-C13	-159.7(3)	O3'#3-K1-O2-C17#1	-130.8(3)
C10-N3-C11-C13#1	159.7(3)	O1-K1-O2-C17#1	148.2(2)
C15#3-C15-O1-C16	-177.4(3)	O1#3-K1-O2-C17#1	161.53(16)
C15#3-C15-O1-K1	48.8(3)	O1#1-K1-O2-C17#1	-18.47(16)
O3'#1-K1-O1-C15	-113.2(3)	O1#2-K1-O2-C17#1	-31.8(2)
O3'#2-K1-O1-C15	82.5(3)	O2#2-K1-O2-C17#1	6.66(18)
O3'-K1-O1-C15	-97.5(3)	O3#1-K1-O2-C17#1	62.6(4)
O3'#3-K1-O1-C15	66.8(3)	O3-K1-O2-C17#1	67.2(4)
O1#3-K1-O1-C15	-17.36(15)	O3'#1-K1-O2-C17	-80.6(3)

O3'#2-K1-O2-C17	130.8(3)	C18-O3-C21-C20	39.9(15)
O3'-K1-O2-C17	-49.2(3)	K1-O3-C21-C20	-74.5(12)
O3'#3-K1-O2-C17	99.4(3)	C19-C20-C21-O3	-50.9(14)
O1-K1-O2-C17	18.47(16)	O3'#1-K1-O3'-C21'	-36.8(13)
O1#3-K1-O2-C17	31.8(2)	O3'#2-K1-O3'-C21'	34(7)
O1#1-K1-O2-C17	-148.2(2)	O3'#3-K1-O3'-C21'	143.2(13)
O1#2-K1-O2-C17	-161.53(16)	O1-K1-O3'-C21'	174.1(13)
O2#2-K1-O2-C17	-123.11(17)	O1#3-K1-O3'-C21'	112.1(13)
O3#1-K1-O2-C17	-67.2(4)	O1#1-K1-O3'-C21'	-67.9(13)
O3-K1-O2-C17	-62.6(4)	O1#2-K1-O3'-C21'	-5.9(13)
O3'#1-K1-O3-C21	33.0(8)	O2-K1-O3'-C21'	-130.5(12)
O3'#2-K1-O3-C21	-85.1(9)	O2#2-K1-O3'-C21'	49.5(12)
O3'-K1-O3-C21	94.8(9)	O3#1-K1-O3'-C21'	-95.7(14)
O3'#3-K1-O3-C21	-147.0(8)	O3-K1-O3'-C21'	-103.3(16)
O1-K1-O3-C21	-174.7(8)	O3'#1-K1-O3'-C18'	91.3(12)
O1#3-K1-O3-C21	129.6(8)	O3'#2-K1-O3'-C18'	162(7)
O1#1-K1-O3-C21	-50.4(8)	O3'#3-K1-O3'-C18'	-88.7(12)
O1#2-K1-O3-C21	5.3(8)	O1-K1-O3'-C18'	-57.8(11)
O2-K1-O3-C21	-112.3(8)	O1#3-K1-O3'-C18'	-119.9(12)
O2#2-K1-O3-C21	67.7(8)	O1#1-K1-O3'-C18'	60.1(12)
O3#1-K1-O3-C21	-22.8(8)	O1#2-K1-O3'-C18'	122.2(11)
O3'#1-K1-O3-C18	-85.3(9)	O2-K1-O3'-C18'	-2.4(12)
O3'#2-K1-O3-C18	156.5(8)	O2#2-K1-O3'-C18'	177.6(12)
O3'-K1-O3-C18	-23.5(8)	O3#1-K1-O3'-C18'	32.4(13)
O3'#3-K1-O3-C18	94.7(9)	O3-K1-O3'-C18'	24.8(11)
O1-K1-O3-C18	66.9(8)	C21'-O3'-C18'-C19'	44(2)
O1#3-K1-O3-C18	11.3(8)	K1-O3'-C18'-C19'	-90.4(15)
O1#1-K1-O3-C18	-168.7(8)	C21'-O3'-C18'-K1	134(2)
O1#2-K1-O3-C18	-113.1(8)	O3'#1-K1-C18'-O3'	-55.7(12)
O2-K1-O3-C18	129.4(8)	O3'#2-K1-C18'-O3'	180.0
O2#2-K1-O3-C18	-50.6(8)	O3'#3-K1-C18'-O3'	124.3(12)
O3#1-K1-O3-C18	-141.1(8)	O1-K1-C18'-O3'	115.7(12)
C21-O3-C18-C19	-11.7(16)	O1#3-K1-C18'-O3'	57.2(11)
K1-O3-C18-C19	108.6(13)	O1#1-K1-C18'-O3'	-122.8(11)
O3-C18-C19-C20	-21.1(17)	O1#2-K1-C18'-O3'	-64.3(12)
C18-C19-C20-C21	45.2(16)	O2-K1-C18'-O3'	177.6(12)

O2#2-K1-C18'-O3'	-2.4(12)	C28#1-K2-O4-C22	55.7(8)
O3#1-K1-C18'-O3'	-105.9(16)	O6#5-K2-O4-C22	-111.1(5)
O3-K1-C18'-O3'	-110(2)	O6#4-K2-O4-C22	-97.0(5)
O3#1-K1-C18'-C19'	40.9(11)	O6'-K2-O4-C22	83.0(5)
O3#2-K1-C18'-C19'	-83.4(14)	O6#1-K2-O4-C22	68.9(5)
O3'-K1-C18'-C19'	96.6(14)	O5#4-K2-O4-C22	-31.4(2)
O3#3-K1-C18'-C19'	-139.1(11)	O5-K2-O4-C22	148.6(2)
O1-K1-C18'-C19'	-147.7(14)	O4#4-K2-O4-C22	174(4)
O1#3-K1-C18'-C19'	153.9(13)	O4#5-K2-O4-C22	-17.28(18)
O1#1-K1-C18'-C19'	-26.1(13)	C22-O4-C23-C24	178.6(3)
O1#2-K1-C18'-C19'	32.3(14)	K2-O4-C23-C24	-48.4(3)
O2-K1-C18'-C19'	-85.8(13)	O4-C23-C24-O5	65.8(4)
O2#2-K1-C18'-C19'	94.2(13)	C23-C24-O5-C24#1	179.1(2)
O3#1-K1-C18'-C19'	-9.3(10)	C23-C24-O5-K2	-49.1(4)
O3-K1-C18'-C19'	-13.1(13)	C28#4-K2-O5-C24#1	62.7(8)
O3'-C18'-C19'-C20'	-28(3)	C28#5-K2-O5-C24#1	69.3(8)
K1-C18'-C19'-C20'	-74.8(18)	C28#1-K2-O5-C24#1	-110.7(8)
C18'-C19'-C20'-C21'	5(3)	O6#5-K2-O5-C24#1	51.5(5)
C18'-O3'-C21'-C20'	-41(3)	O6#4-K2-O5-C24#1	80.5(5)
K1-O3'-C21'-C20'	87(2)	O6'-K2-O5-C24#1	-99.5(5)
C19'-C20'-C21'-O3'	20(3)	O6#1-K2-O5-C24#1	-128.5(5)
C22#5-C22-O4-C23	-178.4(3)	O5#4-K2-O5-C24#1	-90.2(2)
C22#5-C22-O4-K2	48.8(4)	O4-K2-O5-C24#1	149.0(3)
C28#4-K2-O4-C23	101.2(6)	O4#4-K2-O5-C24#1	-31.0(3)
C28#5-K2-O4-C23	104.4(8)	O4#5-K2-O5-C24#1	163.0(2)
C28#1-K2-O4-C23	-75.6(8)	C28#4-K2-O5-C24	-69.3(8)
O6#5-K2-O4-C23	117.5(4)	C28#5-K2-O5-C24	-62.7(8)
O6#4-K2-O4-C23	131.6(5)	C28#1-K2-O5-C24	117.3(8)
O6'-K2-O4-C23	-48.3(5)	O6#5-K2-O5-C24	-80.5(5)
O6#1-K2-O4-C23	-62.5(4)	O6#4-K2-O5-C24	-51.5(5)
O5#4-K2-O4-C23	-162.8(2)	O6'-K2-O5-C24	128.5(5)
O5-K2-O4-C23	17.2(2)	O6#1-K2-O5-C24	99.5(5)
O4#4-K2-O4-C23	42(4)	O5#4-K2-O5-C24	137.8(2)
O4#5-K2-O4-C23	-148.7(3)	O4-K2-O5-C24	17.0(2)
C28#4-K2-O4-C22	-127.4(6)	O4#4-K2-O5-C24	-163.0(2)
C28#5-K2-O4-C22	-124.3(8)	O4#5-K2-O5-C24	31.0(3)

C28'#4-K2-O6-C25	108(23)	K2-O6-C28-C27	-102(2)
C28'#5-K2-O6-C25	60(6)	C28'#4-K2-O6'-C25'	-80(2)
C28'#1-K2-O6-C25	-120(6)	C28'#5-K2-O6'-C25'	-68(3)
O6'#5-K2-O6-C25	155.4(11)	C28'#1-K2-O6'-C25'	112(3)
O6'#4-K2-O6-C25	99.3(13)	O6'#5-K2-O6'-C25'	-136.8(19)
O6'-K2-O6-C25	-80.7(13)	O6'#4-K2-O6'-C25'	-76(21)
O6'#1-K2-O6-C25	-24.6(11)	O6'#1-K2-O6'-C25'	43.2(19)
O5#4-K2-O6-C25	134.8(10)	O5#4-K2-O6'-C25'	137.2(18)
O5-K2-O6-C25	-45.2(10)	O5-K2-O6'-C25'	-42.8(18)
O4-K2-O6-C25	16.3(10)	O4-K2-O6'-C25'	12.7(19)
O4#4-K2-O6-C25	-163.7(10)	O4#4-K2-O6'-C25'	-167.3(19)
O4#5-K2-O6-C25	72.4(9)	O4#5-K2-O6'-C25'	74.2(19)
C28'#4-K2-O6-C28	-138(23)	C28'#4-K2-O6'-C28'	180.002(2)
C28'#5-K2-O6-C28	175(5)	C28'#5-K2-O6'-C28'	-168(3)
C28'#1-K2-O6-C28	-5(5)	C28'#1-K2-O6'-C28'	12(3)
O6'#5-K2-O6-C28	-89.9(13)	O6'#5-K2-O6'-C28'	123.0(16)
O6'#4-K2-O6-C28	-145.9(11)	O6'#4-K2-O6'-C28'	-176(25)
O6'-K2-O6-C28	34.1(11)	O6'#1-K2-O6'-C28'	-57.0(16)
O6'#1-K2-O6-C28	90.1(13)	O5#4-K2-O6'-C28'	36.9(16)
O5#4-K2-O6-C28	-110.5(10)	O5-K2-O6'-C28'	-143.1(16)
O5-K2-O6-C28	69.5(10)	O4-K2-O6'-C28'	-87.5(16)
O4-K2-O6-C28	131.1(10)	O4#4-K2-O6'-C28'	92.5(16)
O4#4-K2-O6-C28	-48.9(10)	O4#5-K2-O6'-C28'	-26.1(16)
O4#5-K2-O6-C28	-172.9(10)	C28'-O6'-C25'-C26'	18(3)
C28-O6-C25-C26	-28(3)	K2-O6'-C25'-C26'	-65(3)
K2-O6-C25-C26	92(2)	O6'-C25'-C26'-C27'	-25(3)
O6-C25-C26-C27	30(3)	C25'-C26'-C27'-C28'	24(4)
C25-C26-C27-C28	-23(3)	C26'-C27'-C28'-O6'	-13(4)
C26-C27-C28-O6	6(3)	C25'-O6'-C28'-C27'	-1(5)
C25-O6-C28-C27	12(3)	K2-O6'-C28'-C27'	124(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z #2 -x,-y+1,-z #3 -x,-y+1,z #4 -x+1,-y+1,-z

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

REFERENCE NUMBER: 04172 [**R&D1**]

CRYSTAL STRUCTURE REPORT

$C_{67} H_{93} Co K_2 O_{14.5}$

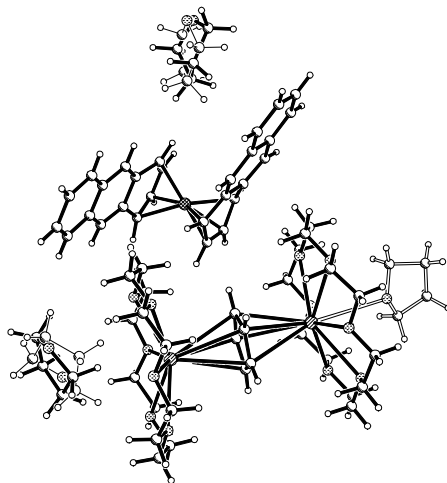
or

$\{[K(18\text{-crown-6})]_2[Cp] \cdot 1.5THF\}[Co(C_{14}H_{10})_2] \cdot THF$

Report prepared for:

W. Brennessel, Prof. J. Ellis

July 14, 2004



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Data collection

A crystal (approximate dimensions 0.42 x 0.18 x 0.12 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Siemens SMART Platform CCD diffractometer for a data collection at 173(2) K. A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 72 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 45 seconds and a detector distance of 4.90 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.84 Å. Three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).¹ Final cell constants were calculated from the xyz centroids of 3702 strong reflections from the actual data collection after integration (SAINT).² Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97³ and refined using SHELXL-97.⁴ The space group *C2/c* 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 $R1 = 0.0635$ and $wR2 = 0.1814$ (F^2 , all data).

Structure description

The structure is similar to the one suggested. It is a double salt of KCp and K[Co(C₁₄H₁₀)₂]. The potassium cations are complexed by 18-crown-6 ethers. Between K1 and K2 lies a Cp anion, making the entire unit a +1 cation. The outer portions of the potassium cations (outer axial positions) are occupied by THF solvent molecules, one of which is disordered over a two-fold axis (50:50). There is one additional THF solvent molecule in the asymmetric unit. The Co(C₁₄H₁₀)₂ anion is similar to those seen in previous structures. All atoms, except for the THF solvent molecule noted above, lie on general positions. The other two THF solvent molecules are modeled as disordered, each over two positions (60:40 and 73:27). Due to the disorders, all THF solvent molecules were restrained to be ideal.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-

-
- ¹ An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
 - ² SAINT V6.2, Bruker Analytical X-Ray Systems, Madison, WI (2001).
 - ³ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
 - ⁴ SHELXTL V6.10, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

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

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

where $w = q / [\sigma^2(F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$

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

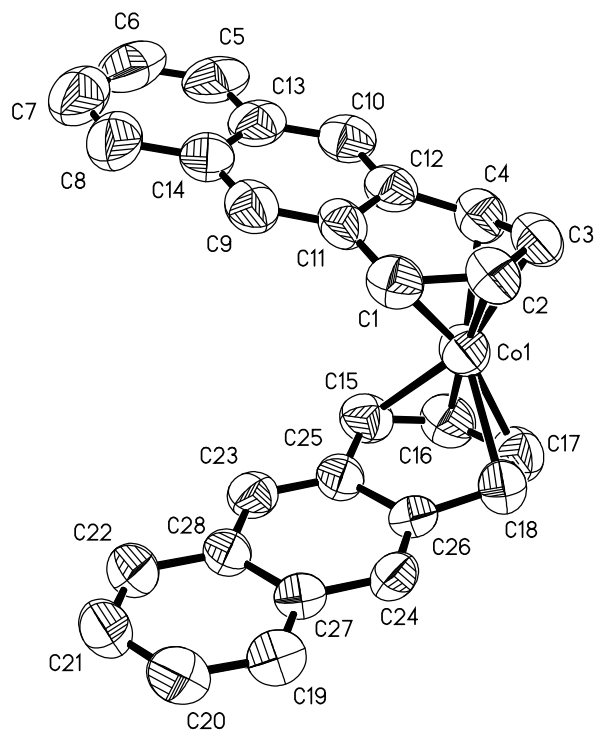
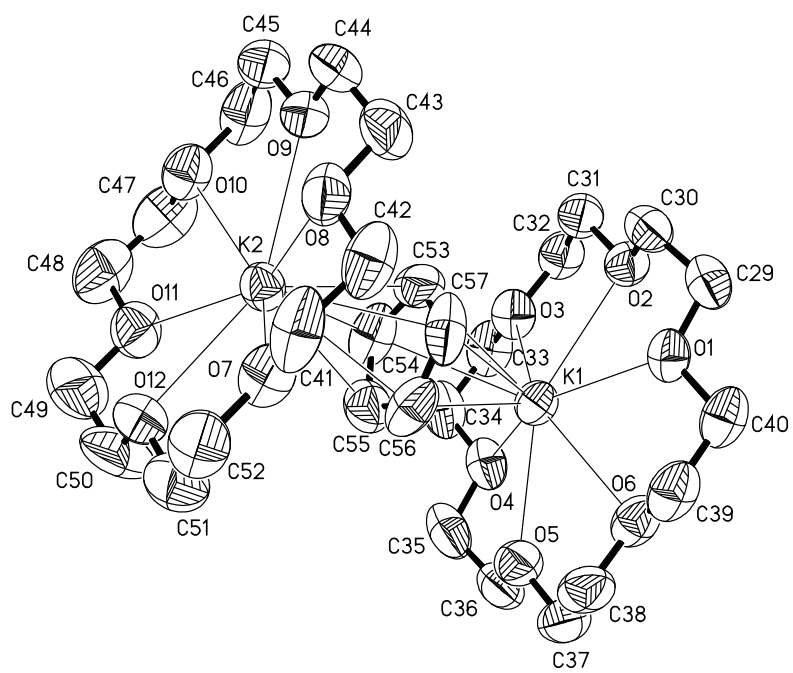


Table 1. Crystal data and structure refinement for 04172.

Identification code	04172	
Empirical formula	C ₆₇ H ₉₃ Co K ₂ O _{14.50}	
Formula weight	1267.54	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	$a = 27.534(3)$ Å	$\alpha = 90^\circ$
	$b = 9.7976(9)$ Å	$\beta = 96.106(2)^\circ$
	$c = 49.465(5)$ Å	$\gamma = 90^\circ$
Volume	13268(2) Å ³	
Z	8	
Density (calculated)	1.269 Mg/m ³	
Absorption coefficient	0.447 mm ⁻¹	
$F(000)$	5408	
Crystal color, morphology	red-black, needle	
Crystal size	0.42 x 0.18 x 0.12 mm ³	
Theta range for data collection	1.49 to 25.05°	
Index ranges	$-25 \leq h \leq 32$, $-11 \leq k \leq 11$, $-58 \leq l \leq 58$	
Reflections collected	37286	
Independent reflections	11749 [$R(\text{int}) = 0.0557$]	
Observed reflections	5887	
Completeness to $\theta = 25.05^\circ$	99.8%	
Absorption correction	Multi-scan	
Max. and min. transmission	1.000000 and 0.796189	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11749 / 81 / 799	
Goodness-of-fit on F^2	1.005	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0635$, $wR2 = 0.1532$	
R indices (all data)	$R1 = 0.1284$, $wR2 = 0.1814$	
Extinction coefficient	0.00026(5)	
Largest diff. peak and hole	0.363 and -0.345 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04172. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	1647(1)	589(1)	1076(1)	65(1)
C1	973(2)	772(5)	1243(1)	64(1)
C2	1061(2)	-512(5)	1128(1)	70(1)
C3	1485(2)	-1244(5)	1231(1)	69(1)
C4	1789(2)	-598(5)	1441(1)	68(1)
C5	1870(2)	2128(6)	2299(1)	90(2)
C6	1701(3)	3181(8)	2445(1)	105(2)
C7	1289(3)	3918(7)	2339(2)	110(2)
C8	1063(2)	3602(6)	2090(1)	94(2)
C9	995(2)	2146(5)	1668(1)	67(1)
C10	1813(2)	669(5)	1884(1)	69(1)
C11	1172(2)	1132(4)	1516(1)	61(1)
C12	1600(2)	365(4)	1625(1)	61(1)
C13	1640(2)	1759(5)	2042(1)	73(1)
C14	1223(2)	2517(5)	1930(1)	73(1)
C15	1932(2)	2589(5)	1091(1)	67(1)
C16	2248(2)	1586(5)	1003(1)	75(1)
C17	2089(2)	798(5)	777(1)	76(1)
C18	1614(2)	1071(5)	651(1)	68(1)
C19	312(2)	4453(5)	378(1)	71(1)
C20	53(2)	5595(5)	434(1)	78(1)
C21	209(2)	6383(5)	665(1)	76(1)
C22	614(2)	6010(5)	833(1)	70(1)
C23	1293(2)	4378(4)	958(1)	58(1)
C24	995(2)	2847(4)	499(1)	62(1)
C25	1544(2)	3191(4)	910(1)	56(1)
C26	1381(2)	2386(4)	674(1)	57(1)
C27	730(2)	4046(4)	547(1)	59(1)
C28	882(2)	4835(4)	783(1)	58(1)
K1	-1340(1)	334(1)	754(1)	59(1)
K2	-748(1)	-2325(1)	1766(1)	60(1)

O1	-581(1)	-676(3)	443(1)	66(1)
O2	-481(1)	1969(3)	658(1)	67(1)
O3	-1243(1)	3099(3)	931(1)	69(1)
O4	-2191(1)	2107(3)	789(1)	75(1)
O5	-2300(1)	-540(4)	571(1)	78(1)
O6	-1540(1)	-1621(3)	307(1)	74(1)
O7	-777(1)	-5129(3)	1615(1)	79(1)
O8	153(1)	-3834(4)	1679(1)	79(1)
O9	193(1)	-1147(4)	1873(1)	78(1)
O10	-535(1)	-190(3)	2182(1)	78(1)
O11	-1444(1)	-1464(4)	2117(1)	86(1)
O12	-1478(1)	-4193(4)	1938(1)	85(1)
C29	-167(2)	156(5)	419(1)	75(1)
C30	-83(2)	1032(5)	663(1)	70(1)
C31	-406(2)	2966(5)	868(1)	73(1)
C32	-839(2)	3869(5)	857(1)	76(1)
C33	-1669(2)	3900(5)	947(1)	81(2)
C34	-2067(2)	2979(5)	1013(1)	81(2)
C35	-2605(2)	1256(6)	816(1)	93(2)
C36	-2694(2)	389(6)	570(1)	87(2)
C37	-2380(2)	-1540(6)	361(1)	90(2)
C38	-1940(2)	-2422(5)	370(1)	86(2)
C39	-1124(2)	-2412(5)	270(1)	81(2)
C40	-723(2)	-1458(5)	208(1)	74(1)
C41	-338(3)	-5809(5)	1581(1)	98(2)
C42	16(2)	-4818(6)	1474(1)	88(2)
C43	493(2)	-2866(7)	1599(1)	92(2)
C44	617(2)	-1887(7)	1829(1)	98(2)
C45	280(2)	-150(7)	2078(1)	95(2)
C46	-161(3)	670(6)	2090(1)	105(2)
C47	-974(3)	519(6)	2214(1)	105(2)
C48	-1316(2)	-457(7)	2321(1)	110(2)
C49	-1771(2)	-2428(8)	2206(1)	116(2)
C50	-1900(2)	-3410(8)	1982(2)	122(2)
C51	-1590(2)	-5175(7)	1741(1)	106(2)
C52	-1146(3)	-5998(5)	1713(1)	105(2)

C53	-735(2)	-317(7)	1300(1)	88(2)
C54	-1188(3)	-102(5)	1376(1)	84(2)
C55	-1481(2)	-1145(7)	1291(1)	83(2)
C56	-1221(3)	-2056(5)	1159(1)	83(2)
C57	-751(2)	-1563(7)	1163(1)	90(2)
O13	-313(5)	-3880(10)	2329(2)	137(3)
C58	-211(5)	-5306(9)	2299(2)	88(2)
C59	87(6)	-5720(8)	2560(2)	88(2)
C60	250(10)	-4370(13)	2696(3)	137(3)
C61	149(4)	-3375(9)	2455(2)	88(2)
O14	-1589(3)	3958(7)	111(1)	136(2)
C62	-1800(4)	2647(9)	146(2)	104(3)
C63	-1685(4)	1721(12)	-82(3)	122(4)
C64	-1220(5)	2341(8)	-174(3)	122(3)
C65	-1175(5)	3704(12)	-36(3)	122(3)
O14'	-1239(8)	1440(20)	-113(4)	136(2)
C62'	-1186(18)	2820(30)	-204(7)	122(3)
C63'	-1243(17)	3710(30)	44(8)	122(3)
C64'	-1509(10)	2760(30)	225(4)	104(3)
C65'	-1669(11)	1610(40)	26(8)	122(4)
O15	2696(4)	6733(15)	1978(3)	103(2)
C66	2252(5)	6850(20)	2104(3)	114(4)
C67	1863(5)	6360(20)	1884(4)	86(3)
C68	2135(7)	5260(20)	1743(6)	133(4)
C69	2615(6)	6000(30)	1726(3)	107(3)
O15'	2479(3)	7227(8)	1963(2)	103(2)
C66'	2004(4)	6654(13)	1981(2)	114(4)
C67'	1897(3)	5688(11)	1744(2)	86(3)
C68'	2396(4)	5257(13)	1685(3)	133(4)
C69'	2749(3)	6289(13)	1816(3)	107(3)

Table 3. Bond lengths [Å] and angles [°] for 04172.

Co(1)-C(2)	1.980(5)	C(15)-C(16)	1.412(6)
Co(1)-C(16)	1.987(5)	C(15)-C(25)	1.444(6)
Co(1)-C(17)	2.021(5)	C(15)-H(15A)	1.0000
Co(1)-C(3)	2.022(4)	C(16)-C(17)	1.390(6)
Co(1)-C(15)	2.109(4)	C(16)-H(16A)	1.0000
Co(1)-C(1)	2.118(4)	C(17)-C(18)	1.413(6)
Co(1)-C(18)	2.146(5)	C(17)-H(17A)	1.0000
Co(1)-C(4)	2.149(5)	C(18)-C(26)	1.448(6)
C(1)-C(2)	1.413(6)	C(18)-H(18A)	1.0000
C(1)-C(11)	1.447(6)	C(19)-C(20)	1.369(6)
C(1)-H(1A)	1.0000	C(19)-C(27)	1.408(6)
C(2)-C(3)	1.417(6)	C(19)-H(19A)	0.9500
C(2)-H(2A)	1.0000	C(20)-C(21)	1.408(7)
C(3)-C(4)	1.413(6)	C(20)-H(20A)	0.9500
C(3)-H(3A)	1.0000	C(21)-C(22)	1.365(7)
C(4)-C(12)	1.444(6)	C(21)-H(21A)	0.9500
C(4)-H(4A)	1.0000	C(22)-C(28)	1.405(6)
C(5)-C(6)	1.368(8)	C(22)-H(22A)	0.9500
C(5)-C(13)	1.409(7)	C(23)-C(25)	1.385(6)
C(5)-H(5A)	0.9500	C(23)-C(28)	1.421(6)
C(6)-C(7)	1.399(9)	C(23)-H(23A)	0.9500
C(6)-H(6A)	0.9500	C(24)-C(26)	1.373(6)
C(7)-C(8)	1.356(8)	C(24)-C(27)	1.416(6)
C(7)-H(7A)	0.9500	C(24)-H(24A)	0.9500
C(8)-C(14)	1.422(7)	C(25)-C(26)	1.442(6)
C(8)-H(8A)	0.9500	C(27)-C(28)	1.423(6)
C(9)-C(11)	1.367(6)	K(1)-O(5)	2.834(3)
C(9)-C(14)	1.424(7)	K(1)-O(3)	2.851(3)
C(9)-H(9A)	0.9500	K(1)-O(1)	2.893(3)
C(10)-C(12)	1.386(6)	K(1)-O(6)	2.930(3)
C(10)-C(13)	1.433(7)	K(1)-O(2)	2.937(3)
C(10)-H(10A)	0.9500	K(1)-O(4)	2.938(3)
C(11)-C(12)	1.450(6)	K(1)-C(56)	3.077(5)
C(13)-C(14)	1.428(7)	K(1)-C(57)	3.080(5)

K(1)-C(53)	3.087(5)	O(11)-C(49)	1.406(7)
K(1)-C(55)	3.090(5)	O(11)-C(48)	1.429(6)
K(1)-C(54)	3.094(5)	O(12)-C(51)	1.379(6)
K(1)-C(64')	3.53(3)	O(12)-C(50)	1.427(7)
K(2)-O(9)	2.836(3)	C(29)-C(30)	1.480(6)
K(2)-O(11)	2.845(3)	C(29)-H(29A)	0.9900
K(2)-O(7)	2.846(3)	C(29)-H(29B)	0.9900
K(2)-O(12)	2.911(3)	C(30)-H(30A)	0.9900
K(2)-O(10)	2.949(3)	C(30)-H(30B)	0.9900
K(2)-O(8)	2.959(3)	C(31)-C(32)	1.480(6)
K(2)-C(53)	3.034(5)	C(31)-H(31A)	0.9900
K(2)-C(54)	3.071(5)	C(31)-H(31B)	0.9900
K(2)-C(57)	3.076(5)	C(32)-H(32A)	0.9900
K(2)-C(55)	3.149(5)	C(32)-H(32B)	0.9900
K(2)-C(56)	3.156(5)	C(33)-C(34)	1.483(7)
K(2)-O(13)	3.285(10)	C(33)-H(33A)	0.9900
O(1)-C(40)	1.413(5)	C(33)-H(33B)	0.9900
O(1)-C(29)	1.418(5)	C(34)-H(34A)	0.9900
O(2)-C(31)	1.425(5)	C(34)-H(34B)	0.9900
O(2)-C(30)	1.428(5)	C(35)-C(36)	1.484(7)
O(3)-C(33)	1.421(5)	C(35)-H(35A)	0.9900
O(3)-C(32)	1.423(5)	C(35)-H(35B)	0.9900
O(4)-C(34)	1.412(6)	C(36)-H(36A)	0.9900
O(4)-C(35)	1.430(6)	C(36)-H(36B)	0.9900
O(5)-C(36)	1.415(6)	C(37)-C(38)	1.484(7)
O(5)-C(37)	1.429(6)	C(37)-H(37A)	0.9900
O(6)-C(39)	1.411(6)	C(37)-H(37B)	0.9900
O(6)-C(38)	1.413(6)	C(38)-H(38A)	0.9900
O(7)-C(41)	1.405(6)	C(38)-H(38B)	0.9900
O(7)-C(52)	1.450(6)	C(39)-C(40)	1.503(7)
O(8)-C(43)	1.420(6)	C(39)-H(39A)	0.9900
O(8)-C(42)	1.421(6)	C(39)-H(39B)	0.9900
O(9)-C(45)	1.408(6)	C(40)-H(40A)	0.9900
O(9)-C(44)	1.409(6)	C(40)-H(40B)	0.9900
O(10)-C(47)	1.415(6)	C(41)-C(42)	1.511(7)
O(10)-C(46)	1.443(6)	C(41)-H(41A)	0.9900

C(41)-H(41B)	0.9900	C(56)-H(56A)	0.9500
C(42)-H(42A)	0.9900	C(57)-H(57A)	0.9500
C(42)-H(42B)	0.9900	O(13)-C(58)	1.436(5)
C(43)-C(44)	1.501(7)	O(13)-C(61)	1.444(5)
C(43)-H(43A)	0.9900	C(58)-C(59)	1.511(8)
C(43)-H(43B)	0.9900	C(58)-H(58A)	0.9900
C(44)-H(44A)	0.9900	C(58)-H(58B)	0.9900
C(44)-H(44B)	0.9900	C(59)-C(60)	1.528(10)
C(45)-C(46)	1.462(8)	C(59)-H(59A)	0.9900
C(45)-H(45A)	0.9900	C(59)-H(59B)	0.9900
C(45)-H(45B)	0.9900	C(60)-C(61)	1.540(9)
C(46)-H(46A)	0.9900	C(60)-K(2)#1	3.494(12)
C(46)-H(46B)	0.9900	C(60)-H(60A)	0.9900
C(47)-C(48)	1.480(8)	C(60)-H(60B)	0.9900
C(47)-H(47A)	0.9900	C(61)-H(61A)	0.9900
C(47)-H(47B)	0.9900	C(61)-H(61B)	0.9900
C(48)-H(48A)	0.9900	O(14)-C(62)	1.427(5)
C(48)-H(48B)	0.9900	O(14)-C(65)	1.438(5)
C(49)-C(50)	1.480(8)	C(62)-C(63)	1.505(7)
C(49)-H(49A)	0.9900	C(62)-H(62A)	0.9900
C(49)-H(49B)	0.9900	C(62)-H(62B)	0.9900
C(50)-H(50A)	0.9900	C(63)-C(64)	1.528(8)
C(50)-H(50B)	0.9900	C(63)-H(63A)	0.9900
C(51)-C(52)	1.482(8)	C(63)-H(63B)	0.9900
C(51)-H(51A)	0.9900	C(64)-C(65)	1.498(7)
C(51)-H(51B)	0.9900	C(64)-H(64A)	0.9900
C(52)-H(52A)	0.9900	C(64)-H(64B)	0.9900
C(52)-H(52B)	0.9900	C(65)-H(65A)	0.9900
C(53)-C(54)	1.357(7)	C(65)-H(65B)	0.9900
C(53)-C(57)	1.396(8)	O(14')-C(62')	1.442(5)
C(53)-H(53A)	0.9500	O(14')-C(65')	1.443(5)
C(54)-C(55)	1.341(7)	C(62')-C(63')	1.524(9)
C(54)-H(54A)	0.9500	C(62')-H(62C)	0.9900
C(55)-C(56)	1.356(7)	C(62')-H(62D)	0.9900
C(55)-H(55A)	0.9500	C(63')-C(64')	1.529(9)
C(56)-C(57)	1.379(7)	C(63')-H(63C)	0.9900

C(63')-H(63D)	0.9900	C(16)-Co(1)-C(3)	136.7(2)
C(64')-C(65')	1.526(9)	C(17)-Co(1)-C(3)	122.8(2)
C(64')-H(64C)	0.9900	C(2)-Co(1)-C(15)	143.80(19)
C(64')-H(64D)	0.9900	C(16)-Co(1)-C(15)	40.18(18)
C(65')-H(65C)	0.9900	C(17)-Co(1)-C(15)	71.42(19)
C(65')-H(65D)	0.9900	C(3)-Co(1)-C(15)	155.29(19)
O(15)-C(66)	1.433(5)	C(2)-Co(1)-C(1)	40.15(17)
O(15)-C(69)	1.438(5)	C(16)-Co(1)-C(1)	144.1(2)
C(66)-C(67)	1.519(8)	C(17)-Co(1)-C(1)	153.8(2)
C(66)-H(66A)	0.9900	C(3)-Co(1)-C(1)	71.88(18)
C(66)-H(66B)	0.9900	C(15)-Co(1)-C(1)	104.24(19)
C(67)-C(68)	1.524(9)	C(2)-Co(1)-C(18)	107.3(2)
C(67)-H(67A)	0.9900	C(16)-Co(1)-C(18)	70.3(2)
C(67)-H(67B)	0.9900	C(17)-Co(1)-C(18)	39.49(18)
C(68)-C(69)	1.515(8)	C(3)-Co(1)-C(18)	125.38(19)
C(68)-H(68A)	0.9900	C(15)-Co(1)-C(18)	78.87(18)
C(68)-H(68B)	0.9900	C(1)-Co(1)-C(18)	114.57(18)
C(69)-H(69A)	0.9900	C(2)-Co(1)-C(4)	70.92(19)
C(69)-H(69B)	0.9900	C(16)-Co(1)-C(4)	109.80(19)
O(15')-C(69')	1.430(5)	C(17)-Co(1)-C(4)	126.85(19)
O(15')-C(66')	1.434(5)	C(3)-Co(1)-C(4)	39.45(17)
C(66')-C(67')	1.513(7)	C(15)-Co(1)-C(4)	116.07(18)
C(66')-H(66C)	0.9900	C(1)-Co(1)-C(4)	78.79(17)
C(66')-H(66D)	0.9900	C(18)-Co(1)-C(4)	158.01(18)
C(67')-C(68')	1.496(8)	C(2)-C(1)-C(11)	122.0(4)
C(67')-H(67C)	0.9900	C(2)-C(1)-Co(1)	64.6(3)
C(67')-H(67D)	0.9900	C(11)-C(1)-Co(1)	97.1(3)
C(68')-C(69')	1.501(7)	C(2)-C(1)-H(1A)	118.5
C(68')-H(68C)	0.9900	C(11)-C(1)-H(1A)	118.5
C(68')-H(68D)	0.9900	Co(1)-C(1)-H(1A)	118.5
C(69')-H(69C)	0.9900	C(1)-C(2)-C(3)	118.4(4)
C(69')-H(69D)	0.9900	C(1)-C(2)-Co(1)	75.2(3)
C(2)-Co(1)-C(16)	175.5(2)	C(3)-C(2)-Co(1)	70.8(3)
C(2)-Co(1)-C(17)	135.4(2)	C(1)-C(2)-H(2A)	120.7
C(16)-Co(1)-C(17)	40.56(19)	C(3)-C(2)-H(2A)	120.7
C(2)-Co(1)-C(3)	41.46(18)	Co(1)-C(2)-H(2A)	120.7

C(4)-C(3)-C(2)	116.0(4)	C(5)-C(13)-C(14)	118.9(5)
C(4)-C(3)-Co(1)	75.1(3)	C(5)-C(13)-C(10)	122.7(5)
C(2)-C(3)-Co(1)	67.7(3)	C(14)-C(13)-C(10)	118.5(5)
C(4)-C(3)-H(3A)	121.9	C(8)-C(14)-C(9)	124.3(5)
C(2)-C(3)-H(3A)	121.9	C(8)-C(14)-C(13)	117.1(5)
Co(1)-C(3)-H(3A)	121.9	C(9)-C(14)-C(13)	118.6(5)
C(3)-C(4)-C(12)	122.1(4)	C(16)-C(15)-C(25)	122.2(4)
C(3)-C(4)-Co(1)	65.4(3)	C(16)-C(15)-Co(1)	65.3(3)
C(12)-C(4)-Co(1)	97.4(3)	C(25)-C(15)-Co(1)	96.3(3)
C(3)-C(4)-H(4A)	118.3	C(16)-C(15)-H(15A)	118.4
C(12)-C(4)-H(4A)	118.3	C(25)-C(15)-H(15A)	118.4
Co(1)-C(4)-H(4A)	118.3	Co(1)-C(15)-H(15A)	118.4
C(6)-C(5)-C(13)	121.6(6)	C(17)-C(16)-C(15)	118.9(5)
C(6)-C(5)-H(5A)	119.2	C(17)-C(16)-Co(1)	71.0(3)
C(13)-C(5)-H(5A)	119.2	C(15)-C(16)-Co(1)	74.6(3)
C(5)-C(6)-C(7)	120.0(6)	C(17)-C(16)-H(16A)	120.4
C(5)-C(6)-H(6A)	120.0	C(15)-C(16)-H(16A)	120.4
C(7)-C(6)-H(6A)	120.0	Co(1)-C(16)-H(16A)	120.4
C(8)-C(7)-C(6)	119.8(6)	C(16)-C(17)-C(18)	116.6(5)
C(8)-C(7)-H(7A)	120.1	C(16)-C(17)-Co(1)	68.4(3)
C(6)-C(7)-H(7A)	120.1	C(18)-C(17)-Co(1)	75.0(3)
C(7)-C(8)-C(14)	122.5(6)	C(16)-C(17)-H(17A)	121.6
C(7)-C(8)-H(8A)	118.7	C(18)-C(17)-H(17A)	121.6
C(14)-C(8)-H(8A)	118.7	Co(1)-C(17)-H(17A)	121.6
C(11)-C(9)-C(14)	122.4(5)	C(17)-C(18)-C(26)	122.0(5)
C(11)-C(9)-H(9A)	118.8	C(17)-C(18)-Co(1)	65.5(3)
C(14)-C(9)-H(9A)	118.8	C(26)-C(18)-Co(1)	95.3(3)
C(12)-C(10)-C(13)	122.1(5)	C(17)-C(18)-H(18A)	118.5
C(12)-C(10)-H(10A)	119.0	C(26)-C(18)-H(18A)	118.5
C(13)-C(10)-H(10A)	119.0	Co(1)-C(18)-H(18A)	118.5
C(9)-C(11)-C(1)	124.6(4)	C(20)-C(19)-C(27)	121.4(5)
C(9)-C(11)-C(12)	119.8(4)	C(20)-C(19)-H(19A)	119.3
C(1)-C(11)-C(12)	115.5(4)	C(27)-C(19)-H(19A)	119.3
C(10)-C(12)-C(4)	125.2(4)	C(19)-C(20)-C(21)	119.5(5)
C(10)-C(12)-C(11)	118.6(4)	C(19)-C(20)-H(20A)	120.2
C(4)-C(12)-C(11)	116.0(4)	C(21)-C(20)-H(20A)	120.2

C(22)-C(21)-C(20)	120.2(5)	O(1)-K(1)-O(4)	149.21(9)
C(22)-C(21)-H(21A)	119.9	O(6)-K(1)-O(4)	110.11(11)
C(20)-C(21)-H(21A)	119.9	O(2)-K(1)-O(4)	110.39(9)
C(21)-C(22)-C(28)	121.6(5)	O(5)-K(1)-C(56)	90.51(14)
C(21)-C(22)-H(22A)	119.2	O(3)-K(1)-C(56)	121.54(11)
C(28)-C(22)-H(22A)	119.2	O(1)-K(1)-C(56)	92.99(15)
C(25)-C(23)-C(28)	122.7(4)	O(6)-K(1)-C(56)	89.54(11)
C(25)-C(23)-H(23A)	118.7	O(2)-K(1)-C(56)	119.22(15)
C(28)-C(23)-H(23A)	118.7	O(4)-K(1)-C(56)	116.21(15)
C(26)-C(24)-C(27)	123.1(4)	O(5)-K(1)-C(57)	115.81(17)
C(26)-C(24)-H(24A)	118.5	O(3)-K(1)-C(57)	110.25(16)
C(27)-C(24)-H(24A)	118.5	O(1)-K(1)-C(57)	77.45(11)
C(23)-C(25)-C(26)	118.7(4)	O(6)-K(1)-C(57)	98.31(15)
C(23)-C(25)-C(15)	126.0(4)	O(2)-K(1)-C(57)	93.34(16)
C(26)-C(25)-C(15)	115.1(4)	O(4)-K(1)-C(57)	133.28(11)
C(24)-C(26)-C(25)	118.9(4)	C(56)-K(1)-C(57)	25.88(14)
C(24)-C(26)-C(18)	124.2(4)	O(5)-K(1)-C(53)	127.92(12)
C(25)-C(26)-C(18)	116.7(4)	O(3)-K(1)-C(53)	84.45(14)
C(19)-C(27)-C(24)	122.6(4)	O(1)-K(1)-C(53)	92.36(16)
C(19)-C(27)-C(28)	119.0(4)	O(6)-K(1)-C(53)	124.43(16)
C(24)-C(27)-C(28)	118.4(4)	O(2)-K(1)-C(53)	83.41(12)
C(22)-C(28)-C(23)	123.4(4)	O(4)-K(1)-C(53)	115.43(17)
C(22)-C(28)-C(27)	118.3(4)	C(56)-K(1)-C(53)	42.44(14)
C(23)-C(28)-C(27)	118.3(4)	C(57)-K(1)-C(53)	26.16(14)
O(5)-K(1)-O(3)	116.02(10)	O(5)-K(1)-C(55)	86.23(12)
O(5)-K(1)-O(1)	115.42(10)	O(3)-K(1)-C(55)	101.40(15)
O(3)-K(1)-O(1)	115.99(9)	O(1)-K(1)-C(55)	117.38(13)
O(5)-K(1)-O(6)	57.85(10)	O(6)-K(1)-C(55)	108.13(15)
O(3)-K(1)-O(6)	148.92(9)	O(2)-K(1)-C(55)	124.87(13)
O(1)-K(1)-O(6)	57.73(10)	O(4)-K(1)-C(55)	92.98(13)
O(5)-K(1)-O(2)	148.61(9)	C(56)-K(1)-C(55)	25.41(13)
O(3)-K(1)-O(2)	58.68(9)	C(57)-K(1)-C(55)	41.99(13)
O(1)-K(1)-O(2)	57.46(9)	C(53)-K(1)-C(55)	41.80(14)
O(6)-K(1)-O(2)	109.01(9)	O(5)-K(1)-C(54)	107.35(16)
O(5)-K(1)-O(4)	58.29(10)	O(3)-K(1)-C(54)	80.05(12)
O(3)-K(1)-O(4)	57.93(10)	O(1)-K(1)-C(54)	116.86(14)

O(6)-K(1)-C(54)	130.88(12)	O(12)-K(2)-C(53)	133.92(13)
O(2)-K(1)-C(54)	102.11(15)	O(10)-K(2)-C(53)	93.02(15)
O(4)-K(1)-C(54)	92.67(13)	O(8)-K(2)-C(53)	97.80(16)
C(56)-K(1)-C(54)	41.63(13)	O(9)-K(2)-C(54)	96.89(16)
C(57)-K(1)-C(54)	41.95(13)	O(11)-K(2)-C(54)	85.80(14)
C(53)-K(1)-C(54)	25.36(14)	O(7)-K(2)-C(54)	121.41(12)
C(55)-K(1)-C(54)	25.06(14)	O(12)-K(2)-C(54)	112.99(16)
O(5)-K(1)-C(64')	85.5(4)	O(10)-K(2)-C(54)	88.33(12)
O(3)-K(1)-C(64')	65.7(4)	O(8)-K(2)-C(54)	122.95(14)
O(1)-K(1)-C(64')	83.3(4)	C(53)-K(2)-C(54)	25.67(14)
O(6)-K(1)-C(64')	83.2(4)	O(9)-K(2)-C(57)	89.41(16)
O(2)-K(1)-C(64')	63.8(4)	O(11)-K(2)-C(57)	125.98(12)
O(4)-K(1)-C(64')	66.6(4)	O(7)-K(2)-C(57)	88.95(15)
C(56)-K(1)-C(64')	172.8(4)	O(12)-K(2)-C(57)	120.35(17)
C(57)-K(1)-C(64')	155.9(4)	O(10)-K(2)-C(57)	118.99(17)
C(53)-K(1)-C(64')	143.6(4)	O(8)-K(2)-C(57)	84.01(11)
C(55)-K(1)-C(64')	159.3(4)	C(53)-K(2)-C(57)	26.39(15)
C(54)-K(1)-C(64')	145.5(4)	C(54)-K(2)-C(57)	42.15(13)
O(9)-K(2)-O(11)	115.28(11)	O(9)-K(2)-C(55)	119.33(13)
O(9)-K(2)-O(7)	116.17(11)	O(11)-K(2)-C(55)	85.80(13)
O(11)-K(2)-O(7)	116.42(11)	O(7)-K(2)-C(55)	99.23(15)
O(9)-K(2)-O(12)	147.94(10)	O(12)-K(2)-C(55)	92.35(13)
O(11)-K(2)-O(12)	58.53(11)	O(10)-K(2)-C(55)	108.91(15)
O(7)-K(2)-O(12)	57.96(11)	O(8)-K(2)-C(55)	123.76(13)
O(9)-K(2)-O(10)	58.08(10)	C(53)-K(2)-C(55)	41.70(14)
O(11)-K(2)-O(10)	57.38(11)	C(54)-K(2)-C(55)	24.87(14)
O(7)-K(2)-O(10)	150.02(9)	C(57)-K(2)-C(55)	41.57(13)
O(12)-K(2)-O(10)	109.54(10)	O(9)-K(2)-C(56)	114.80(14)
O(9)-K(2)-O(8)	57.73(11)	O(11)-K(2)-C(56)	108.65(15)
O(11)-K(2)-O(8)	149.99(10)	O(7)-K(2)-C(56)	80.39(11)
O(7)-K(2)-O(8)	58.65(11)	O(12)-K(2)-C(56)	95.91(14)
O(12)-K(2)-O(8)	110.14(11)	O(10)-K(2)-C(56)	129.50(12)
O(10)-K(2)-O(8)	110.38(10)	O(8)-K(2)-C(56)	99.83(14)
O(9)-K(2)-C(53)	78.07(12)	C(53)-K(2)-C(56)	42.19(14)
O(11)-K(2)-C(53)	109.53(17)	C(54)-K(2)-C(56)	41.21(13)
O(7)-K(2)-C(53)	115.35(15)	C(57)-K(2)-C(56)	25.52(14)

C(55)-K(2)-C(56)	24.84(13)	C(45)-O(9)-C(44)	112.8(4)
O(9)-K(2)-O(13)	77.7(3)	C(45)-O(9)-K(2)	119.9(3)
O(11)-K(2)-O(13)	80.2(2)	C(44)-O(9)-K(2)	121.1(3)
O(7)-K(2)-O(13)	76.87(18)	C(47)-O(10)-C(46)	113.3(5)
O(12)-K(2)-O(13)	70.3(3)	C(47)-O(10)-K(2)	108.5(3)
O(10)-K(2)-O(13)	73.17(18)	C(46)-O(10)-K(2)	106.7(3)
O(8)-K(2)-O(13)	69.8(2)	C(49)-O(11)-C(48)	111.2(5)
C(53)-K(2)-O(13)	155.7(3)	C(49)-O(11)-K(2)	119.1(3)
C(54)-K(2)-O(13)	160.9(2)	C(48)-O(11)-K(2)	120.3(3)
C(57)-K(2)-O(13)	153.8(2)	C(51)-O(12)-C(50)	111.1(5)
C(55)-K(2)-O(13)	161.7(3)	C(51)-O(12)-K(2)	110.0(3)
C(56)-K(2)-O(13)	157.2(2)	C(50)-O(12)-K(2)	107.8(3)
C(40)-O(1)-C(29)	113.2(3)	O(1)-C(29)-C(30)	108.6(4)
C(40)-O(1)-K(1)	118.0(3)	O(1)-C(29)-H(29A)	110.0
C(29)-O(1)-K(1)	118.8(2)	C(30)-C(29)-H(29A)	110.0
C(31)-O(2)-C(30)	112.2(3)	O(1)-C(29)-H(29B)	110.0
C(31)-O(2)-K(1)	108.2(2)	C(30)-C(29)-H(29B)	110.0
C(30)-O(2)-K(1)	106.0(2)	H(29A)-C(29)-H(29B)	108.3
C(33)-O(3)-C(32)	113.3(4)	O(2)-C(30)-C(29)	107.8(4)
C(33)-O(3)-K(1)	119.5(3)	O(2)-C(30)-H(30A)	110.1
C(32)-O(3)-K(1)	118.4(3)	C(29)-C(30)-H(30A)	110.1
C(34)-O(4)-C(35)	114.0(4)	O(2)-C(30)-H(30B)	110.1
C(34)-O(4)-K(1)	106.1(3)	C(29)-C(30)-H(30B)	110.1
C(35)-O(4)-K(1)	108.0(3)	H(30A)-C(30)-H(30B)	108.5
C(36)-O(5)-C(37)	112.4(4)	O(2)-C(31)-C(32)	109.2(4)
C(36)-O(5)-K(1)	119.7(3)	O(2)-C(31)-H(31A)	109.8
C(37)-O(5)-K(1)	120.4(3)	C(32)-C(31)-H(31A)	109.8
C(39)-O(6)-C(38)	112.7(4)	O(2)-C(31)-H(31B)	109.8
C(39)-O(6)-K(1)	111.5(3)	C(32)-C(31)-H(31B)	109.8
C(38)-O(6)-K(1)	106.7(3)	H(31A)-C(31)-H(31B)	108.3
C(41)-O(7)-C(52)	113.8(4)	O(3)-C(32)-C(31)	108.8(4)
C(41)-O(7)-K(2)	119.2(3)	O(3)-C(32)-H(32A)	109.9
C(52)-O(7)-K(2)	118.6(3)	C(31)-C(32)-H(32A)	109.9
C(43)-O(8)-C(42)	112.7(4)	O(3)-C(32)-H(32B)	109.9
C(43)-O(8)-K(2)	107.2(3)	C(31)-C(32)-H(32B)	109.9
C(42)-O(8)-K(2)	106.3(3)	H(32A)-C(32)-H(32B)	108.3

O(3)-C(33)-C(34)	108.1(4)	O(6)-C(39)-C(40)	108.0(4)
O(3)-C(33)-H(33A)	110.1	O(6)-C(39)-H(39A)	110.1
C(34)-C(33)-H(33A)	110.1	C(40)-C(39)-H(39A)	110.1
O(3)-C(33)-H(33B)	110.1	O(6)-C(39)-H(39B)	110.1
C(34)-C(33)-H(33B)	110.1	C(40)-C(39)-H(39B)	110.1
H(33A)-C(33)-H(33B)	108.4	H(39A)-C(39)-H(39B)	108.4
O(4)-C(34)-C(33)	108.6(4)	O(1)-C(40)-C(39)	108.3(4)
O(4)-C(34)-H(34A)	110.0	O(1)-C(40)-H(40A)	110.0
C(33)-C(34)-H(34A)	110.0	C(39)-C(40)-H(40A)	110.0
O(4)-C(34)-H(34B)	110.0	O(1)-C(40)-H(40B)	110.0
C(33)-C(34)-H(34B)	110.0	C(39)-C(40)-H(40B)	110.0
H(34A)-C(34)-H(34B)	108.4	H(40A)-C(40)-H(40B)	108.4
O(4)-C(35)-C(36)	108.6(4)	O(7)-C(41)-C(42)	109.4(4)
O(4)-C(35)-H(35A)	110.0	O(7)-C(41)-H(41A)	109.8
C(36)-C(35)-H(35A)	110.0	C(42)-C(41)-H(41A)	109.8
O(4)-C(35)-H(35B)	110.0	O(7)-C(41)-H(41B)	109.8
C(36)-C(35)-H(35B)	110.0	C(42)-C(41)-H(41B)	109.8
H(35A)-C(35)-H(35B)	108.4	H(41A)-C(41)-H(41B)	108.2
O(5)-C(36)-C(35)	107.9(4)	O(8)-C(42)-C(41)	108.6(4)
O(5)-C(36)-H(36A)	110.1	O(8)-C(42)-H(42A)	110.0
C(35)-C(36)-H(36A)	110.1	C(41)-C(42)-H(42A)	110.0
O(5)-C(36)-H(36B)	110.1	O(8)-C(42)-H(42B)	110.0
C(35)-C(36)-H(36B)	110.1	C(41)-C(42)-H(42B)	110.0
H(36A)-C(36)-H(36B)	108.4	H(42A)-C(42)-H(42B)	108.4
O(5)-C(37)-C(38)	108.3(4)	O(8)-C(43)-C(44)	108.5(4)
O(5)-C(37)-H(37A)	110.0	O(8)-C(43)-H(43A)	110.0
C(38)-C(37)-H(37A)	110.0	C(44)-C(43)-H(43A)	110.0
O(5)-C(37)-H(37B)	110.0	O(8)-C(43)-H(43B)	110.0
C(38)-C(37)-H(37B)	110.0	C(44)-C(43)-H(43B)	110.0
H(37A)-C(37)-H(37B)	108.4	H(43A)-C(43)-H(43B)	108.4
O(6)-C(38)-C(37)	108.8(4)	O(9)-C(44)-C(43)	108.8(4)
O(6)-C(38)-H(38A)	109.9	O(9)-C(44)-H(44A)	109.9
C(37)-C(38)-H(38A)	109.9	C(43)-C(44)-H(44A)	109.9
O(6)-C(38)-H(38B)	109.9	O(9)-C(44)-H(44B)	109.9
C(37)-C(38)-H(38B)	109.9	C(43)-C(44)-H(44B)	109.9
H(38A)-C(38)-H(38B)	108.3	H(44A)-C(44)-H(44B)	108.3

O(9)-C(45)-C(46)	109.4(5)	O(12)-C(51)-C(52)	108.8(5)
O(9)-C(45)-H(45A)	109.8	O(12)-C(51)-H(51A)	109.9
C(46)-C(45)-H(45A)	109.8	C(52)-C(51)-H(51A)	109.9
O(9)-C(45)-H(45B)	109.8	O(12)-C(51)-H(51B)	109.9
C(46)-C(45)-H(45B)	109.8	C(52)-C(51)-H(51B)	109.9
H(45A)-C(45)-H(45B)	108.2	H(51A)-C(51)-H(51B)	108.3
O(10)-C(46)-C(45)	108.4(4)	O(7)-C(52)-C(51)	109.0(4)
O(10)-C(46)-H(46A)	110.0	O(7)-C(52)-H(52A)	109.9
C(45)-C(46)-H(46A)	110.0	C(51)-C(52)-H(52A)	109.9
O(10)-C(46)-H(46B)	110.0	O(7)-C(52)-H(52B)	109.9
C(45)-C(46)-H(46B)	110.0	C(51)-C(52)-H(52B)	109.9
H(46A)-C(46)-H(46B)	108.4	H(52A)-C(52)-H(52B)	108.3
O(10)-C(47)-C(48)	107.8(5)	C(54)-C(53)-C(57)	106.8(5)
O(10)-C(47)-H(47A)	110.2	C(54)-C(53)-K(2)	78.7(3)
C(48)-C(47)-H(47A)	110.2	C(57)-C(53)-K(2)	78.5(3)
O(10)-C(47)-H(47B)	110.2	C(54)-C(53)-K(1)	77.6(3)
C(48)-C(47)-H(47B)	110.2	C(57)-C(53)-K(1)	76.6(3)
H(47A)-C(47)-H(47B)	108.5	K(2)-C(53)-K(1)	138.65(19)
O(11)-C(48)-C(47)	108.1(5)	C(54)-C(53)-H(53A)	126.6
O(11)-C(48)-H(48A)	110.1	C(57)-C(53)-H(53A)	126.6
C(47)-C(48)-H(48A)	110.1	K(2)-C(53)-H(53A)	109.4
O(11)-C(48)-H(48B)	110.1	K(1)-C(53)-H(53A)	112.0
C(47)-C(48)-H(48B)	110.1	C(55)-C(54)-C(53)	109.5(5)
H(48A)-C(48)-H(48B)	108.4	C(55)-C(54)-K(2)	80.8(3)
O(11)-C(49)-C(50)	108.4(5)	C(53)-C(54)-K(2)	75.6(3)
O(11)-C(49)-H(49A)	110.0	C(55)-C(54)-K(1)	77.3(3)
C(50)-C(49)-H(49A)	110.0	C(53)-C(54)-K(1)	77.0(3)
O(11)-C(49)-H(49B)	110.0	K(2)-C(54)-K(1)	136.52(18)
C(50)-C(49)-H(49B)	110.0	C(55)-C(54)-H(54A)	125.2
H(49A)-C(49)-H(49B)	108.4	C(53)-C(54)-H(54A)	125.2
O(12)-C(50)-C(49)	109.2(5)	K(2)-C(54)-H(54A)	110.7
O(12)-C(50)-H(50A)	109.8	K(1)-C(54)-H(54A)	112.7
C(49)-C(50)-H(50A)	109.8	C(54)-C(55)-C(56)	108.8(5)
O(12)-C(50)-H(50B)	109.8	C(54)-C(55)-K(1)	77.7(3)
C(49)-C(50)-H(50B)	109.8	C(56)-C(55)-K(1)	76.8(3)
H(50A)-C(50)-H(50B)	108.3	C(54)-C(55)-K(2)	74.3(3)

C(56)-C(55)-K(2)	77.9(3)	C(58)-C(59)-H(59A)	110.9
K(1)-C(55)-K(2)	133.26(18)	C(60)-C(59)-H(59A)	110.9
C(54)-C(55)-H(55A)	125.6	C(58)-C(59)-H(59B)	110.9
C(56)-C(55)-H(55A)	125.6	C(60)-C(59)-H(59B)	110.9
K(1)-C(55)-H(55A)	112.3	H(59A)-C(59)-H(59B)	108.9
K(2)-C(55)-H(55A)	114.4	C(59)-C(60)-C(61)	100.9(8)
C(55)-C(56)-C(57)	107.8(5)	C(59)-C(60)-K(2)#1	154.7(7)
C(55)-C(56)-K(1)	77.8(3)	C(61)-C(60)-K(2)#1	104.4(7)
C(57)-C(56)-K(1)	77.2(3)	C(59)-C(60)-H(60A)	111.6
C(55)-C(56)-K(2)	77.3(3)	C(61)-C(60)-H(60A)	111.6
C(57)-C(56)-K(2)	74.0(3)	K(2)#1-C(60)-H(60A)	57.0
K(1)-C(56)-K(2)	133.52(18)	C(59)-C(60)-H(60B)	111.6
C(55)-C(56)-H(56A)	126.1	C(61)-C(60)-H(60B)	111.6
C(57)-C(56)-H(56A)	126.1	K(2)#1-C(60)-H(60B)	59.9
K(1)-C(56)-H(56A)	111.6	H(60A)-C(60)-H(60B)	109.4
K(2)-C(56)-H(56A)	114.9	O(13)-C(61)-C(60)	101.3(10)
C(56)-C(57)-C(53)	107.0(5)	O(13)-C(61)-H(61A)	111.5
C(56)-C(57)-K(2)	80.5(3)	C(60)-C(61)-H(61A)	111.5
C(53)-C(57)-K(2)	75.1(3)	O(13)-C(61)-H(61B)	111.5
C(56)-C(57)-K(1)	76.9(3)	C(60)-C(61)-H(61B)	111.5
C(53)-C(57)-K(1)	77.2(3)	H(61A)-C(61)-H(61B)	109.3
K(2)-C(57)-K(1)	136.96(17)	C(62)-O(14)-C(65)	105.1(7)
C(56)-C(57)-H(57A)	126.5	O(14)-C(62)-C(63)	109.3(7)
C(53)-C(57)-H(57A)	126.5	O(14)-C(62)-H(62A)	109.8
K(2)-C(57)-H(57A)	110.8	C(63)-C(62)-H(62A)	109.8
K(1)-C(57)-H(57A)	112.1	O(14)-C(62)-H(62B)	109.8
C(58)-O(13)-C(61)	101.8(8)	C(63)-C(62)-H(62B)	109.8
C(58)-O(13)-K(2)	114.9(6)	H(62A)-C(62)-H(62B)	108.3
C(61)-O(13)-K(2)	115.7(8)	C(62)-C(63)-C(64)	103.5(7)
O(13)-C(58)-C(59)	105.5(9)	C(62)-C(63)-H(63A)	111.1
O(13)-C(58)-H(58A)	110.6	C(64)-C(63)-H(63A)	111.1
C(59)-C(58)-H(58A)	110.6	C(62)-C(63)-H(63B)	111.1
O(13)-C(58)-H(58B)	110.6	C(64)-C(63)-H(63B)	111.1
C(59)-C(58)-H(58B)	110.6	H(63A)-C(63)-H(63B)	109.0
H(58A)-C(58)-H(58B)	108.8	C(65)-C(64)-C(63)	104.5(7)
C(58)-C(59)-C(60)	104.5(8)	C(65)-C(64)-H(64A)	110.8

C(63)-C(64)-H(64A)	110.8	O(14')-C(65')-H(65D)	111.5
C(65)-C(64)-H(64B)	110.8	C(64')-C(65')-H(65D)	111.5
C(63)-C(64)-H(64B)	110.8	H(65C)-C(65')-H(65D)	109.3
H(64A)-C(64)-H(64B)	108.9	C(66)-O(15)-C(69)	110.9(11)
O(14)-C(65)-C(64)	110.6(7)	O(15)-C(66)-C(67)	103.4(10)
O(14)-C(65)-H(65A)	109.5	O(15)-C(66)-H(66A)	111.1
C(64)-C(65)-H(65A)	109.5	C(67)-C(66)-H(66A)	111.1
O(14)-C(65)-H(65B)	109.5	O(15)-C(66)-H(66B)	111.1
C(64)-C(65)-H(65B)	109.5	C(67)-C(66)-H(66B)	111.1
H(65A)-C(65)-H(65B)	108.1	H(66A)-C(66)-H(66B)	109.0
C(62')-O(14')-C(65')	98.7(19)	C(66)-C(67)-C(68)	102.0(11)
O(14')-C(62')-C(63')	105.2(17)	C(66)-C(67)-H(67A)	111.4
O(14')-C(62')-H(62C)	110.7	C(68)-C(67)-H(67A)	111.4
C(63')-C(62')-H(62C)	110.7	C(66)-C(67)-H(67B)	111.4
O(14')-C(62')-H(62D)	110.7	C(68)-C(67)-H(67B)	111.4
C(63')-C(62')-H(62D)	110.7	H(67A)-C(67)-H(67B)	109.2
H(62C)-C(62')-H(62D)	108.8	C(69)-C(68)-C(67)	99.4(11)
C(62')-C(63')-C(64')	102.8(12)	C(69)-C(68)-H(68A)	111.9
C(62')-C(63')-H(63C)	111.2	C(67)-C(68)-H(68A)	111.9
C(64')-C(63')-H(63C)	111.2	C(69)-C(68)-H(68B)	111.9
C(62')-C(63')-H(63D)	111.2	C(67)-C(68)-H(68B)	111.9
C(64')-C(63')-H(63D)	111.2	H(68A)-C(68)-H(68B)	109.6
H(63C)-C(63')-H(63D)	109.1	O(15)-C(69)-C(68)	104.2(11)
C(65')-C(64')-C(63')	101.2(13)	O(15)-C(69)-H(69A)	110.9
C(65')-C(64')-K(1)	89(2)	C(68)-C(69)-H(69A)	110.9
C(63')-C(64')-K(1)	144(3)	O(15)-C(69)-H(69B)	110.9
C(65')-C(64')-H(64C)	111.5	C(68)-C(69)-H(69B)	110.9
C(63')-C(64')-H(64C)	111.5	H(69A)-C(69)-H(69B)	108.9
K(1)-C(64')-H(64C)	34.2	C(69')-O(15')-C(66')	107.9(7)
C(65')-C(64')-H(64D)	111.5	O(15')-C(66')-C(67')	107.5(7)
C(63')-C(64')-H(64D)	111.5	O(15')-C(66')-H(66C)	110.2
K(1)-C(64')-H(64D)	95.7	C(67')-C(66')-H(66C)	110.2
H(64C)-C(64')-H(64D)	109.4	O(15')-C(66')-H(66D)	110.2
O(14')-C(65')-C(64')	101.5(15)	C(67')-C(66')-H(66D)	110.2
O(14')-C(65')-H(65C)	111.5	H(66C)-C(66')-H(66D)	108.5
C(64')-C(65')-H(65C)	111.5	C(68')-C(67')-C(66')	102.7(7)

C(68')-C(67')-H(67C)	111.2	C(69')-C(68')-H(68D)	110.3
C(66')-C(67')-H(67C)	111.2	H(68C)-C(68')-H(68D)	108.6
C(68')-C(67')-H(67D)	111.2	O(15')-C(69')-C(68')	107.8(7)
C(66')-C(67')-H(67D)	111.2	O(15')-C(69')-H(69C)	110.2
H(67C)-C(67')-H(67D)	109.1	C(68')-C(69')-H(69C)	110.2
C(67')-C(68')-C(69')	107.0(7)	O(15')-C(69')-H(69D)	110.2
C(67')-C(68')-H(68C)	110.3	C(68')-C(69')-H(69D)	110.2
C(69')-C(68')-H(68C)	110.3	H(69C)-C(69')-H(69D)	108.5
C(67')-C(68')-H(68D)	110.3		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04172. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	67(1)	58(1)	71(1)	2(1)	10(1)	1(1)
C1	54(3)	68(3)	69(3)	9(2)	2(2)	4(2)
C2	75(3)	56(3)	79(3)	4(2)	8(2)	-1(3)
C3	72(3)	52(3)	84(3)	8(2)	14(3)	2(3)
C4	57(3)	62(3)	86(3)	4(3)	14(2)	4(2)
C5	85(4)	110(5)	80(4)	12(3)	27(3)	-32(4)
C6	124(6)	125(6)	73(4)	-12(4)	34(4)	-53(5)
C7	141(6)	93(5)	106(5)	-22(4)	56(5)	-37(5)
C8	107(4)	77(4)	105(5)	-10(3)	47(4)	-15(3)
C9	60(3)	60(3)	84(3)	7(3)	17(3)	-1(2)
C10	54(3)	76(3)	78(3)	15(3)	12(2)	-5(3)
C11	58(3)	48(3)	80(3)	7(2)	21(2)	0(2)
C12	54(3)	58(3)	71(3)	11(2)	11(2)	-6(2)
C13	74(3)	76(3)	70(3)	3(3)	21(3)	-25(3)
C14	79(4)	63(3)	82(3)	5(3)	32(3)	-11(3)
C15	71(3)	62(3)	67(3)	4(2)	3(2)	-14(3)
C16	66(3)	74(3)	85(4)	7(3)	7(3)	3(3)
C17	75(4)	66(3)	89(4)	3(3)	22(3)	6(3)
C18	80(3)	56(3)	71(3)	-3(2)	16(3)	4(3)
C19	82(3)	70(3)	61(3)	3(2)	12(3)	3(3)
C20	90(4)	71(3)	74(3)	14(3)	12(3)	11(3)
C21	92(4)	54(3)	85(4)	10(3)	27(3)	15(3)
C22	91(4)	51(3)	70(3)	2(2)	20(3)	-1(3)
C23	69(3)	53(3)	54(2)	-1(2)	11(2)	-14(2)
C24	86(3)	56(3)	44(2)	-7(2)	14(2)	-6(3)
C25	62(3)	49(3)	59(3)	2(2)	15(2)	-6(2)
C26	75(3)	54(3)	43(2)	4(2)	15(2)	0(2)
C27	73(3)	56(3)	50(2)	6(2)	16(2)	2(2)
C28	76(3)	43(2)	58(3)	3(2)	22(2)	-5(2)
K1	65(1)	56(1)	57(1)	-3(1)	5(1)	3(1)
K2	67(1)	55(1)	60(1)	-2(1)	14(1)	-5(1)

O1	79(2)	64(2)	57(2)	-2(2)	17(2)	4(2)
O2	72(2)	64(2)	64(2)	-5(2)	7(2)	-7(2)
O3	89(2)	46(2)	72(2)	3(1)	16(2)	6(2)
O4	74(2)	81(2)	74(2)	13(2)	24(2)	12(2)
O5	72(2)	87(2)	71(2)	12(2)	-3(2)	-9(2)
O6	106(3)	56(2)	59(2)	-2(2)	-1(2)	-9(2)
O7	118(3)	47(2)	72(2)	-1(2)	4(2)	0(2)
O8	77(2)	101(3)	59(2)	8(2)	15(2)	17(2)
O9	73(2)	97(2)	64(2)	2(2)	3(2)	-26(2)
O10	104(3)	62(2)	67(2)	-8(2)	8(2)	1(2)
O11	77(2)	106(3)	78(2)	-7(2)	24(2)	10(2)
O12	84(3)	86(2)	85(2)	3(2)	10(2)	-29(2)
C29	68(3)	83(3)	76(3)	10(3)	24(3)	5(3)
C30	59(3)	74(3)	78(3)	11(3)	11(2)	-4(3)
C31	86(4)	64(3)	69(3)	-5(2)	9(3)	-23(3)
C32	100(4)	57(3)	70(3)	-5(2)	8(3)	-11(3)
C33	112(4)	52(3)	80(3)	-2(2)	20(3)	23(3)
C34	93(4)	71(3)	86(4)	8(3)	36(3)	28(3)
C35	68(3)	117(5)	99(4)	35(4)	30(3)	8(3)
C36	59(3)	117(5)	86(4)	31(4)	5(3)	-14(3)
C37	95(4)	98(4)	73(3)	9(3)	-13(3)	-33(4)
C38	109(5)	66(3)	80(3)	-1(3)	-8(3)	-30(4)
C39	126(5)	49(3)	68(3)	-15(2)	11(3)	2(3)
C40	111(4)	52(3)	60(3)	-9(2)	12(3)	16(3)
C41	174(6)	62(3)	60(3)	4(3)	23(4)	26(4)
C42	122(5)	84(4)	60(3)	-6(3)	17(3)	43(4)
C43	57(3)	139(5)	85(4)	15(4)	26(3)	15(3)
C44	55(3)	157(6)	83(4)	18(4)	10(3)	-26(4)
C45	103(5)	106(5)	75(4)	-2(3)	0(3)	-58(4)
C46	183(7)	62(4)	68(3)	-7(3)	5(4)	-45(4)
C47	139(6)	73(4)	100(4)	-32(3)	-4(4)	28(4)
C48	113(5)	138(6)	81(4)	-40(4)	17(4)	35(5)
C49	80(4)	154(6)	122(5)	-13(5)	44(4)	-4(4)
C50	54(4)	143(6)	172(7)	-18(5)	32(4)	-23(4)
C51	117(5)	85(4)	116(5)	-3(4)	16(4)	-34(4)
C52	175(7)	52(3)	89(4)	-7(3)	13(4)	-43(4)

C53	85(4)	103(5)	69(3)	32(3)	-19(3)	-36(4)
C54	140(6)	53(3)	58(3)	-1(2)	9(3)	19(4)
C55	70(3)	103(5)	77(3)	26(3)	9(3)	1(4)
C56	136(5)	52(3)	57(3)	3(2)	-11(3)	1(4)
C57	98(5)	121(5)	57(3)	28(3)	28(3)	58(4)
O13	152(7)	162(10)	92(4)	20(7)	-16(4)	-21(9)
C58	137(7)	63(4)	70(6)	-3(3)	36(5)	-23(4)
C59	137(7)	63(4)	70(6)	-3(3)	36(5)	-23(4)
C60	152(7)	162(10)	92(4)	20(7)	-16(4)	-21(9)
C61	137(7)	63(4)	70(6)	-3(3)	36(5)	-23(4)
O14	157(6)	123(5)	135(5)	-12(4)	42(4)	1(5)
C62	98(8)	134(7)	84(6)	10(5)	26(5)	-19(7)
C63	139(7)	76(5)	157(13)	12(8)	48(8)	5(5)
C64	176(8)	57(9)	144(7)	27(7)	66(6)	14(8)
C65	106(7)	167(8)	103(10)	-49(6)	50(6)	-34(5)
O14'	157(6)	123(5)	135(5)	-12(4)	42(4)	1(5)
C62'	176(8)	57(9)	144(7)	27(7)	66(6)	14(8)
C63'	106(7)	167(8)	103(10)	-49(6)	50(6)	-34(5)
C64'	98(8)	134(7)	84(6)	10(5)	26(5)	-19(7)
C65'	139(7)	76(5)	157(13)	12(8)	48(8)	5(5)
O15	86(6)	101(6)	117(4)	-27(4)	-10(5)	3(4)
C66	127(12)	130(8)	93(11)	-57(7)	44(8)	-54(9)
C67	78(5)	86(8)	93(8)	3(5)	7(6)	-16(6)
C68	65(9)	147(8)	190(11)	-85(7)	25(9)	-34(9)
C69	74(7)	149(10)	90(10)	-50(7)	-25(6)	-13(7)
O15'	86(6)	101(6)	117(4)	-27(4)	-10(5)	3(4)
C66'	127(12)	130(8)	93(11)	-57(7)	44(8)	-54(9)
C67'	78(5)	86(8)	93(8)	3(5)	7(6)	-16(6)
C68'	65(9)	147(8)	190(11)	-85(7)	25(9)	-34(9)
C69'	74(7)	149(10)	90(10)	-50(7)	-25(6)	-13(7)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04172.

	x	y	z	U(eq)
H1A	714	1369	1148	77
H2A	844	-863	968	84
H3A	1580	-2121	1147	82
H4A	2126	-965	1489	82
H5A	2149	1632	2374	108
H6A	1863	3412	2618	126
H7A	1167	4638	2441	132
H8A	789	4127	2019	112
H9A	709	2620	1597	81
H10A	2082	138	1960	82
H15A	2019	3019	1273	80
H16A	2567	1385	1111	90
H17A	2286	17	718	91
H18A	1459	398	516	82
H19A	207	3926	221	85
H20A	-229	5853	318	94
H21A	31	7177	705	91
H22A	716	6559	986	84
H23A	1400	4909	1113	70
H24A	901	2338	339	74
H29A	-223	730	253	90
H29B	123	-423	402	90
H30A	-65	465	829	84
H30B	229	1533	662	84
H31A	-111	3512	844	88
H31B	-356	2509	1047	88
H32A	-772	4644	984	91
H32B	-914	4239	671	91
H33A	-1763	4366	772	97
H33B	-1606	4603	1090	97

H34A	-1958	2433	1177	98
H34B	-2356	3521	1051	98
H35A	-2896	1826	837	112
H35B	-2542	675	980	112
H36A	-3005	-114	572	105
H36B	-2714	963	405	105
H37A	-2438	-1086	181	108
H37B	-2671	-2098	388	108
H38A	-1870	-2826	553	103
H38B	-1998	-3174	237	103
H39A	-1200	-3060	118	97
H39B	-1021	-2942	437	97
H40A	-441	-1985	156	89
H40B	-841	-850	55	89
H41A	-402	-6575	1452	117
H41B	-196	-6187	1758	117
H42A	309	-5312	1427	106
H42B	-139	-4361	1309	106
H43A	350	-2366	1435	111
H43B	792	-3336	1553	111
H44A	738	-2394	1996	118
H44B	876	-1253	1784	118
H45A	554	444	2037	114
H45B	370	-597	2255	114
H46A	-92	1444	2216	126
H46B	-272	1041	1907	126
H47A	-1117	887	2037	126
H47B	-908	1291	2342	126
H48A	-1159	-897	2488	132
H48B	-1612	26	2366	132
H49A	-2068	-1964	2255	140
H49B	-1617	-2913	2368	140
H50A	-2163	-4023	2030	146
H50B	-2020	-2913	1814	146
H51A	-1703	-4735	1566	127
H51B	-1855	-5770	1794	127

H52A	-1022	-6392	1892	126
H52B	-1226	-6757	1584	126
H53A	-460	268	1334	105
H54A	-1283	668	1475	100
H55A	-1816	-1232	1319	100
H56A	-1341	-2885	1078	100
H57A	-487	-1991	1086	109
H58A	-24	-5458	2141	106
H58B	-518	-5838	2271	106
H59A	373	-6275	2522	106
H59B	-113	-6253	2677	106
H60A	601	-4387	2765	165
H60B	54	-4141	2846	165
H61A	122	-2422	2518	106
H61B	406	-3429	2330	106
H62A	-2158	2735	145	125
H62B	-1667	2255	322	125
H63A	-1953	1721	-232	146
H63B	-1627	774	-17	146
H64A	-933	1762	-117	147
H64B	-1250	2446	-374	147
H65A	-872	3728	91	147
H65B	-1153	4428	-174	147
H62C	-1441	3045	-354	147
H62D	-861	2961	-268	147
H63C	-1439	4532	-6	147
H63D	-921	3985	136	147
H64C	-1287	2416	381	125
H64D	-1792	3215	293	125
H65C	-1749	770	123	146
H65D	-1955	1888	-101	146
H66A	2193	7810	2155	137
H66B	2262	6269	2268	137
H67A	1753	7112	1758	103
H67B	1578	5981	1964	103
H68A	2178	4421	1853	160

H68B	1970	5044	1560	160
H69A	2882	5341	1707	128
H69B	2591	6634	1569	128
H66C	1756	7387	1973	137
H66D	1999	6155	2155	137
H67C	1702	4897	1794	103
H67D	1721	6158	1586	103
H68C	2415	5229	1486	160
H68D	2473	4337	1761	160
H69C	3003	5830	1941	128
H69D	2912	6780	1676	128

Table 6. Torsion angles [°] for 04172.

C16-Co1-C1-C2	178.0(3)	C15-Co1-C3-C4	-9.6(6)
C17-Co1-C1-C2	95.3(5)	C1-Co1-C3-C4	-94.3(3)
C3-Co1-C1-C2	-33.4(3)	C18-Co1-C3-C4	157.9(3)
C15-Co1-C1-C2	172.0(3)	C16-Co1-C3-C2	-174.0(3)
C18-Co1-C1-C2	88.0(3)	C17-Co1-C3-C2	-123.4(3)
C4-Co1-C1-C2	-73.6(3)	C15-Co1-C3-C2	117.1(5)
C2-Co1-C1-C11	122.1(4)	C1-Co1-C3-C2	32.4(3)
C16-Co1-C1-C11	-59.9(4)	C18-Co1-C3-C2	-75.3(3)
C17-Co1-C1-C11	-142.7(4)	C4-Co1-C3-C2	126.8(4)
C3-Co1-C1-C11	88.7(3)	C2-C3-C4-C12	27.6(6)
C15-Co1-C1-C11	-65.9(3)	Co1-C3-C4-C12	83.2(4)
C18-Co1-C1-C11	-150.0(3)	C2-C3-C4-Co1	-55.5(3)
C4-Co1-C1-C11	48.4(3)	C2-Co1-C4-C3	34.1(3)
C11-C1-C2-C3	-24.2(6)	C16-Co1-C4-C3	-141.2(3)
Co1-C1-C2-C3	58.1(4)	C17-Co1-C4-C3	-98.9(3)
C11-C1-C2-Co1	-82.3(4)	C15-Co1-C4-C3	175.5(3)
C16-Co1-C2-C1	-165(3)	C1-Co1-C4-C3	75.0(3)
C17-Co1-C2-C1	-141.2(3)	C18-Co1-C4-C3	-54.9(6)
C3-Co1-C2-C1	127.8(4)	C2-Co1-C4-C12	-87.8(3)
C15-Co1-C2-C1	-13.1(5)	C16-Co1-C4-C12	96.9(3)
C18-Co1-C2-C1	-107.9(3)	C17-Co1-C4-C12	139.2(3)
C4-Co1-C2-C1	95.2(3)	C3-Co1-C4-C12	-121.9(4)
C16-Co1-C2-C3	67(3)	C15-Co1-C4-C12	53.6(3)
C17-Co1-C2-C3	91.0(4)	C1-Co1-C4-C12	-46.9(3)
C15-Co1-C2-C3	-140.9(3)	C18-Co1-C4-C12	-176.8(4)
C1-Co1-C2-C3	-127.8(4)	C13-C5-C6-C7	0.3(8)
C18-Co1-C2-C3	124.3(3)	C5-C6-C7-C8	-1.3(9)
C4-Co1-C2-C3	-32.6(3)	C6-C7-C8-C14	1.4(9)
C1-C2-C3-C4	-0.8(6)	C14-C9-C11-C1	-176.0(4)
Co1-C2-C3-C4	59.5(4)	C14-C9-C11-C12	1.9(6)
C1-C2-C3-Co1	-60.3(4)	C2-C1-C11-C9	-159.7(4)
C2-Co1-C3-C4	-126.8(4)	Co1-C1-C11-C9	135.8(4)
C16-Co1-C3-C4	59.3(4)	C2-C1-C11-C12	22.3(6)
C17-Co1-C3-C4	109.9(3)	Co1-C1-C11-C12	-42.2(4)

C13-C10-C12-C4	171.9(4)	Co1-C15-C16-C17	57.5(4)
C13-C10-C12-C11	-3.3(6)	C25-C15-C16-Co1	-81.4(4)
C3-C4-C12-C10	155.7(4)	C2-Co1-C16-C17	26(3)
Co1-C4-C12-C10	-138.7(4)	C3-Co1-C16-C17	88.6(4)
C3-C4-C12-C11	-29.0(6)	C15-Co1-C16-C17	-128.6(4)
Co1-C4-C12-C11	36.6(4)	C1-Co1-C16-C17	-137.6(3)
C9-C11-C12-C10	1.2(6)	C18-Co1-C16-C17	-32.6(3)
C1-C11-C12-C10	179.3(4)	C4-Co1-C16-C17	124.0(3)
C9-C11-C12-C4	-174.5(4)	C2-Co1-C16-C15	154(3)
C1-C11-C12-C4	3.6(5)	C17-Co1-C16-C15	128.6(4)
C6-C5-C13-C14	0.6(7)	C3-Co1-C16-C15	-142.8(3)
C6-C5-C13-C10	179.4(4)	C1-Co1-C16-C15	-9.0(5)
C12-C10-C13-C5	-176.4(4)	C18-Co1-C16-C15	96.1(3)
C12-C10-C13-C14	2.4(6)	C4-Co1-C16-C15	-107.3(3)
C7-C8-C14-C9	179.5(5)	C15-C16-C17-C18	0.2(7)
C7-C8-C14-C13	-0.6(7)	Co1-C16-C17-C18	59.4(4)
C11-C9-C14-C8	177.1(4)	C15-C16-C17-Co1	-59.3(4)
C11-C9-C14-C13	-2.8(6)	C2-Co1-C17-C16	-177.3(3)
C5-C13-C14-C8	-0.4(6)	C3-Co1-C17-C16	-125.3(3)
C10-C13-C14-C8	-179.3(4)	C15-Co1-C17-C16	32.1(3)
C5-C13-C14-C9	179.5(4)	C1-Co1-C17-C16	116.7(5)
C10-C13-C14-C9	0.6(6)	C18-Co1-C17-C16	127.1(4)
C2-Co1-C15-C16	-176.7(3)	C4-Co1-C17-C16	-77.0(3)
C17-Co1-C15-C16	-32.4(3)	C2-Co1-C17-C18	55.6(4)
C3-Co1-C15-C16	97.1(5)	C16-Co1-C17-C18	-127.1(4)
C1-Co1-C15-C16	174.6(3)	C3-Co1-C17-C18	107.5(3)
C18-Co1-C15-C16	-72.6(3)	C15-Co1-C17-C18	-95.0(3)
C4-Co1-C15-C16	90.3(3)	C1-Co1-C17-C18	-10.5(6)
C2-Co1-C15-C25	-54.0(4)	C4-Co1-C17-C18	155.9(3)
C16-Co1-C15-C25	122.7(4)	C16-C17-C18-C26	24.5(7)
C17-Co1-C15-C25	90.3(3)	Co1-C17-C18-C26	80.5(4)
C3-Co1-C15-C25	-140.2(4)	C16-C17-C18-Co1	-56.0(4)
C1-Co1-C15-C25	-62.7(3)	C2-Co1-C18-C17	-142.6(3)
C18-Co1-C15-C25	50.1(3)	C16-Co1-C18-C17	33.4(3)
C4-Co1-C15-C25	-147.0(3)	C3-Co1-C18-C17	-100.5(3)
C25-C15-C16-C17	-23.9(7)	C15-Co1-C18-C17	74.2(3)

C1-Co1-C18-C17	174.9(3)	C19-C27-C28-C22	-1.3(6)
C4-Co1-C18-C17	-60.9(6)	C24-C27-C28-C22	-178.9(4)
C2-Co1-C18-C26	94.5(3)	C19-C27-C28-C23	177.4(4)
C16-Co1-C18-C26	-89.5(3)	C24-C27-C28-C23	-0.2(6)
C17-Co1-C18-C26	-122.9(4)	O5-K1-O1-C40	4.5(3)
C3-Co1-C18-C26	136.6(3)	O3-K1-O1-C40	-136.0(3)
C15-Co1-C18-C26	-48.6(3)	O6-K1-O1-C40	9.0(3)
C1-Co1-C18-C26	52.1(3)	O2-K1-O1-C40	-140.3(3)
C4-Co1-C18-C26	176.2(4)	O4-K1-O1-C40	-65.6(3)
C27-C19-C20-C21	0.3(7)	C56-K1-O1-C40	96.5(3)
C19-C20-C21-C22	-0.1(7)	C57-K1-O1-C40	117.4(3)
C20-C21-C22-C28	-0.8(7)	C53-K1-O1-C40	139.0(3)
C28-C23-C25-C26	0.0(6)	C55-K1-O1-C40	104.0(3)
C28-C23-C25-C15	-173.6(4)	C54-K1-O1-C40	132.2(3)
C16-C15-C25-C23	-164.0(4)	C64'-K1-O1-C40	-77.3(5)
Co1-C15-C25-C23	131.4(4)	O5-K1-O1-C29	148.0(3)
C16-C15-C25-C26	22.2(6)	O3-K1-O1-C29	7.4(3)
Co1-C15-C25-C26	-42.4(4)	O6-K1-O1-C29	152.4(3)
C27-C24-C26-C25	-3.3(6)	O2-K1-O1-C29	3.1(3)
C27-C24-C26-C18	170.7(4)	O4-K1-O1-C29	77.8(3)
C23-C25-C26-C24	2.1(6)	C56-K1-O1-C29	-120.0(3)
C15-C25-C26-C24	176.4(4)	C57-K1-O1-C29	-99.2(3)
C23-C25-C26-C18	-172.4(4)	C53-K1-O1-C29	-77.6(3)
C15-C25-C26-C18	1.9(5)	C55-K1-O1-C29	-112.6(3)
C17-C18-C26-C24	160.4(4)	C54-K1-O1-C29	-84.4(3)
Co1-C18-C26-C24	-135.3(4)	C64'-K1-O1-C29	66.2(5)
C17-C18-C26-C25	-25.5(6)	O5-K1-O2-C31	117.7(3)
Co1-C18-C26-C25	38.8(4)	O3-K1-O2-C31	28.3(3)
C20-C19-C27-C24	177.9(4)	O1-K1-O2-C31	-156.2(3)
C20-C19-C27-C28	0.5(6)	O6-K1-O2-C31	176.6(3)
C26-C24-C27-C19	-175.1(4)	O4-K1-O2-C31	55.6(3)
C26-C24-C27-C28	2.4(6)	C56-K1-O2-C31	-82.8(3)
C21-C22-C28-C23	-177.2(4)	C57-K1-O2-C31	-83.4(3)
C21-C22-C28-C27	1.5(6)	C53-K1-O2-C31	-59.2(3)
C25-C23-C28-C22	177.7(4)	C55-K1-O2-C31	-53.5(3)
C25-C23-C28-C27	-1.0(6)	C54-K1-O2-C31	-41.9(3)

C64'-K1-O2-C31	104.6(5)	O1-K1-O4-C34	-121.5(3)
O5-K1-O2-C30	-121.8(3)	O6-K1-O4-C34	178.2(3)
O3-K1-O2-C30	148.9(3)	O2-K1-O4-C34	-61.4(3)
O1-K1-O2-C30	-35.7(2)	C56-K1-O4-C34	78.4(3)
O6-K1-O2-C30	-62.8(3)	C57-K1-O4-C34	54.4(4)
O4-K1-O2-C30	176.1(2)	C53-K1-O4-C34	31.0(3)
C56-K1-O2-C30	37.7(3)	C55-K1-O4-C34	67.7(3)
C57-K1-O2-C30	37.1(3)	C54-K1-O4-C34	42.6(3)
C53-K1-O2-C30	61.4(3)	C64'-K1-O4-C34	-108.9(5)
C55-K1-O2-C30	67.1(3)	O5-K1-O4-C35	28.8(3)
C54-K1-O2-C30	78.6(3)	O3-K1-O4-C35	-156.5(3)
C64'-K1-O2-C30	-134.9(5)	O1-K1-O4-C35	115.9(3)
O5-K1-O3-C33	5.9(3)	O6-K1-O4-C35	55.7(3)
O1-K1-O3-C33	146.3(3)	O2-K1-O4-C35	176.1(3)
O6-K1-O3-C33	76.2(4)	C56-K1-O4-C35	-44.2(3)
O2-K1-O3-C33	150.5(3)	C57-K1-O4-C35	-68.1(4)
O4-K1-O3-C33	0.9(3)	C53-K1-O4-C35	-91.6(3)
C56-K1-O3-C33	-102.2(3)	C55-K1-O4-C35	-54.9(3)
C57-K1-O3-C33	-128.2(3)	C54-K1-O4-C35	-80.0(3)
C53-K1-O3-C33	-123.8(3)	C64'-K1-O4-C35	128.5(5)
C55-K1-O3-C33	-85.4(3)	O3-K1-O5-C36	0.5(3)
C54-K1-O3-C33	-98.6(3)	O1-K1-O5-C36	-140.1(3)
C64'-K1-O3-C33	77.6(5)	O6-K1-O5-C36	-144.5(3)
O5-K1-O3-C32	-139.2(3)	O2-K1-O5-C36	-71.5(4)
O1-K1-O3-C32	1.1(3)	O4-K1-O5-C36	5.4(3)
O6-K1-O3-C32	-68.9(4)	C56-K1-O5-C36	126.4(3)
O2-K1-O3-C32	5.4(3)	C57-K1-O5-C36	132.1(3)
O4-K1-O3-C32	-144.2(3)	C53-K1-O5-C36	104.6(4)
C56-K1-O3-C32	112.7(3)	C55-K1-O5-C36	101.3(3)
C57-K1-O3-C32	86.7(3)	C54-K1-O5-C36	87.7(3)
C53-K1-O3-C32	91.1(3)	C64'-K1-O5-C36	-59.7(5)
C55-K1-O3-C32	129.5(3)	O3-K1-O5-C37	147.7(3)
C54-K1-O3-C32	116.3(3)	O1-K1-O5-C37	7.2(3)
C64'-K1-O3-C32	-67.6(5)	O6-K1-O5-C37	2.8(3)
O5-K1-O4-C34	151.4(3)	O2-K1-O5-C37	75.8(4)
O3-K1-O4-C34	-33.9(3)	O4-K1-O5-C37	152.7(3)

C56-K1-O5-C37	-86.4(3)	C55-K2-O7-C41	125.4(3)
C57-K1-O5-C37	-80.7(3)	C56-K2-O7-C41	109.1(3)
C53-K1-O5-C37	-108.2(4)	O13-K2-O7-C41	-72.9(4)
C55-K1-O5-C37	-111.4(3)	O9-K2-O7-C52	142.5(3)
C54-K1-O5-C37	-125.1(3)	O11-K2-O7-C52	1.6(4)
C64'-K1-O5-C37	87.6(5)	O12-K2-O7-C52	-1.3(3)
O5-K1-O6-C39	-158.0(3)	O10-K2-O7-C52	71.6(4)
O3-K1-O6-C39	114.2(3)	O8-K2-O7-C52	147.7(4)
O1-K1-O6-C39	26.7(3)	C53-K2-O7-C52	-128.8(4)
O2-K1-O6-C39	53.8(3)	C54-K2-O7-C52	-100.3(4)
O4-K1-O6-C39	175.0(3)	C57-K2-O7-C52	-128.7(4)
C56-K1-O6-C39	-67.1(3)	C55-K2-O7-C52	-88.2(4)
C57-K1-O6-C39	-42.7(3)	C56-K2-O7-C52	-104.5(4)
C53-K1-O6-C39	-41.3(3)	O13-K2-O7-C52	73.5(4)
C55-K1-O6-C39	-84.7(3)	O9-K2-O8-C43	-32.8(3)
C54-K1-O6-C39	-72.5(3)	O11-K2-O8-C43	-118.0(3)
C64'-K1-O6-C39	113.0(5)	O7-K2-O8-C43	152.7(3)
O5-K1-O6-C38	-34.6(3)	O12-K2-O8-C43	-179.5(3)
O3-K1-O6-C38	-122.3(3)	O10-K2-O8-C43	-58.4(3)
O1-K1-O6-C38	150.2(3)	C53-K2-O8-C43	37.7(3)
O2-K1-O6-C38	177.2(3)	C54-K2-O8-C43	43.3(3)
O4-K1-O6-C38	-61.5(3)	C57-K2-O8-C43	60.3(3)
C56-K1-O6-C38	56.3(3)	C55-K2-O8-C43	73.2(3)
C57-K1-O6-C38	80.8(3)	C56-K2-O8-C43	80.4(3)
C53-K1-O6-C38	82.1(3)	O13-K2-O8-C43	-120.7(4)
C55-K1-O6-C38	38.7(3)	O9-K2-O8-C42	-153.5(3)
C54-K1-O6-C38	50.9(4)	O11-K2-O8-C42	121.3(3)
C64'-K1-O6-C38	-123.6(5)	O7-K2-O8-C42	32.0(3)
O9-K2-O7-C41	-3.9(3)	O12-K2-O8-C42	59.8(3)
O11-K2-O7-C41	-144.8(3)	O10-K2-O8-C42	-179.1(3)
O12-K2-O7-C41	-147.7(3)	C53-K2-O8-C42	-82.9(3)
O10-K2-O7-C41	-74.8(4)	C54-K2-O8-C42	-77.4(3)
O8-K2-O7-C41	1.3(3)	C57-K2-O8-C42	-60.4(3)
C53-K2-O7-C41	84.8(3)	C55-K2-O8-C42	-47.5(3)
C54-K2-O7-C41	113.3(3)	C56-K2-O8-C42	-40.3(3)
C57-K2-O7-C41	84.9(3)	O13-K2-O8-C42	118.6(4)

O11-K2-O9-C45	-3.6(4)	O12-K2-O10-C46	178.1(3)
O7-K2-O9-C45	-144.9(4)	O8-K2-O10-C46	56.7(4)
O12-K2-O9-C45	-74.1(4)	C53-K2-O10-C46	-42.8(4)
O10-K2-O9-C45	1.3(4)	C54-K2-O10-C46	-68.1(4)
O8-K2-O9-C45	-150.1(4)	C57-K2-O10-C46	-37.9(4)
C53-K2-O9-C45	102.5(4)	C55-K2-O10-C46	-82.3(4)
C54-K2-O9-C45	85.0(4)	C56-K2-O10-C46	-66.2(4)
C57-K2-O9-C45	126.6(4)	O13-K2-O10-C46	116.9(4)
C55-K2-O9-C45	96.3(4)	O9-K2-O11-C49	-140.6(4)
C56-K2-O9-C45	123.8(4)	O7-K2-O11-C49	0.6(4)
O13-K2-O9-C45	-76.4(4)	O12-K2-O11-C49	3.5(4)
O11-K2-O9-C44	146.8(3)	O10-K2-O11-C49	-145.5(4)
O7-K2-O9-C44	5.5(3)	O8-K2-O11-C49	-71.8(5)
O12-K2-O9-C44	76.3(4)	C53-K2-O11-C49	133.7(4)
O10-K2-O9-C44	151.7(3)	C54-K2-O11-C49	123.8(4)
O8-K2-O9-C44	0.2(3)	C57-K2-O11-C49	110.2(4)
C53-K2-O9-C44	-107.1(4)	C55-K2-O11-C49	98.9(4)
C54-K2-O9-C44	-124.6(3)	C56-K2-O11-C49	89.0(4)
C57-K2-O9-C44	-83.1(3)	O13-K2-O11-C49	-69.3(4)
C55-K2-O9-C44	-113.3(3)	O9-K2-O11-C48	2.8(4)
C56-K2-O9-C44	-85.8(3)	O7-K2-O11-C48	144.0(4)
O13-K2-O9-C44	74.0(4)	O12-K2-O11-C48	146.9(4)
O9-K2-O10-C47	153.5(4)	O10-K2-O11-C48	-2.1(4)
O11-K2-O10-C47	-31.8(3)	O8-K2-O11-C48	71.6(5)
O7-K2-O10-C47	-118.8(4)	C53-K2-O11-C48	-82.9(4)
O12-K2-O10-C47	-59.5(4)	C54-K2-O11-C48	-92.8(4)
O8-K2-O10-C47	179.0(3)	C57-K2-O11-C48	-106.4(4)
C53-K2-O10-C47	79.5(4)	C55-K2-O11-C48	-117.7(4)
C54-K2-O10-C47	54.3(4)	C56-K2-O11-C48	-127.6(4)
C57-K2-O10-C47	84.5(4)	O13-K2-O11-C48	74.1(4)
C55-K2-O10-C47	40.1(4)	O9-K2-O12-C51	-120.9(4)
C56-K2-O10-C47	56.2(4)	O11-K2-O12-C51	151.1(4)
O13-K2-O10-C47	-120.8(4)	O7-K2-O12-C51	-32.0(4)
O9-K2-O10-C46	31.1(3)	O10-K2-O12-C51	178.4(4)
O11-K2-O10-C46	-154.1(4)	O8-K2-O12-C51	-60.0(4)
O7-K2-O10-C46	118.8(4)	C53-K2-O12-C51	63.7(5)

C54-K2-O12-C51	81.7(4)	C36-O5-C37-C38	177.4(4)
C57-K2-O12-C51	35.0(4)	K1-O5-C37-C38	28.0(5)
C55-K2-O12-C51	67.4(4)	C39-O6-C38-C37	-170.8(4)
C56-K2-O12-C51	42.8(4)	K1-O6-C38-C37	66.4(4)
O13-K2-O12-C51	-118.5(4)	O5-C37-C38-O6	-64.5(5)
O9-K2-O12-C50	117.9(4)	C38-O6-C39-C40	-179.3(4)
O11-K2-O12-C50	29.8(4)	K1-O6-C39-C40	-59.4(4)
O7-K2-O12-C50	-153.2(4)	C29-O1-C40-C39	173.4(4)
O10-K2-O12-C50	57.2(4)	K1-O1-C40-C39	-41.2(4)
O8-K2-O12-C50	178.8(4)	O6-C39-C40-O1	67.5(5)
C53-K2-O12-C50	-57.6(4)	C52-O7-C41-C42	179.2(4)
C54-K2-O12-C50	-39.5(4)	K2-O7-C41-C42	-32.9(5)
C57-K2-O12-C50	-86.3(4)	C43-O8-C42-C41	179.1(4)
C55-K2-O12-C50	-53.8(4)	K2-O8-C42-C41	-63.8(4)
C56-K2-O12-C50	-78.4(4)	O7-C41-C42-O8	67.3(5)
O13-K2-O12-C50	120.2(4)	C42-O8-C43-C44	-179.5(4)
C40-O1-C29-C30	174.1(4)	K2-O8-C43-C44	64.0(4)
K1-O1-C29-C30	29.0(5)	C45-O9-C44-C43	-177.0(4)
C31-O2-C30-C29	-173.1(4)	K2-O9-C44-C43	30.7(5)
K1-O2-C30-C29	69.0(4)	O8-C43-C44-O9	-64.8(6)
O1-C29-C30-O2	-67.2(5)	C44-O9-C45-C46	173.7(4)
C30-O2-C31-C32	-178.0(4)	K2-O9-C45-C46	-33.7(6)
K1-O2-C31-C32	-61.4(4)	C47-O10-C46-C45	177.2(4)
C33-O3-C32-C31	175.3(4)	K2-O10-C46-C45	-63.5(4)
K1-O3-C32-C31	-37.5(4)	O9-C45-C46-O10	66.7(5)
O2-C31-C32-O3	67.8(5)	C46-O10-C47-C48	-177.4(4)
C32-O3-C33-C34	177.5(4)	K2-O10-C47-C48	64.3(5)
K1-O3-C33-C34	30.8(5)	C49-O11-C48-C47	-179.9(5)
C35-O4-C34-C33	-174.2(4)	K2-O11-C48-C47	34.1(6)
K1-O4-C34-C33	67.1(4)	O10-C47-C48-O11	-66.4(6)
O3-C33-C34-O4	-67.4(5)	C48-O11-C49-C50	178.2(5)
C34-O4-C35-C36	-179.6(4)	K2-O11-C49-C50	-35.3(7)
K1-O4-C35-C36	-62.0(4)	C51-O12-C50-C49	176.6(5)
C37-O5-C36-C35	172.4(4)	K2-O12-C50-C49	-62.9(6)
K1-O5-C36-C35	-37.9(5)	O11-C49-C50-O12	67.1(7)
O4-C35-C36-O5	67.8(5)	C50-O12-C51-C52	-177.3(5)

K2-O12-C51-C52	63.5(5)	O3-K1-C53-C54	78.4(4)
C41-O7-C52-C51	179.9(5)	O1-K1-C53-C54	-165.7(4)
K2-O7-C52-C51	31.7(6)	O6-K1-C53-C54	-114.0(4)
O12-C51-C52-O7	-64.3(6)	O2-K1-C53-C54	137.5(4)
O9-K2-C53-C54	-136.3(4)	O4-K1-C53-C54	28.0(4)
O11-K2-C53-C54	-23.4(4)	C56-K1-C53-C54	-73.8(4)
O7-K2-C53-C54	110.2(4)	C57-K1-C53-C54	-110.9(5)
O12-K2-C53-C54	41.3(5)	C55-K1-C53-C54	-35.6(3)
O10-K2-C53-C54	-79.8(4)	C64'-K1-C53-C54	112.5(7)
O8-K2-C53-C54	169.2(4)	O5-K1-C53-C57	70.5(5)
C57-K2-C53-C54	110.0(5)	O3-K1-C53-C57	-170.6(4)
C55-K2-C53-C54	35.6(3)	O1-K1-C53-C57	-54.7(4)
C56-K2-C53-C54	73.1(3)	O6-K1-C53-C57	-3.0(5)
O13-K2-C53-C54	-133.7(6)	O2-K1-C53-C57	-111.6(4)
O9-K2-C53-C57	113.7(4)	O4-K1-C53-C57	138.9(4)
O11-K2-C53-C57	-133.4(4)	C56-K1-C53-C57	37.1(3)
O7-K2-C53-C57	0.2(5)	C55-K1-C53-C57	75.4(4)
O12-K2-C53-C57	-68.8(5)	C54-K1-C53-C57	110.9(5)
O10-K2-C53-C57	170.2(4)	C64'-K1-C53-C57	-136.6(7)
O8-K2-C53-C57	59.1(4)	O5-K1-C53-K2	16.0(5)
C54-K2-C53-C57	-110.0(5)	O3-K1-C53-K2	134.8(4)
C55-K2-C53-C57	-74.4(4)	O1-K1-C53-K2	-109.3(4)
C56-K2-C53-C57	-36.9(3)	O6-K1-C53-K2	-57.6(5)
O13-K2-C53-C57	116.3(6)	O2-K1-C53-K2	-166.1(4)
O9-K2-C53-K1	167.7(4)	O4-K1-C53-K2	84.4(4)
O11-K2-C53-K1	-79.5(4)	C56-K1-C53-K2	-17.4(3)
O7-K2-C53-K1	54.2(5)	C57-K1-C53-K2	-54.5(3)
O12-K2-C53-K1	-14.8(6)	C55-K1-C53-K2	20.9(3)
O10-K2-C53-K1	-135.9(4)	C54-K1-C53-K2	56.4(3)
O8-K2-C53-K1	113.1(4)	C64'-K1-C53-K2	168.9(7)
C54-K2-C53-K1	-56.1(3)	C57-C53-C54-C55	-0.5(6)
C57-K2-C53-K1	53.9(3)	K2-C53-C54-C55	-74.6(4)
C55-K2-C53-K1	-20.5(3)	K1-C53-C54-C55	71.3(4)
C56-K2-C53-K1	17.0(3)	C57-C53-C54-K2	74.2(3)
O13-K2-C53-K1	170.2(5)	K1-C53-C54-K2	145.86(15)
O5-K1-C53-C54	-40.5(5)	C57-C53-C54-K1	-71.7(3)

K2-C53-C54-K1	-145.86(15)	O2-K1-C54-C55	-157.2(4)
O9-K2-C54-C55	155.9(4)	O4-K1-C54-C55	91.3(4)
O11-K2-C54-C55	-89.1(4)	C56-K1-C54-C55	-36.5(3)
O7-K2-C54-C55	29.5(4)	C57-K1-C54-C55	-75.8(4)
O12-K2-C54-C55	-35.9(4)	C53-K1-C54-C55	-113.8(5)
O10-K2-C54-C55	-146.5(4)	C64'-K1-C54-C55	141.9(8)
O8-K2-C54-C55	100.2(4)	O5-K1-C54-C53	147.6(4)
C53-K2-C54-C55	113.0(5)	O3-K1-C54-C53	-98.1(4)
C57-K2-C54-C55	74.5(4)	O1-K1-C54-C53	16.1(4)
C56-K2-C54-C55	35.7(3)	O6-K1-C54-C53	85.4(5)
O13-K2-C54-C55	-131.9(9)	O2-K1-C54-C53	-43.4(4)
O9-K2-C54-C53	42.9(4)	O4-K1-C54-C53	-154.9(4)
O11-K2-C54-C53	157.9(4)	C56-K1-C54-C53	77.3(4)
O7-K2-C54-C53	-83.5(4)	C57-K1-C54-C53	38.0(3)
O12-K2-C54-C53	-148.9(4)	C55-K1-C54-C53	113.8(5)
O10-K2-C54-C53	100.5(4)	C64'-K1-C54-C53	-104.3(8)
O8-K2-C54-C53	-12.8(4)	O5-K1-C54-K2	95.4(4)
C57-K2-C54-C53	-38.5(3)	O3-K1-C54-K2	-150.3(4)
C55-K2-C54-C53	-113.0(5)	O1-K1-C54-K2	-36.1(4)
C56-K2-C54-C53	-77.3(4)	O6-K1-C54-K2	33.2(5)
O13-K2-C54-C53	115.1(9)	O2-K1-C54-K2	-95.6(4)
O9-K2-C54-K1	95.6(4)	O4-K1-C54-K2	152.9(4)
O11-K2-C54-K1	-149.4(4)	C56-K1-C54-K2	25.1(3)
O7-K2-C54-K1	-30.9(5)	C57-K1-C54-K2	-14.2(3)
O12-K2-C54-K1	-96.3(4)	C53-K1-C54-K2	-52.2(3)
O10-K2-C54-K1	153.1(4)	C55-K1-C54-K2	61.6(3)
O8-K2-C54-K1	39.8(4)	C64'-K1-C54-K2	-156.5(8)
C53-K2-C54-K1	52.6(3)	C53-C54-C55-C56	0.1(6)
C57-K2-C54-K1	14.1(3)	K2-C54-C55-C56	-71.0(4)
C55-K2-C54-K1	-60.3(3)	K1-C54-C55-C56	71.2(3)
C56-K2-C54-K1	-24.6(3)	C53-C54-C55-K1	-71.1(4)
O13-K2-C54-K1	167.7(8)	K2-C54-C55-K1	-142.19(15)
O5-K1-C54-C55	33.8(4)	C53-C54-C55-K2	71.1(4)
O3-K1-C54-C55	148.1(4)	K1-C54-C55-K2	142.19(15)
O1-K1-C54-C55	-97.7(4)	O5-K1-C55-C54	-147.9(4)
O6-K1-C54-C55	-28.4(5)	O3-K1-C55-C54	-32.1(4)

O1-K1-C55-C54	95.4(4)	C57-K2-C55-C54	-77.0(4)
O6-K1-C55-C54	157.8(4)	C56-K2-C55-C54	-113.7(5)
O2-K1-C55-C54	27.6(4)	O13-K2-C55-C54	129.1(7)
O4-K1-C55-C54	-89.9(4)	O9-K2-C55-C56	86.1(4)
C56-K1-C55-C54	112.9(5)	O11-K2-C55-C56	-157.2(4)
C57-K1-C55-C54	75.6(4)	O7-K2-C55-C56	-41.1(4)
C53-K1-C55-C54	36.0(3)	O12-K2-C55-C56	-99.0(4)
C64'-K1-C55-C54	-81.1(12)	O10-K2-C55-C56	149.4(4)
O5-K1-C55-C56	99.2(4)	O8-K2-C55-C56	17.2(4)
O3-K1-C55-C56	-145.0(4)	C53-K2-C55-C56	76.9(4)
O1-K1-C55-C56	-17.6(4)	C54-K2-C55-C56	113.7(5)
O6-K1-C55-C56	44.8(4)	C57-K2-C55-C56	36.7(3)
O2-K1-C55-C56	-85.4(4)	O13-K2-C55-C56	-117.1(7)
O4-K1-C55-C56	157.1(4)	O9-K2-C55-K1	27.6(4)
C57-K1-C55-C56	-37.3(3)	O11-K2-C55-K1	144.4(3)
C53-K1-C55-C56	-76.9(4)	O7-K2-C55-K1	-99.5(3)
C54-K1-C55-C56	-112.9(5)	O12-K2-C55-K1	-157.4(3)
C64'-K1-C55-C56	165.9(12)	O10-K2-C55-K1	91.0(3)
O5-K1-C55-K2	158.0(3)	O8-K2-C55-K1	-41.2(4)
O3-K1-C55-K2	-86.2(3)	C53-K2-C55-K1	18.5(3)
O1-K1-C55-K2	41.2(4)	C54-K2-C55-K1	55.3(3)
O6-K1-C55-K2	103.6(3)	C57-K2-C55-K1	-21.7(3)
O2-K1-C55-K2	-26.6(4)	C56-K2-C55-K1	-58.4(3)
O4-K1-C55-K2	-144.1(3)	O13-K2-C55-K1	-175.5(6)
C56-K1-C55-K2	58.8(3)	C54-C55-C56-C57	0.2(6)
C57-K1-C55-K2	21.5(3)	K1-C55-C56-C57	72.1(3)
C53-K1-C55-K2	-18.1(3)	K2-C55-C56-C57	-68.3(3)
C54-K1-C55-K2	-54.1(3)	C54-C55-C56-K1	-71.8(4)
C64'-K1-C55-K2	-135.3(12)	K2-C55-C56-K1	-140.42(15)
O9-K2-C55-C54	-27.7(4)	C54-C55-C56-K2	68.6(4)
O11-K2-C55-C54	89.1(4)	K1-C55-C56-K2	140.42(15)
O7-K2-C55-C54	-154.8(4)	O5-K1-C56-C55	-80.1(4)
O12-K2-C55-C54	147.3(4)	O3-K1-C56-C55	41.3(4)
O10-K2-C55-C54	35.7(4)	O1-K1-C56-C55	164.4(4)
O8-K2-C55-C54	-96.5(4)	O6-K1-C56-C55	-137.9(4)
C53-K2-C55-C54	-36.8(3)	O2-K1-C56-C55	110.4(4)

O4-K1-C56-C55	-25.6(4)	O9-K2-C56-C57	6.4(4)
C57-K1-C56-C55	111.7(5)	O11-K2-C56-C57	137.1(4)
C53-K1-C56-C55	74.2(4)	O7-K2-C56-C57	-108.1(4)
C54-K1-C56-C55	35.9(3)	O12-K2-C56-C57	-164.2(4)
C64'-K1-C56-C55	-137(3)	O10-K2-C56-C57	74.4(4)
O5-K1-C56-C57	168.2(4)	O8-K2-C56-C57	-52.5(4)
O3-K1-C56-C57	-70.5(4)	C53-K2-C56-C57	38.3(3)
O1-K1-C56-C57	52.7(4)	C54-K2-C56-C57	77.3(4)
O6-K1-C56-C57	110.3(4)	C55-K2-C56-C57	113.0(5)
O2-K1-C56-C57	-1.3(4)	O13-K2-C56-C57	-113.1(7)
O4-K1-C56-C57	-137.4(4)	O9-K2-C56-K1	-47.5(4)
C53-K1-C56-C57	-37.5(3)	O11-K2-C56-K1	83.3(3)
C55-K1-C56-C57	-111.7(5)	O7-K2-C56-K1	-162.0(4)
C54-K1-C56-C57	-75.8(4)	O12-K2-C56-K1	142.0(3)
C64'-K1-C56-C57	111(3)	O10-K2-C56-K1	20.6(4)
O5-K1-C56-K2	-139.1(3)	O8-K2-C56-K1	-106.3(3)
O3-K1-C56-K2	-17.7(4)	C53-K2-C56-K1	-15.5(3)
O1-K1-C56-K2	105.4(3)	C54-K2-C56-K1	23.4(3)
O6-K1-C56-K2	163.1(3)	C57-K2-C56-K1	-53.8(3)
O2-K1-C56-K2	51.4(4)	C55-K2-C56-K1	59.2(3)
O4-K1-C56-K2	-84.6(4)	O13-K2-C56-K1	-167.0(7)
C57-K1-C56-K2	52.7(3)	C55-C56-C57-C53	-0.5(5)
C53-K1-C56-K2	15.2(3)	K1-C56-C57-C53	72.0(3)
C55-K1-C56-K2	-59.0(3)	K2-C56-C57-C53	-71.1(3)
C54-K1-C56-K2	-23.1(3)	C55-C56-C57-K2	70.6(3)
C64'-K1-C56-K2	164(3)	K1-C56-C57-K2	143.11(15)
O9-K2-C56-C55	-106.7(4)	C55-C56-C57-K1	-72.5(3)
O11-K2-C56-C55	24.1(4)	K2-C56-C57-K1	-143.11(15)
O7-K2-C56-C55	138.8(4)	C54-C53-C57-C56	0.6(5)
O12-K2-C56-C55	82.8(4)	K2-C53-C57-C56	74.9(3)
O10-K2-C56-C55	-38.6(5)	K1-C53-C57-C56	-71.8(3)
O8-K2-C56-C55	-165.5(4)	C54-C53-C57-K2	-74.3(3)
C53-K2-C56-C55	-74.7(4)	K1-C53-C57-K2	-146.70(15)
C54-K2-C56-C55	-35.7(3)	C54-C53-C57-K1	72.4(3)
C57-K2-C56-C55	-113.0(5)	K2-C53-C57-K1	146.70(15)
O13-K2-C56-C55	133.8(7)	O9-K2-C57-C56	-174.2(4)

O11-K2-C57-C56	-52.9(5)	C53-K1-C57-C56	111.2(4)
O7-K2-C57-C56	69.6(4)	C55-K1-C57-C56	36.6(3)
O12-K2-C57-C56	18.3(4)	C54-K1-C57-C56	74.4(3)
O10-K2-C57-C56	-121.8(4)	C64'-K1-C57-C56	-163.4(10)
O8-K2-C57-C56	128.2(4)	O5-K1-C57-C53	-124.3(4)
C53-K2-C57-C56	-110.6(5)	O3-K1-C57-C53	9.9(4)
C54-K2-C57-C56	-73.3(3)	O1-K1-C57-C53	123.3(4)
C55-K2-C57-C56	-35.6(3)	O6-K1-C57-C53	177.5(4)
O13-K2-C57-C56	126.0(6)	O2-K1-C57-C53	67.7(4)
O9-K2-C57-C53	-63.6(4)	O4-K1-C57-C53	-54.6(5)
O11-K2-C57-C53	57.7(5)	C56-K1-C57-C53	-111.2(4)
O7-K2-C57-C53	-179.8(4)	C55-K1-C57-C53	-74.6(3)
O12-K2-C57-C53	128.9(4)	C54-K1-C57-C53	-36.7(3)
O10-K2-C57-C53	-11.2(5)	C64'-K1-C57-C53	85.5(10)
O8-K2-C57-C53	-121.2(4)	O5-K1-C57-K2	-73.3(4)
C54-K2-C57-C53	37.3(3)	O3-K1-C57-K2	61.0(4)
C55-K2-C57-C53	75.0(4)	O1-K1-C57-K2	174.3(4)
C56-K2-C57-C53	110.6(5)	O6-K1-C57-K2	-131.5(4)
O13-K2-C57-C53	-123.3(6)	O2-K1-C57-K2	118.7(4)
O9-K2-C57-K1	-115.3(4)	O4-K1-C57-K2	-3.6(6)
O11-K2-C57-K1	6.1(5)	C56-K1-C57-K2	-60.2(3)
O7-K2-C57-K1	128.5(4)	C53-K1-C57-K2	51.0(3)
O12-K2-C57-K1	77.3(4)	C55-K1-C57-K2	-23.6(3)
O10-K2-C57-K1	-62.9(5)	C54-K1-C57-K2	14.3(3)
O8-K2-C57-K1	-172.9(4)	C64'-K1-C57-K2	136.5(10)
C53-K2-C57-K1	-51.7(3)	O9-K2-O13-C58	-111.2(9)
C54-K2-C57-K1	-14.3(3)	O11-K2-O13-C58	130.1(9)
C55-K2-C57-K1	23.3(3)	O7-K2-O13-C58	9.8(9)
C56-K2-C57-K1	59.0(3)	O12-K2-O13-C58	70.1(9)
O13-K2-C57-K1	-175.0(5)	O10-K2-O13-C58	-171.2(10)
O5-K1-C57-C56	-13.1(4)	O8-K2-O13-C58	-51.3(9)
O3-K1-C57-C56	121.1(4)	C53-K2-O13-C58	-113.7(9)
O1-K1-C57-C56	-125.5(4)	C54-K2-O13-C58	173.6(8)
O6-K1-C57-C56	-71.4(4)	C57-K2-O13-C58	-49.0(13)
O2-K1-C57-C56	178.9(4)	C55-K2-O13-C58	89.4(11)
O4-K1-C57-C56	56.6(5)	C56-K2-O13-C58	14.9(15)

O9-K2-O13-C61	7.1(7)	O6-K1-C64'-C65'	6.9(12)
O11-K2-O13-C61	-111.7(8)	O2-K1-C64'-C65'	122.0(14)
O7-K2-O13-C61	128.1(8)	O4-K1-C64'-C65'	-108.5(13)
O12-K2-O13-C61	-171.6(8)	C56-K1-C64'-C65'	6(4)
O10-K2-O13-C61	-52.9(7)	C57-K1-C64'-C65'	102.2(15)
O8-K2-O13-C61	67.0(8)	C53-K1-C64'-C65'	149.9(11)
C53-K2-O13-C61	4.6(12)	C55-K1-C64'-C65'	-118.0(14)
C54-K2-O13-C61	-68.1(14)	C54-K1-C64'-C65'	-165.7(10)
C57-K2-O13-C61	69.2(9)	O5-K1-C64'-C63'	-160(2)
C55-K2-O13-C61	-152.3(7)	O3-K1-C64'-C63'	79(2)
C56-K2-O13-C61	133.1(7)	O1-K1-C64'-C63'	-43(2)
C61-O13-C58-C59	41.5(12)	O6-K1-C64'-C63'	-101(2)
K2-O13-C58-C59	167.3(8)	O2-K1-C64'-C63'	14(2)
O13-C58-C59-C60	-14.7(16)	O4-K1-C64'-C63'	143(2)
C58-C59-C60-C61	-15.8(19)	C56-K1-C64'-C63'	-102(4)
C58-C59-C60-K2#1	168(3)	C57-K1-C64'-C63'	-6(3)
C58-O13-C61-C60	-51.6(16)	C53-K1-C64'-C63'	42(2)
K2-O13-C61-C60	-176.8(9)	C55-K1-C64'-C63'	133.6(19)
C59-C60-C61-O13	41.0(19)	C54-K1-C64'-C63'	86(2)
K2#1-C60-C61-O13	-140.6(7)	C62'-O14'-C65'-C64'	-55(3)
C65-O14-C62-C63	-27.3(13)	C63'-C64'-C65'-O14'	42(3)
O14-C62-C63-C64	24.6(13)	K1-C64'-C65'-O14'	-103(2)
C62-C63-C64-C65	-11.9(15)	C69-O15-C66-C67	-10(3)
C62-O14-C65-C64	19.2(14)	O15-C66-C67-C68	34(2)
C63-C64-C65-O14	-4.0(16)	C66-C67-C68-C69	-44(2)
C65'-O14'-C62'-C63'	47(4)	C66-O15-C69-C68	-18(3)
O14'-C62'-C63'-C64'	-20(4)	C67-C68-C69-O15	38(3)
C62'-C63'-C64'-C65'	-13(4)	C69'-O15'-C66'-C67'	-25.2(14)
C62'-C63'-C64'-K1	92(4)	O15'-C66'-C67'-C68'	26.8(15)
O5-K1-C64'-C65'	-51.2(13)	C66'-C67'-C68'-C69'	-18.5(16)
O3-K1-C64'-C65'	-172.4(14)	C66'-O15'-C69'-C68'	12.9(16)
O1-K1-C64'-C65'	65.1(13)	C67'-C68'-C69'-O15'	4.3(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

REFERENCE NUMBER: 05267 [**R&D2**]

CRYSTAL STRUCTURE REPORT

$C_{36} H_{54} Co K N_2 O_6$

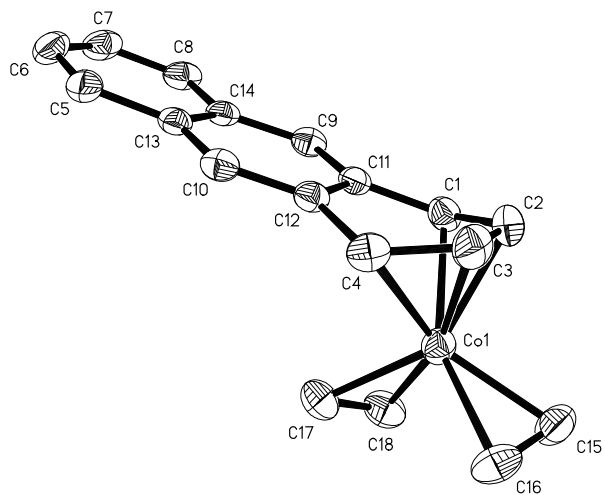
or

$[K(\text{cryptand-222})][Co(C_2H_4)_2(C_{14}H_{10})]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

September 06, 2005



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Data collection

A crystal (approximate dimensions 0.50 x 0.20 x 0.20 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 61 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 15 seconds and a detector distance of 4.99 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.78 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 3885 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ 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. Hydrogen atoms on C1, C2, C3, and C4 were found from the difference map and refined with individual isotropic displacement parameters. All remaining hydrogen atoms, including those of the ethylene ligands (due to disorder), were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0403$ and $wR2 = 0.1154$ (F^2 , all data).

Structure description

The structure is the one suggested. All atoms lie on general positions and the cation and anion are well separated. The ethylene ligands are modeled as disordered over two positions (64:36), with no restraints or constraints applied in order to avoid a presupposed model (i.e., the C—C distances are not necessarily equal). This leads to a slight range in the bondlengths, but all values lie within three standard uncertainties. The dihedral (fold) angle of the anthracene ligand is 26.24(13) degrees. There are two twist angles (due to the disorder) of 82.4 and 80.5 degrees—the geometry of the anion is essentially tetrahedral.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-

- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
- ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
- ³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
- ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
- ⁵ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

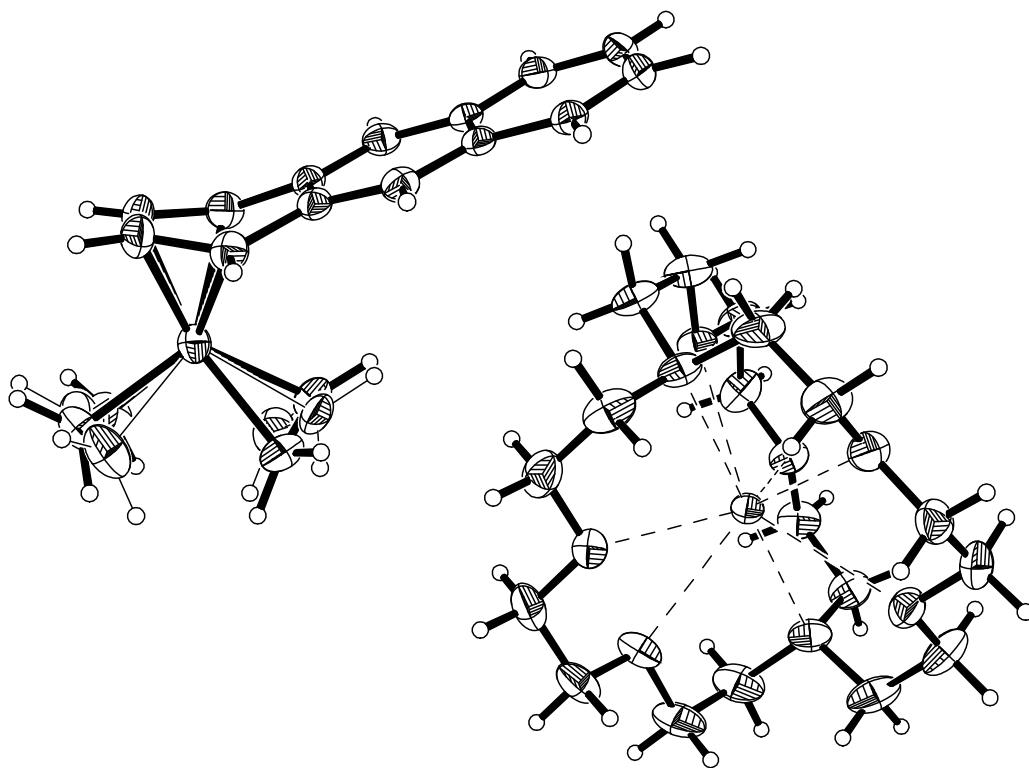
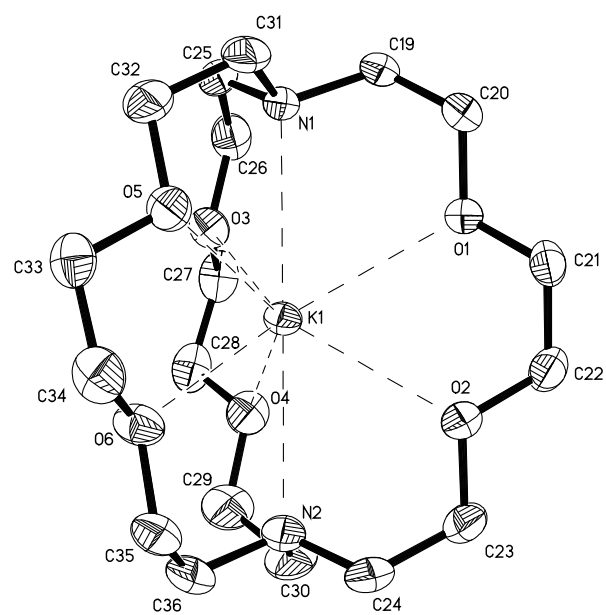
$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

$$\text{where } w = q / [\sigma^2 (F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

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



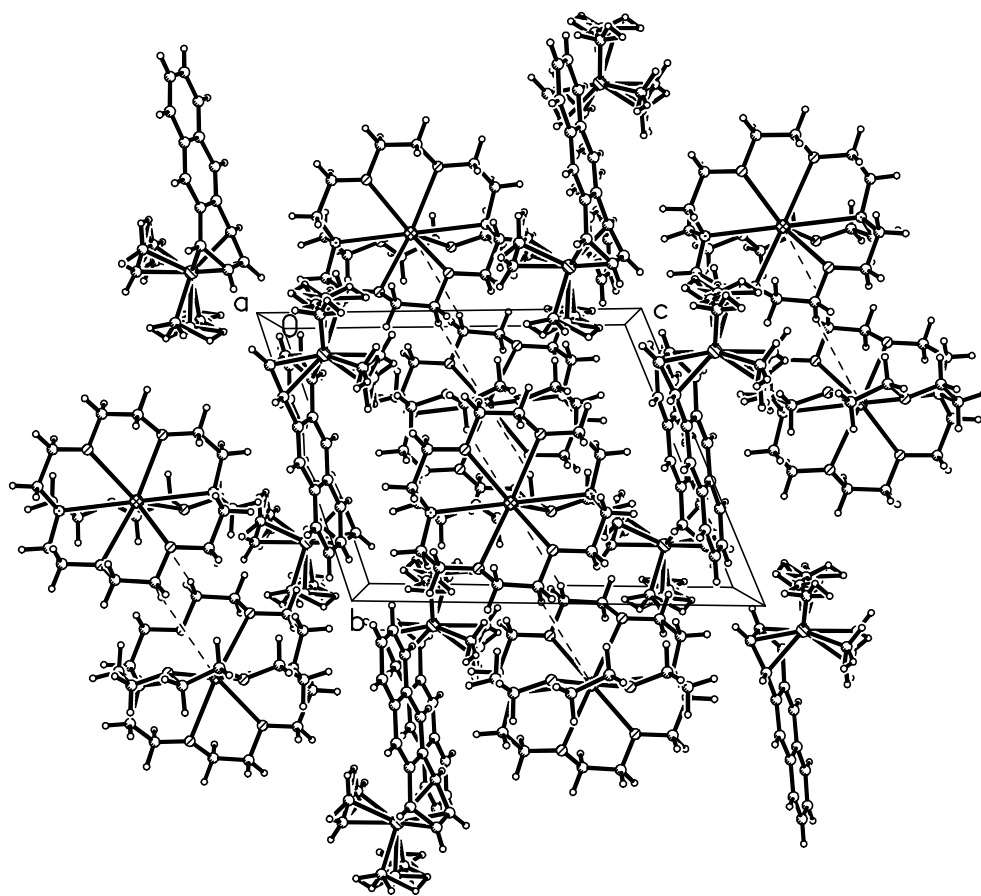
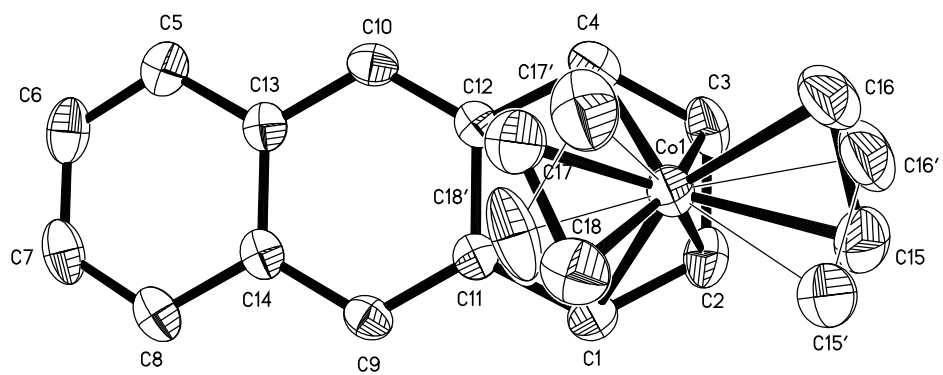


Table 1. Crystal data and structure refinement for 05267.

Identification code	05267	
Empirical formula	C ₃₆ H ₅₄ Co K N ₂ O ₆	
Formula weight	708.84	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 12.4181(9) Å	α = 66.162(1)°
	<i>b</i> = 12.550(1) Å	β = 77.387(1)°
	<i>c</i> = 14.420(1) Å	γ = 61.227(1)°
Volume	1800.9(2) Å ³	
<i>Z</i>	2	
Density (calculated)	1.307 Mg/m ³	
Absorption coefficient	0.638 mm ⁻¹	
<i>F</i> (000)	756	
Crystal color, morphology	metallic red, square prism	
Crystal size	0.50 x 0.20 x 0.20 mm ³	
Theta range for data collection	1.54 to 27.10°	
Index ranges	-15 ≤ <i>h</i> ≤ 15, -16 ≤ <i>k</i> ≤ 16, -18 ≤ <i>l</i> ≤ 18	
Reflections collected	20620	
Independent reflections	7836 [<i>R</i> (int) = 0.0294]	
Observed reflections	5880	
Completeness to theta = 27.10°	98.8%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8831 and 0.7410	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	7836 / 0 / 468	
Goodness-of-fit on <i>F</i> ²	1.039	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0403, <i>wR</i> 2 = 0.1025	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0623, <i>wR</i> 2 = 0.1154	
Largest diff. peak and hole	0.480 and -0.447 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05267. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	202(1)	8471(1)	8607(1)	28(1)
C1	178(2)	6962(2)	10037(2)	29(1)
C2	58(2)	8098(2)	10111(2)	35(1)
C3	1011(2)	8465(2)	9682(2)	35(1)
C4	2013(2)	7654(2)	9226(2)	31(1)
C5	4995(2)	3007(2)	9792(2)	31(1)
C6	5210(2)	1732(2)	10112(2)	37(1)
C7	4238(2)	1393(2)	10463(2)	36(1)
C8	3055(2)	2328(2)	10506(2)	31(1)
C9	1605(2)	4631(2)	10279(2)	26(1)
C10	3535(2)	5325(2)	9514(2)	26(1)
C11	1378(2)	5909(2)	9995(2)	24(1)
C12	2366(2)	6272(2)	9580(2)	24(1)
C13	3794(2)	3998(2)	9823(2)	25(1)
C14	2801(2)	3652(2)	10195(2)	25(1)
C15	-1323(6)	10185(7)	8293(5)	40(2)
C16	-292(7)	10311(6)	7692(6)	41(2)
C17	929(5)	7652(7)	7541(4)	36(2)
C18	-321(6)	7962(7)	7686(4)	38(1)
C15'	-1571(12)	9818(12)	8264(11)	48(3)
C16'	-813(15)	10447(11)	8005(10)	45(3)
C17'	623(10)	8452(13)	7153(8)	48(3)
C18'	337(16)	7416(11)	7809(8)	47(3)
K1	3276(1)	3210(1)	5177(1)	25(1)
N1	2978(2)	2868(2)	7348(1)	32(1)
N2	3569(2)	3539(2)	3014(2)	37(1)
O1	5136(1)	3090(2)	6121(1)	32(1)
O2	5605(2)	2870(2)	4188(1)	34(1)
O3	1216(2)	5100(2)	5834(1)	35(1)
O4	1828(2)	5635(2)	3750(1)	41(1)
O5	3046(2)	944(2)	6624(1)	37(1)

O6	2798(2)	1608(2)	4549(1)	38(1)
C19	3854(2)	3183(3)	7607(2)	37(1)
C20	5138(2)	2584(3)	7196(2)	39(1)
C21	6348(2)	2595(3)	5698(2)	40(1)
C22	6303(2)	3225(3)	4567(2)	42(1)
C23	5650(2)	3317(3)	3105(2)	40(1)
C24	4879(2)	2932(3)	2752(2)	41(1)
C25	1719(2)	3757(3)	7562(2)	42(1)
C26	1263(2)	5110(3)	6801(2)	44(1)
C27	748(2)	6387(2)	5105(2)	43(1)
C28	648(2)	6351(2)	4115(2)	42(1)
C29	1768(3)	5699(3)	2746(2)	54(1)
C30	3026(3)	4930(3)	2391(2)	51(1)
C31	3216(3)	1523(3)	7957(2)	43(1)
C32	2580(3)	994(3)	7610(2)	45(1)
C33	2456(2)	457(2)	6268(2)	38(1)
C34	3005(3)	357(2)	5269(2)	43(1)
C35	3227(3)	1559(3)	3565(2)	50(1)
C36	2954(3)	2901(3)	2824(2)	51(1)

Table 3. Bond lengths [Å] and angles [°] for 05267.

Co(1)-C(16)	1.994(6)	C(10)-C(13)	1.423(3)
Co(1)-C(17)	2.003(4)	C(10)-H(10A)	0.9500
Co(1)-C(18')	2.010(9)	C(11)-C(12)	1.438(3)
Co(1)-C(2)	2.012(3)	C(13)-C(14)	1.425(3)
Co(1)-C(18)	2.014(5)	C(15)-C(16)	1.419(8)
Co(1)-C(3)	2.018(3)	C(15)-H(15A)	0.9900
Co(1)-C(15)	2.021(6)	C(15)-H(15B)	0.9900
Co(1)-C(15')	2.041(13)	C(16)-H(16A)	0.9900
Co(1)-C(16')	2.054(11)	C(16)-H(16B)	0.9900
Co(1)-C(17')	2.054(9)	C(17)-C(18)	1.395(9)
Co(1)-C(1)	2.171(2)	C(17)-H(17A)	0.9900
Co(1)-C(4)	2.196(2)	C(17)-H(17B)	0.9900
C(1)-C(2)	1.405(3)	C(18)-H(18A)	0.9900
C(1)-C(11)	1.450(3)	C(18)-H(18B)	0.9900
C(1)-H(1)	0.90(3)	C(15')-C(16')	1.404(15)
C(2)-C(3)	1.404(4)	C(15')-H(15C)	0.9900
C(2)-H(2)	0.95(3)	C(15')-H(15D)	0.9900
C(3)-C(4)	1.407(4)	C(16')-H(16C)	0.9900
C(3)-H(3)	0.87(3)	C(16')-H(16D)	0.9900
C(4)-C(12)	1.453(3)	C(17')-C(18')	1.420(17)
C(4)-H(4)	0.86(3)	C(17')-H(17C)	0.9900
C(5)-C(6)	1.375(3)	C(17')-H(17D)	0.9900
C(5)-C(13)	1.416(3)	C(18')-H(18C)	0.9900
C(5)-H(5A)	0.9500	C(18')-H(18D)	0.9900
C(6)-C(7)	1.395(4)	K(1)-O(3)	2.8251(17)
C(6)-H(6A)	0.9500	K(1)-O(4)	2.8311(17)
C(7)-C(8)	1.377(3)	K(1)-O(6)	2.8413(17)
C(7)-H(7A)	0.9500	K(1)-O(2)	2.8429(17)
C(8)-C(14)	1.421(3)	K(1)-O(1)	2.8431(16)
C(8)-H(8A)	0.9500	K(1)-O(5)	2.8721(17)
C(9)-C(11)	1.380(3)	K(1)-N(2)	2.940(2)
C(9)-C(14)	1.420(3)	K(1)-N(1)	2.946(2)
C(9)-H(9A)	0.9500	N(1)-C(31)	1.464(3)
C(10)-C(12)	1.377(3)	N(1)-C(25)	1.475(3)

N(1)-C(19)	1.480(3)	C(27)-C(28)	1.480(4)
N(2)-C(24)	1.463(3)	C(27)-H(27A)	0.9900
N(2)-C(36)	1.468(3)	C(27)-H(27B)	0.9900
N(2)-C(30)	1.474(3)	C(28)-H(28A)	0.9900
O(1)-C(20)	1.418(3)	C(28)-H(28B)	0.9900
O(1)-C(21)	1.424(3)	C(29)-C(30)	1.495(4)
O(2)-C(22)	1.423(3)	C(29)-H(29A)	0.9900
O(2)-C(23)	1.428(3)	C(29)-H(29B)	0.9900
O(3)-C(26)	1.413(3)	C(30)-H(30A)	0.9900
O(3)-C(27)	1.429(3)	C(30)-H(30B)	0.9900
O(4)-C(28)	1.417(3)	C(31)-C(32)	1.503(4)
O(4)-C(29)	1.433(3)	C(31)-H(31A)	0.9900
O(5)-C(33)	1.421(3)	C(31)-H(31B)	0.9900
O(5)-C(32)	1.428(3)	C(32)-H(32A)	0.9900
O(6)-C(35)	1.418(3)	C(32)-H(32B)	0.9900
O(6)-C(34)	1.420(3)	C(33)-C(34)	1.480(4)
C(19)-C(20)	1.501(4)	C(33)-H(33A)	0.9900
C(19)-H(19A)	0.9900	C(33)-H(33B)	0.9900
C(19)-H(19B)	0.9900	C(34)-H(34A)	0.9900
C(20)-H(20A)	0.9900	C(34)-H(34B)	0.9900
C(20)-H(20B)	0.9900	C(35)-C(36)	1.499(4)
C(21)-C(22)	1.497(4)	C(35)-H(35A)	0.9900
C(21)-H(21A)	0.9900	C(35)-H(35B)	0.9900
C(21)-H(21B)	0.9900	C(36)-H(36A)	0.9900
C(22)-H(22A)	0.9900	C(36)-H(36B)	0.9900
C(22)-H(22B)	0.9900	C(16)-Co(1)-C(17)	97.7(3)
C(23)-C(24)	1.505(4)	C(16)-Co(1)-C(18')	109.4(4)
C(23)-H(23A)	0.9900	C(17)-Co(1)-C(18')	25.3(4)
C(23)-H(23B)	0.9900	C(16)-Co(1)-C(2)	117.6(2)
C(24)-H(24A)	0.9900	C(17)-Co(1)-C(2)	143.8(2)
C(24)-H(24B)	0.9900	C(18')-Co(1)-C(2)	130.9(4)
C(25)-C(26)	1.499(4)	C(16)-Co(1)-C(18)	95.6(3)
C(25)-H(25A)	0.9900	C(17)-Co(1)-C(18)	40.6(2)
C(25)-H(25B)	0.9900	C(18')-Co(1)-C(18)	22.1(3)
C(26)-H(26A)	0.9900	C(2)-Co(1)-C(18)	134.25(18)
C(26)-H(26B)	0.9900	C(16)-Co(1)-C(3)	98.7(2)

C(17)-Co(1)-C(3)	130.76(19)	C(18')-Co(1)-C(1)	91.9(4)
C(18')-Co(1)-C(3)	143.6(4)	C(2)-Co(1)-C(1)	39.03(9)
C(2)-Co(1)-C(3)	40.78(11)	C(18)-Co(1)-C(1)	99.33(19)
C(18)-Co(1)-C(3)	164.6(2)	C(3)-Co(1)-C(1)	69.75(10)
C(16)-Co(1)-C(15)	41.4(2)	C(15)-Co(1)-C(1)	116.6(2)
C(17)-Co(1)-C(15)	118.9(3)	C(15')-Co(1)-C(1)	108.1(4)
C(18')-Co(1)-C(15)	112.7(4)	C(16')-Co(1)-C(1)	135.2(5)
C(2)-Co(1)-C(15)	94.4(2)	C(17')-Co(1)-C(1)	131.2(4)
C(18)-Co(1)-C(15)	90.8(3)	C(16)-Co(1)-C(4)	110.2(2)
C(3)-Co(1)-C(15)	103.7(2)	C(17)-Co(1)-C(4)	92.10(18)
C(16)-Co(1)-C(15')	55.6(4)	C(18')-Co(1)-C(4)	107.7(5)
C(17)-Co(1)-C(15')	109.2(5)	C(2)-Co(1)-C(4)	69.35(10)
C(18')-Co(1)-C(15')	96.8(5)	C(18)-Co(1)-C(4)	129.6(2)
C(2)-Co(1)-C(15')	97.9(4)	C(3)-Co(1)-C(4)	38.72(10)
C(18)-Co(1)-C(15')	74.7(4)	C(15)-Co(1)-C(4)	136.8(3)
C(3)-Co(1)-C(15')	118.4(4)	C(15')-Co(1)-C(4)	155.1(4)
C(15)-Co(1)-C(15')	19.4(3)	C(16')-Co(1)-C(4)	120.1(4)
C(16)-Co(1)-C(16')	19.6(3)	C(17')-Co(1)-C(4)	103.1(3)
C(17)-Co(1)-C(16')	112.6(4)	C(1)-Co(1)-C(4)	76.03(9)
C(18')-Co(1)-C(16')	117.4(5)	C(2)-C(1)-C(11)	121.1(2)
C(2)-Co(1)-C(16')	103.6(4)	C(2)-C(1)-Co(1)	64.36(14)
C(18)-Co(1)-C(16')	98.6(4)	C(11)-C(1)-Co(1)	101.17(15)
C(3)-Co(1)-C(16')	96.8(4)	C(2)-C(1)-H(1)	119.1(16)
C(15)-Co(1)-C(16')	22.9(3)	C(11)-C(1)-H(1)	115.9(16)
C(15')-Co(1)-C(16')	40.1(4)	Co(1)-C(1)-H(1)	123.3(16)
C(16)-Co(1)-C(17')	73.5(4)	C(3)-C(2)-C(1)	117.2(2)
C(17)-Co(1)-C(17')	24.4(3)	C(3)-C(2)-Co(1)	69.87(15)
C(18')-Co(1)-C(17')	40.9(5)	C(1)-C(2)-Co(1)	76.61(15)
C(2)-Co(1)-C(17')	167.9(4)	C(3)-C(2)-H(2)	120.7(17)
C(18)-Co(1)-C(17')	43.4(3)	C(1)-C(2)-H(2)	121.9(17)
C(3)-Co(1)-C(17')	137.0(3)	Co(1)-C(2)-H(2)	120.0(17)
C(15)-Co(1)-C(17')	97.4(4)	C(2)-C(3)-C(4)	117.1(2)
C(15')-Co(1)-C(17')	92.4(6)	C(2)-C(3)-Co(1)	69.35(15)
C(16')-Co(1)-C(17')	88.3(5)	C(4)-C(3)-Co(1)	77.49(15)
C(16)-Co(1)-C(1)	153.8(2)	C(2)-C(3)-H(3)	123.1(18)
C(17)-Co(1)-C(1)	107.7(2)	C(4)-C(3)-H(3)	119.6(18)

Co(1)-C(3)-H(3)	120.3(18)	C(8)-C(14)-C(13)	118.6(2)
C(3)-C(4)-C(12)	120.9(2)	C(16)-C(15)-Co(1)	68.3(4)
C(3)-C(4)-Co(1)	63.79(14)	C(16)-C(15)-H(15A)	116.8
C(12)-C(4)-Co(1)	101.29(15)	Co(1)-C(15)-H(15A)	116.8
C(3)-C(4)-H(4)	119.1(17)	C(16)-C(15)-H(15B)	116.8
C(12)-C(4)-H(4)	115.8(17)	Co(1)-C(15)-H(15B)	116.8
Co(1)-C(4)-H(4)	124.3(17)	H(15A)-C(15)-H(15B)	113.9
C(6)-C(5)-C(13)	121.0(2)	C(15)-C(16)-Co(1)	70.3(3)
C(6)-C(5)-H(5A)	119.5	C(15)-C(16)-H(16A)	116.6
C(13)-C(5)-H(5A)	119.5	Co(1)-C(16)-H(16A)	116.6
C(5)-C(6)-C(7)	120.3(2)	C(15)-C(16)-H(16B)	116.6
C(5)-C(6)-H(6A)	119.8	Co(1)-C(16)-H(16B)	116.6
C(7)-C(6)-H(6A)	119.8	H(16A)-C(16)-H(16B)	113.6
C(8)-C(7)-C(6)	120.5(2)	C(18)-C(17)-Co(1)	70.1(3)
C(8)-C(7)-H(7A)	119.7	C(18)-C(17)-H(17A)	116.6
C(6)-C(7)-H(7A)	119.7	Co(1)-C(17)-H(17A)	116.6
C(7)-C(8)-C(14)	120.7(2)	C(18)-C(17)-H(17B)	116.6
C(7)-C(8)-H(8A)	119.6	Co(1)-C(17)-H(17B)	116.6
C(14)-C(8)-H(8A)	119.6	H(17A)-C(17)-H(17B)	113.6
C(11)-C(9)-C(14)	121.6(2)	C(17)-C(18)-Co(1)	69.2(3)
C(11)-C(9)-H(9A)	119.2	C(17)-C(18)-H(18A)	116.7
C(14)-C(9)-H(9A)	119.2	Co(1)-C(18)-H(18A)	116.7
C(12)-C(10)-C(13)	122.1(2)	C(17)-C(18)-H(18B)	116.7
C(12)-C(10)-H(10A)	119.0	Co(1)-C(18)-H(18B)	116.7
C(13)-C(10)-H(10A)	119.0	H(18A)-C(18)-H(18B)	113.7
C(9)-C(11)-C(12)	119.6(2)	C(16')-C(15')-Co(1)	70.5(7)
C(9)-C(11)-C(1)	124.6(2)	C(16')-C(15')-H(15C)	116.6
C(12)-C(11)-C(1)	115.8(2)	Co(1)-C(15')-H(15C)	116.6
C(10)-C(12)-C(11)	119.2(2)	C(16')-C(15')-H(15D)	116.6
C(10)-C(12)-C(4)	125.4(2)	Co(1)-C(15')-H(15D)	116.6
C(11)-C(12)-C(4)	115.3(2)	H(15C)-C(15')-H(15D)	113.6
C(5)-C(13)-C(10)	122.8(2)	C(15')-C(16')-Co(1)	69.5(7)
C(5)-C(13)-C(14)	118.8(2)	C(15')-C(16')-H(16C)	116.7
C(10)-C(13)-C(14)	118.4(2)	Co(1)-C(16')-H(16C)	116.7
C(9)-C(14)-C(8)	122.2(2)	C(15')-C(16')-H(16D)	116.7
C(9)-C(14)-C(13)	119.07(19)	Co(1)-C(16')-H(16D)	116.7

H(16C)-C(16')-H(16D)	113.7	O(6)-K(1)-N(1)	118.47(5)
C(18')-C(17')-Co(1)	67.9(5)	O(2)-K(1)-N(1)	119.08(5)
C(18')-C(17')-H(17C)	116.9	O(1)-K(1)-N(1)	60.99(5)
Co(1)-C(17')-H(17C)	116.9	O(5)-K(1)-N(1)	61.02(5)
C(18')-C(17')-H(17D)	116.9	N(2)-K(1)-N(1)	179.65(6)
Co(1)-C(17')-H(17D)	116.9	C(31)-N(1)-C(25)	110.0(2)
H(17C)-C(17')-H(17D)	113.9	C(31)-N(1)-C(19)	109.6(2)
C(17')-C(18')-Co(1)	71.3(5)	C(25)-N(1)-C(19)	108.5(2)
C(17')-C(18')-H(18C)	116.5	C(31)-N(1)-K(1)	109.63(15)
Co(1)-C(18')-H(18C)	116.5	C(25)-N(1)-K(1)	109.55(14)
C(17')-C(18')-H(18D)	116.5	C(19)-N(1)-K(1)	109.45(13)
Co(1)-C(18')-H(18D)	116.5	C(24)-N(2)-C(36)	109.2(2)
H(18C)-C(18')-H(18D)	113.5	C(24)-N(2)-C(30)	109.6(2)
O(3)-K(1)-O(4)	59.68(5)	C(36)-N(2)-C(30)	109.8(2)
O(3)-K(1)-O(6)	116.37(5)	C(24)-N(2)-K(1)	109.04(14)
O(4)-K(1)-O(6)	98.14(5)	C(36)-N(2)-K(1)	109.15(15)
O(3)-K(1)-O(2)	139.08(5)	C(30)-N(2)-K(1)	110.06(16)
O(4)-K(1)-O(2)	97.83(5)	C(20)-O(1)-C(21)	111.22(18)
O(6)-K(1)-O(2)	99.38(5)	C(20)-O(1)-K(1)	117.20(13)
O(3)-K(1)-O(1)	98.53(5)	C(21)-O(1)-K(1)	116.04(13)
O(4)-K(1)-O(1)	117.13(5)	C(22)-O(2)-C(23)	111.81(19)
O(6)-K(1)-O(1)	139.88(5)	C(22)-O(2)-K(1)	114.91(13)
O(2)-K(1)-O(1)	59.41(5)	C(23)-O(2)-K(1)	117.29(14)
O(3)-K(1)-O(5)	98.33(5)	C(26)-O(3)-C(27)	111.0(2)
O(4)-K(1)-O(5)	139.17(5)	C(26)-O(3)-K(1)	117.21(14)
O(6)-K(1)-O(5)	58.85(5)	C(27)-O(3)-K(1)	115.62(15)
O(2)-K(1)-O(5)	117.75(5)	C(28)-O(4)-C(29)	110.9(2)
O(1)-K(1)-O(5)	98.86(5)	C(28)-O(4)-K(1)	115.27(14)
O(3)-K(1)-N(2)	118.91(6)	C(29)-O(4)-K(1)	118.44(16)
O(4)-K(1)-N(2)	60.67(6)	C(33)-O(5)-C(32)	110.88(19)
O(6)-K(1)-N(2)	61.18(6)	C(33)-O(5)-K(1)	115.13(14)
O(2)-K(1)-N(2)	61.08(5)	C(32)-O(5)-K(1)	116.08(14)
O(1)-K(1)-N(2)	119.24(5)	C(35)-O(6)-C(34)	111.4(2)
O(5)-K(1)-N(2)	118.63(6)	C(35)-O(6)-K(1)	117.29(15)
O(3)-K(1)-N(1)	61.21(5)	C(34)-O(6)-K(1)	116.64(14)
O(4)-K(1)-N(1)	119.52(6)	N(1)-C(19)-C(20)	114.0(2)

N(1)-C(19)-H(19A)	108.7	N(1)-C(25)-H(25A)	108.7
C(20)-C(19)-H(19A)	108.7	C(26)-C(25)-H(25A)	108.7
N(1)-C(19)-H(19B)	108.7	N(1)-C(25)-H(25B)	108.7
C(20)-C(19)-H(19B)	108.7	C(26)-C(25)-H(25B)	108.7
H(19A)-C(19)-H(19B)	107.6	H(25A)-C(25)-H(25B)	107.6
O(1)-C(20)-C(19)	109.4(2)	O(3)-C(26)-C(25)	110.2(2)
O(1)-C(20)-H(20A)	109.8	O(3)-C(26)-H(26A)	109.6
C(19)-C(20)-H(20A)	109.8	C(25)-C(26)-H(26A)	109.6
O(1)-C(20)-H(20B)	109.8	O(3)-C(26)-H(26B)	109.6
C(19)-C(20)-H(20B)	109.8	C(25)-C(26)-H(26B)	109.6
H(20A)-C(20)-H(20B)	108.2	H(26A)-C(26)-H(26B)	108.1
O(1)-C(21)-C(22)	109.0(2)	O(3)-C(27)-C(28)	109.7(2)
O(1)-C(21)-H(21A)	109.9	O(3)-C(27)-H(27A)	109.7
C(22)-C(21)-H(21A)	109.9	C(28)-C(27)-H(27A)	109.7
O(1)-C(21)-H(21B)	109.9	O(3)-C(27)-H(27B)	109.7
C(22)-C(21)-H(21B)	109.9	C(28)-C(27)-H(27B)	109.7
H(21A)-C(21)-H(21B)	108.3	H(27A)-C(27)-H(27B)	108.2
O(2)-C(22)-C(21)	109.3(2)	O(4)-C(28)-C(27)	110.0(2)
O(2)-C(22)-H(22A)	109.8	O(4)-C(28)-H(28A)	109.7
C(21)-C(22)-H(22A)	109.8	C(27)-C(28)-H(28A)	109.7
O(2)-C(22)-H(22B)	109.8	O(4)-C(28)-H(28B)	109.7
C(21)-C(22)-H(22B)	109.8	C(27)-C(28)-H(28B)	109.7
H(22A)-C(22)-H(22B)	108.3	H(28A)-C(28)-H(28B)	108.2
O(2)-C(23)-C(24)	109.2(2)	O(4)-C(29)-C(30)	109.3(2)
O(2)-C(23)-H(23A)	109.8	O(4)-C(29)-H(29A)	109.8
C(24)-C(23)-H(23A)	109.8	C(30)-C(29)-H(29A)	109.8
O(2)-C(23)-H(23B)	109.8	O(4)-C(29)-H(29B)	109.8
C(24)-C(23)-H(23B)	109.8	C(30)-C(29)-H(29B)	109.8
H(23A)-C(23)-H(23B)	108.3	H(29A)-C(29)-H(29B)	108.3
N(2)-C(24)-C(23)	114.0(2)	N(2)-C(30)-C(29)	113.9(2)
N(2)-C(24)-H(24A)	108.7	N(2)-C(30)-H(30A)	108.8
C(23)-C(24)-H(24A)	108.7	C(29)-C(30)-H(30A)	108.8
N(2)-C(24)-H(24B)	108.7	N(2)-C(30)-H(30B)	108.8
C(23)-C(24)-H(24B)	108.7	C(29)-C(30)-H(30B)	108.8
H(24A)-C(24)-H(24B)	107.6	H(30A)-C(30)-H(30B)	107.7
N(1)-C(25)-C(26)	114.4(2)	N(1)-C(31)-C(32)	114.6(2)

N(1)-C(31)-H(31A)	108.6	O(6)-C(34)-H(34A)	109.7
C(32)-C(31)-H(31A)	108.6	C(33)-C(34)-H(34A)	109.7
N(1)-C(31)-H(31B)	108.6	O(6)-C(34)-H(34B)	109.7
C(32)-C(31)-H(31B)	108.6	C(33)-C(34)-H(34B)	109.7
H(31A)-C(31)-H(31B)	107.6	H(34A)-C(34)-H(34B)	108.2
O(5)-C(32)-C(31)	109.4(2)	O(6)-C(35)-C(36)	109.7(2)
O(5)-C(32)-H(32A)	109.8	O(6)-C(35)-H(35A)	109.7
C(31)-C(32)-H(32A)	109.8	C(36)-C(35)-H(35A)	109.7
O(5)-C(32)-H(32B)	109.8	O(6)-C(35)-H(35B)	109.7
C(31)-C(32)-H(32B)	109.8	C(36)-C(35)-H(35B)	109.7
H(32A)-C(32)-H(32B)	108.2	H(35A)-C(35)-H(35B)	108.2
O(5)-C(33)-C(34)	109.4(2)	N(2)-C(36)-C(35)	114.9(2)
O(5)-C(33)-H(33A)	109.8	N(2)-C(36)-H(36A)	108.5
C(34)-C(33)-H(33A)	109.8	C(35)-C(36)-H(36A)	108.5
O(5)-C(33)-H(33B)	109.8	N(2)-C(36)-H(36B)	108.5
C(34)-C(33)-H(33B)	109.8	C(35)-C(36)-H(36B)	108.5
H(33A)-C(33)-H(33B)	108.3	H(36A)-C(36)-H(36B)	107.5
O(6)-C(34)-C(33)	110.0(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05267. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	30(1)	24(1)	30(1)	-10(1)	1(1)	-12(1)
C1	30(1)	32(1)	25(1)	-11(1)	4(1)	-14(1)
C2	38(1)	31(1)	34(1)	-18(1)	2(1)	-9(1)
C3	44(2)	26(1)	42(2)	-17(1)	-7(1)	-14(1)
C4	34(1)	28(1)	32(1)	-7(1)	-3(1)	-18(1)
C5	30(1)	34(1)	27(1)	-12(1)	-6(1)	-9(1)
C6	38(1)	27(1)	35(1)	-13(1)	-14(1)	2(1)
C7	51(2)	20(1)	32(1)	-7(1)	-14(1)	-8(1)
C8	44(1)	26(1)	24(1)	-6(1)	-9(1)	-17(1)
C9	32(1)	27(1)	21(1)	-6(1)	-1(1)	-17(1)
C10	29(1)	30(1)	22(1)	-6(1)	-2(1)	-17(1)
C11	29(1)	24(1)	17(1)	-6(1)	-1(1)	-12(1)
C12	30(1)	24(1)	20(1)	-7(1)	-2(1)	-13(1)
C13	30(1)	26(1)	17(1)	-8(1)	-4(1)	-11(1)
C14	33(1)	24(1)	16(1)	-6(1)	-5(1)	-12(1)
C15	33(4)	29(4)	44(3)	-7(3)	-5(3)	-6(2)
C16	48(4)	26(3)	43(4)	1(2)	-8(3)	-19(3)
C17	42(3)	42(4)	31(3)	-20(3)	3(2)	-21(3)
C18	46(4)	46(4)	30(2)	-16(3)	-4(2)	-24(3)
C15'	36(6)	30(6)	64(7)	-8(5)	-1(4)	-12(4)
C16'	58(11)	23(5)	46(8)	-5(5)	0(6)	-18(7)
C17'	65(6)	42(7)	34(5)	-14(5)	1(4)	-21(5)
C18'	77(11)	27(6)	44(6)	-16(5)	-23(6)	-16(6)
K1	29(1)	25(1)	21(1)	-6(1)	-3(1)	-11(1)
N1	36(1)	44(1)	22(1)	-10(1)	0(1)	-25(1)
N2	40(1)	46(1)	22(1)	-7(1)	-4(1)	-20(1)
O1	30(1)	42(1)	25(1)	-12(1)	1(1)	-17(1)
O2	36(1)	43(1)	26(1)	-12(1)	3(1)	-22(1)
O3	37(1)	30(1)	39(1)	-14(1)	-4(1)	-13(1)
O4	32(1)	34(1)	39(1)	-2(1)	-9(1)	-7(1)
O5	47(1)	36(1)	32(1)	-4(1)	-5(1)	-26(1)

O6	50(1)	36(1)	33(1)	-16(1)	-3(1)	-19(1)
C19	43(1)	57(2)	24(1)	-16(1)	0(1)	-30(1)
C20	38(1)	55(2)	29(1)	-11(1)	-5(1)	-25(1)
C21	28(1)	60(2)	45(2)	-29(1)	2(1)	-21(1)
C22	37(1)	60(2)	44(2)	-28(1)	13(1)	-31(1)
C23	38(1)	51(2)	29(1)	-11(1)	6(1)	-23(1)
C24	48(2)	51(2)	23(1)	-14(1)	6(1)	-25(1)
C25	39(1)	70(2)	31(1)	-26(1)	12(1)	-32(1)
C26	34(1)	52(2)	55(2)	-35(2)	6(1)	-17(1)
C27	33(1)	24(1)	65(2)	-14(1)	-2(1)	-8(1)
C28	32(1)	27(1)	52(2)	1(1)	-9(1)	-9(1)
C29	50(2)	53(2)	34(2)	3(1)	-18(1)	-13(2)
C30	54(2)	54(2)	25(1)	3(1)	-6(1)	-21(2)
C31	58(2)	51(2)	22(1)	1(1)	-9(1)	-33(1)
C32	64(2)	48(2)	29(1)	-2(1)	-1(1)	-38(2)
C33	40(1)	29(1)	47(2)	-10(1)	-4(1)	-17(1)
C34	53(2)	30(1)	53(2)	-17(1)	-3(1)	-21(1)
C35	63(2)	70(2)	43(2)	-35(2)	7(1)	-41(2)
C36	62(2)	78(2)	28(1)	-18(1)	-5(1)	-42(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 05267.

	x	y	z	U(eq)
H1	-450(20)	6750(20)	10252(19)	33(7)
H2	-660(30)	8630(30)	10400(20)	46(8)
H3	990(20)	9180(30)	9660(20)	41(8)
H4	2580(20)	7890(20)	8915(19)	31(7)
H5A	5663	3226	9546	37
H6A	6024	1079	10094	45
H7A	4393	512	10674	43
H8A	2402	2084	10746	37
H9A	944	4400	10537	31
H10A	4188	5567	9253	32
H15A	-1980	10279	7940	48
H15B	-1632	10587	8822	48
H16A	40	10800	7840	50
H16B	-307	10493	6959	50
H17A	1183	8168	6888	43
H17B	1508	6718	7773	43
H18A	-538	7226	8012	45
H18B	-864	8678	7127	45
H15C	-1920	9847	7694	58
H15D	-2156	9930	8844	58
H16C	-917	10952	8423	54
H16D	-680	10870	7273	54
H17C	19	9152	6629	58
H17D	1490	8221	6915	58
H18C	1026	6532	7974	57
H18D	-441	7461	7689	57
H19A	3877	2886	8355	45
H19B	3548	4137	7342	45
H20A	5686	2779	7439	47
H20B	5450	1630	7438	47

H21A	6691	1643	5890	49
H21B	6886	2781	5963	49
H22A	5920	4180	4378	50
H22B	7147	2942	4267	50
H23A	6510	2932	2857	48
H23B	5334	4273	2830	48
H24A	4981	3167	2006	49
H24B	5189	1978	3054	49
H25A	1690	3797	8240	51
H25B	1154	3396	7589	51
H26A	434	5658	7014	52
H26B	1819	5486	6766	52
H27A	1304	6777	5032	51
H27B	-71	6930	5338	51
H28A	107	5942	4192	51
H28B	278	7246	3621	51
H29A	1445	6614	2281	65
H29B	1207	5346	2748	65
H30A	2986	5021	1683	61
H30B	3575	5298	2390	61
H31A	2953	1463	8669	52
H31B	4113	968	7947	52
H32A	2725	113	8092	54
H32B	1683	1557	7589	54
H33A	1566	1047	6204	46
H33B	2558	-408	6757	46
H34A	3899	-213	5330	52
H34B	2633	-32	5037	52
H35A	2820	1180	3360	59
H35B	4124	1000	3569	59
H36A	3199	2857	2135	61
H36B	2055	3446	2835	61

Table 6. Torsion angles [°] for 05267.

C16-Co1-C1-C2	-33.1(5)	C16-Co1-C2-C1	164.2(3)
C17-Co1-C1-C2	162.0(2)	C17-Co1-C2-C1	-29.8(4)
C18'-Co1-C1-C2	-177.9(5)	C18'-Co1-C2-C1	2.8(7)
C18-Co1-C1-C2	-157.0(2)	C18-Co1-C2-C1	32.6(4)
C3-Co1-C1-C2	34.26(16)	C3-Co1-C2-C1	-126.1(2)
C15-Co1-C1-C2	-61.3(3)	C15-Co1-C2-C1	128.1(3)
C15'-Co1-C1-C2	-80.1(5)	C15'-Co1-C2-C1	109.0(4)
C16'-Co1-C1-C2	-44.6(6)	C16'-Co1-C2-C1	149.4(5)
C17'-Co1-C1-C2	169.7(4)	C17'-Co1-C2-C1	-40.0(14)
C4-Co1-C1-C2	74.33(16)	C4-Co1-C2-C1	-93.16(16)
C16-Co1-C1-C11	-152.4(5)	C1-C2-C3-C4	-0.8(4)
C17-Co1-C1-C11	42.8(2)	Co1-C2-C3-C4	-63.0(2)
C18'-Co1-C1-C11	62.8(5)	C1-C2-C3-Co1	62.2(2)
C2-Co1-C1-C11	-119.3(2)	C16-Co1-C3-C2	122.7(3)
C18-Co1-C1-C11	83.8(2)	C17-Co1-C3-C2	-129.2(3)
C3-Co1-C1-C11	-85.03(16)	C18'-Co1-C3-C2	-96.7(7)
C15-Co1-C1-C11	179.4(3)	C18-Co1-C3-C2	-79.3(7)
C15'-Co1-C1-C11	160.6(5)	C15-Co1-C3-C2	80.8(3)
C16'-Co1-C1-C11	-163.9(6)	C15'-Co1-C3-C2	67.3(5)
C17'-Co1-C1-C11	50.4(4)	C16'-Co1-C3-C2	103.0(5)
C4-Co1-C1-C11	-44.95(15)	C17'-Co1-C3-C2	-162.2(6)
C11-C1-C2-C3	29.2(3)	C1-Co1-C3-C2	-32.87(14)
Co1-C1-C2-C3	-58.6(2)	C4-Co1-C3-C2	-125.7(2)
C11-C1-C2-Co1	87.8(2)	C16-Co1-C3-C4	-111.6(3)
C16-Co1-C2-C3	-69.8(3)	C17-Co1-C3-C4	-3.5(3)
C17-Co1-C2-C3	96.2(3)	C18'-Co1-C3-C4	29.0(8)
C18'-Co1-C2-C3	128.8(7)	C2-Co1-C3-C4	125.7(2)
C18-Co1-C2-C3	158.7(3)	C18-Co1-C3-C4	46.4(7)
C15-Co1-C2-C3	-105.8(3)	C15-Co1-C3-C4	-153.5(3)
C15'-Co1-C2-C3	-125.0(4)	C15'-Co1-C3-C4	-167.1(4)
C16'-Co1-C2-C3	-84.5(5)	C16'-Co1-C3-C4	-131.3(5)
C17'-Co1-C2-C3	86.0(14)	C17'-Co1-C3-C4	-36.5(6)
C1-Co1-C2-C3	126.1(2)	C1-Co1-C3-C4	92.80(16)
C4-Co1-C2-C3	32.89(14)	C2-C3-C4-C12	-29.0(3)

Co1-C3-C4-C12	-87.7(2)	C9-C11-C12-C4	175.1(2)
C2-C3-C4-Co1	58.7(2)	C1-C11-C12-C4	-2.2(3)
C16-Co1-C4-C3	78.4(3)	C3-C4-C12-C10	-152.2(2)
C17-Co1-C4-C3	177.3(3)	Co1-C4-C12-C10	141.7(2)
C18'-Co1-C4-C3	-162.4(4)	C3-C4-C12-C11	30.2(3)
C2-Co1-C4-C3	-34.55(16)	Co1-C4-C12-C11	-35.9(2)
C18-Co1-C4-C3	-165.6(2)	C6-C5-C13-C10	179.0(2)
C15-Co1-C4-C3	39.2(4)	C6-C5-C13-C14	0.1(3)
C15'-Co1-C4-C3	27.9(9)	C12-C10-C13-C5	-177.8(2)
C16'-Co1-C4-C3	59.6(5)	C12-C10-C13-C14	1.1(3)
C17'-Co1-C4-C3	155.4(4)	C11-C9-C14-C8	178.6(2)
C1-Co1-C4-C3	-74.93(16)	C11-C9-C14-C13	1.0(3)
C16-Co1-C4-C12	-162.7(3)	C7-C8-C14-C9	-176.6(2)
C17-Co1-C4-C12	-63.7(3)	C7-C8-C14-C13	1.0(3)
C18'-Co1-C4-C12	-43.4(4)	C5-C13-C14-C9	176.68(19)
C2-Co1-C4-C12	84.43(16)	C10-C13-C14-C9	-2.3(3)
C18-Co1-C4-C12	-46.6(3)	C5-C13-C14-C8	-1.0(3)
C3-Co1-C4-C12	119.0(2)	C10-C13-C14-C8	-179.96(19)
C15-Co1-C4-C12	158.2(3)	C17-Co1-C15-C16	-66.7(5)
C15'-Co1-C4-C12	146.9(9)	C18'-Co1-C15-C16	-94.0(7)
C16'-Co1-C4-C12	178.6(5)	C2-Co1-C15-C16	128.0(4)
C17'-Co1-C4-C12	-85.7(4)	C18-Co1-C15-C16	-97.5(5)
C1-Co1-C4-C12	44.05(15)	C3-Co1-C15-C16	87.7(5)
C13-C5-C6-C7	0.8(4)	C15'-Co1-C15-C16	-130.7(18)
C5-C6-C7-C8	-0.9(4)	C16'-Co1-C15-C16	12.9(11)
C6-C7-C8-C14	-0.1(3)	C17'-Co1-C15-C16	-54.5(5)
C14-C9-C11-C12	1.5(3)	C1-Co1-C15-C16	161.6(4)
C14-C9-C11-C1	178.5(2)	C4-Co1-C15-C16	63.6(5)
C2-C1-C11-C9	155.8(2)	C17-Co1-C16-C15	125.8(5)
Co1-C1-C11-C9	-137.56(19)	C18'-Co1-C16-C15	102.7(6)
C2-C1-C11-C12	-27.1(3)	C2-Co1-C16-C15	-62.5(5)
Co1-C1-C11-C12	39.6(2)	C18-Co1-C16-C15	84.9(5)
C13-C10-C12-C11	1.4(3)	C3-Co1-C16-C15	-100.8(4)
C13-C10-C12-C4	-176.2(2)	C15'-Co1-C16-C15	17.7(6)
C9-C11-C12-C10	-2.7(3)	C16'-Co1-C16-C15	-15.0(14)
C1-C11-C12-C10	-180.0(2)	C17'-Co1-C16-C15	122.6(6)

C1-Co1-C16-C15	-39.7(7)	C18-Co1-C16'-C15'	53.5(9)
C4-Co1-C16-C15	-139.1(4)	C3-Co1-C16'-C15'	-127.1(9)
C16-Co1-C17-C18	-89.6(4)	C15-Co1-C16'-C15'	-17.8(10)
C18'-Co1-C17-C18	30.2(9)	C17'-Co1-C16'-C15'	95.8(9)
C2-Co1-C17-C18	102.8(5)	C1-Co1-C16'-C15'	-59.1(10)
C3-Co1-C17-C18	161.8(3)	C4-Co1-C16'-C15'	-160.0(7)
C15-Co1-C17-C18	-51.8(5)	C16-Co1-C17'-C18'	-150.5(9)
C15'-Co1-C17-C18	-33.5(5)	C17-Co1-C17'-C18'	37.0(10)
C16'-Co1-C17-C18	-76.3(6)	C2-Co1-C17'-C18'	51.7(17)
C17'-Co1-C17-C18	-82.3(9)	C18-Co1-C17'-C18'	-33.0(5)
C1-Co1-C17-C18	83.6(5)	C3-Co1-C17'-C18'	124.4(7)
C4-Co1-C17-C18	159.6(5)	C15-Co1-C17'-C18'	-116.4(9)
C16-Co1-C18-C17	95.3(4)	C15'-Co1-C17'-C18'	-97.6(8)
C18'-Co1-C18-C17	-34.8(12)	C16'-Co1-C17'-C18'	-137.4(9)
C2-Co1-C18-C17	-126.5(4)	C1-Co1-C17'-C18'	19.2(11)
C3-Co1-C18-C17	-62.9(7)	C4-Co1-C17'-C18'	102.0(9)
C15-Co1-C18-C17	136.5(5)	C16-Co1-C18'-C17'	30.0(9)
C15'-Co1-C18-C17	147.3(6)	C17-Co1-C18'-C17'	-35.7(8)
C16'-Co1-C18-C17	114.8(5)	C2-Co1-C18'-C17'	-167.4(6)
C17'-Co1-C18-C17	36.6(4)	C18-Co1-C18'-C17'	83.8(12)
C1-Co1-C18-C17	-106.4(4)	C3-Co1-C18'-C17'	-108.3(8)
C4-Co1-C18-C17	-26.8(6)	C15-Co1-C18'-C17'	74.3(9)
C16-Co1-C15'-C16'	-16.4(7)	C15'-Co1-C18'-C17'	85.9(9)
C17-Co1-C15'-C16'	-102.6(9)	C16'-Co1-C18'-C17'	49.6(10)
C18'-Co1-C15'-C16'	-125.2(9)	C1-Co1-C18'-C17'	-165.7(8)
C2-Co1-C15'-C16'	101.7(8)	C4-Co1-C18'-C17'	-89.8(8)
C18-Co1-C15'-C16'	-124.5(9)	O3-K1-N1-C31	134.96(17)
C3-Co1-C15'-C16'	64.3(9)	O4-K1-N1-C31	148.27(15)
C15-Co1-C15'-C16'	21.0(13)	O6-K1-N1-C31	28.79(17)
C17'-Co1-C15'-C16'	-84.5(9)	O2-K1-N1-C31	-92.12(16)
C1-Co1-C15'-C16'	140.5(8)	O1-K1-N1-C31	-105.16(16)
C4-Co1-C15'-C16'	44.8(14)	O5-K1-N1-C31	15.40(15)
C16-Co1-C16'-C15'	136(2)	N2-K1-N1-C31	25(11)
C17-Co1-C16'-C15'	93.3(10)	O3-K1-N1-C25	14.12(14)
C18'-Co1-C16'-C15'	65.9(11)	O4-K1-N1-C25	27.43(17)
C2-Co1-C16'-C15'	-86.2(9)	O6-K1-N1-C25	-92.05(16)

O2-K1-N1-C25	147.04(15)	O5-K1-O1-C20	-33.10(17)
O1-K1-N1-C25	134.00(16)	N2-K1-O1-C20	-163.11(16)
O5-K1-N1-C25	-105.44(16)	N1-K1-O1-C20	16.58(16)
N2-K1-N1-C25	-96(11)	O3-K1-O1-C21	-158.46(16)
O3-K1-N1-C19	-104.75(17)	O4-K1-O1-C21	-98.24(17)
O4-K1-N1-C19	-91.44(16)	O6-K1-O1-C21	50.51(19)
O6-K1-N1-C19	149.07(15)	O2-K1-O1-C21	-15.43(16)
O2-K1-N1-C19	28.17(18)	O5-K1-O1-C21	101.65(17)
O1-K1-N1-C19	15.13(15)	N2-K1-O1-C21	-28.36(18)
O5-K1-N1-C19	135.68(17)	N1-K1-O1-C21	151.33(18)
N2-K1-N1-C19	145(11)	O3-K1-O2-C22	46.45(19)
O3-K1-N2-C24	150.71(15)	O4-K1-O2-C22	98.18(17)
O4-K1-N2-C24	137.05(18)	O6-K1-O2-C22	-162.17(16)
O6-K1-N2-C24	-103.31(17)	O1-K1-O2-C22	-18.78(16)
O2-K1-N2-C24	17.78(15)	O5-K1-O2-C22	-102.53(17)
O1-K1-N2-C24	30.50(18)	N2-K1-O2-C22	148.33(18)
O5-K1-N2-C24	-89.94(17)	N1-K1-O2-C22	-32.03(18)
N1-K1-N2-C24	-99(11)	O3-K1-O2-C23	-88.02(18)
O3-K1-N2-C36	-90.12(18)	O4-K1-O2-C23	-36.28(17)
O4-K1-N2-C36	-103.78(19)	O6-K1-O2-C23	63.37(17)
O6-K1-N2-C36	15.86(17)	O1-K1-O2-C23	-153.25(18)
O2-K1-N2-C36	136.96(19)	O5-K1-O2-C23	123.00(16)
O1-K1-N2-C36	149.67(17)	N2-K1-O2-C23	13.86(16)
O5-K1-N2-C36	29.23(19)	N1-K1-O2-C23	-166.50(16)
N1-K1-N2-C36	20(11)	O4-K1-O3-C26	-149.74(18)
O3-K1-N2-C30	30.41(18)	O6-K1-O3-C26	126.39(16)
O4-K1-N2-C30	16.75(16)	O2-K1-O3-C26	-85.44(18)
O6-K1-N2-C30	136.39(18)	O1-K1-O3-C26	-33.22(17)
O2-K1-N2-C30	-102.52(18)	O5-K1-O3-C26	67.11(17)
O1-K1-N2-C30	-89.80(17)	N2-K1-O3-C26	-163.54(16)
O5-K1-N2-C30	149.76(16)	N1-K1-O3-C26	16.84(16)
N1-K1-N2-C30	140(11)	O4-K1-O3-C27	-15.86(15)
O3-K1-O1-C20	66.78(17)	O6-K1-O3-C27	-99.73(16)
O4-K1-O1-C20	127.00(16)	O2-K1-O3-C27	48.44(18)
O6-K1-O1-C20	-84.24(18)	O1-K1-O3-C27	100.66(16)
O2-K1-O1-C20	-150.18(18)	O5-K1-O3-C27	-159.01(16)

N2-K1-O3-C27	-29.66(17)	N1-K1-O6-C35	-164.92(18)
N1-K1-O3-C27	150.72(17)	O3-K1-O6-C34	-99.03(17)
O3-K1-O4-C28	-17.22(16)	O4-K1-O6-C34	-159.15(17)
O6-K1-O4-C28	98.64(17)	O2-K1-O6-C34	101.46(17)
O2-K1-O4-C28	-160.65(17)	O1-K1-O6-C34	48.64(19)
O1-K1-O4-C28	-101.10(17)	O5-K1-O6-C34	-15.38(16)
O5-K1-O4-C28	48.0(2)	N2-K1-O6-C34	150.90(18)
N2-K1-O4-C28	148.93(18)	N1-K1-O6-C34	-29.07(18)
N1-K1-O4-C28	-30.74(18)	C31-N1-C19-C20	74.0(3)
O3-K1-O4-C29	-151.9(2)	C25-N1-C19-C20	-165.8(2)
O6-K1-O4-C29	-36.06(19)	K1-N1-C19-C20	-46.3(2)
O2-K1-O4-C29	64.65(19)	C21-O1-C20-C19	177.1(2)
O1-K1-O4-C29	124.20(18)	K1-O1-C20-C19	-46.1(2)
O5-K1-O4-C29	-86.7(2)	N1-C19-C20-O1	63.6(3)
N2-K1-O4-C29	14.23(18)	C20-O1-C21-C22	-176.3(2)
N1-K1-O4-C29	-165.44(18)	K1-O1-C21-C22	46.3(2)
O3-K1-O5-C33	97.80(16)	C23-O2-C22-C21	-173.1(2)
O4-K1-O5-C33	45.45(19)	K1-O2-C22-C21	50.0(2)
O6-K1-O5-C33	-18.04(15)	O1-C21-C22-O2	-63.9(3)
O2-K1-O5-C33	-102.14(16)	C22-O2-C23-C24	-179.1(2)
O1-K1-O5-C33	-162.15(15)	K1-O2-C23-C24	-43.3(3)
N2-K1-O5-C33	-31.74(17)	C36-N2-C24-C23	-168.5(2)
N1-K1-O5-C33	148.20(17)	C30-N2-C24-C23	71.2(3)
O3-K1-O5-C32	-34.11(17)	K1-N2-C24-C23	-49.3(2)
O4-K1-O5-C32	-86.47(18)	O2-C23-C24-N2	64.1(3)
O6-K1-O5-C32	-149.96(18)	C31-N1-C25-C26	-164.9(2)
O2-K1-O5-C32	125.94(16)	C19-N1-C25-C26	75.1(3)
O1-K1-O5-C32	65.94(17)	K1-N1-C25-C26	-44.3(2)
N2-K1-O5-C32	-163.65(16)	C27-O3-C26-C25	178.2(2)
N1-K1-O5-C32	16.28(16)	K1-O3-C26-C25	-45.9(2)
O3-K1-O6-C35	125.12(18)	N1-C25-C26-O3	62.2(3)
O4-K1-O6-C35	65.00(19)	C26-O3-C27-C28	-177.1(2)
O2-K1-O6-C35	-34.38(19)	K1-O3-C27-C28	46.3(2)
O1-K1-O6-C35	-87.2(2)	C29-O4-C28-C27	-174.1(2)
O5-K1-O6-C35	-151.2(2)	K1-O4-C28-C27	47.9(2)
N2-K1-O6-C35	15.05(18)	O3-C27-C28-O4	-62.6(3)

C28-O4-C29-C30	-179.7(2)	C32-O5-C33-C34	-177.2(2)
K1-O4-C29-C30	-43.2(3)	K1-O5-C33-C34	48.5(2)
C24-N2-C30-C29	-167.4(2)	C35-O6-C34-C33	-175.4(2)
C36-N2-C30-C29	72.7(3)	K1-O6-C34-C33	46.3(3)
K1-N2-C30-C29	-47.5(3)	O5-C33-C34-O6	-62.8(3)
O4-C29-C30-N2	61.8(3)	C34-O6-C35-C36	178.1(2)
C25-N1-C31-C32	73.4(3)	K1-O6-C35-C36	-43.8(3)
C19-N1-C31-C32	-167.3(2)	C24-N2-C36-C35	72.3(3)
K1-N1-C31-C32	-47.1(3)	C30-N2-C36-C35	-167.5(2)
C33-O5-C32-C31	-179.5(2)	K1-N2-C36-C35	-46.8(3)
K1-O5-C32-C31	-45.6(3)	O6-C35-C36-N2	62.8(3)
N1-C31-C32-O5	64.4(3)		

Symmetry transformations used to generate equivalent atoms:

REFERENCE NUMBER: 04349 [**R&D3**]

CRYSTAL STRUCTURE REPORT

$C_{28} H_{58} Co K O_{6.5} P_2$

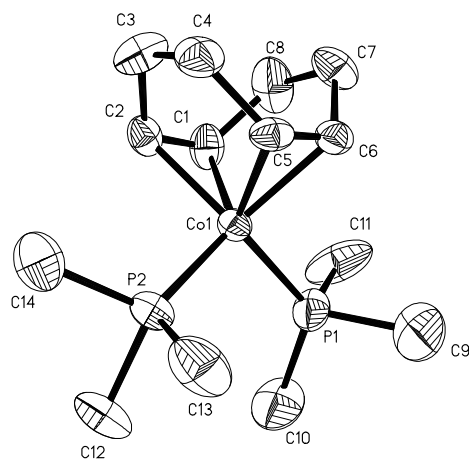
or

$[K(18\text{-crown})(THF)_{1/2}][Co(1,5\text{-COD})(PMe_3)_2]$

Report prepared for:

W. Brennessel, Prof. J. Ellis

December 16, 2004



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Data collection

A crystal (approximate dimensions 0.24 x 0.20 x 0.20 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 54 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 45 seconds and a detector distance of 4.81 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.84 Å. Three major sections of frames were collected with 0.30° steps in ω at three different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from the xyz centroids of 3084 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97⁴ and refined using SHELXL-97.⁵ The space group $P2_12_12$ 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 $R1 = 0.0429$ and $wR2 = 0.1037$ (F^2 , all data).

Structure description

The structure is the one suggested. The axial positions of the potassium 18-crown-6 cation are occupied by the COD ligand of the anion and a solvent THF molecule, which is modeled as doubly disordered over a crystallographic two-fold axis (50:50, 73:37). One of the PMe₃ groups is modeled as disordered (50:50) due to the presence of its nearby symmetry equivalent. The twist angle of 88.7° means that the overall geometry is tetrahedral.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, S146 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
- ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).
- ³ SAINT+ V6.45, Bruker Analytical X-Ray Systems, Madison, WI (2003).
- ⁴ A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).
- ⁵ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

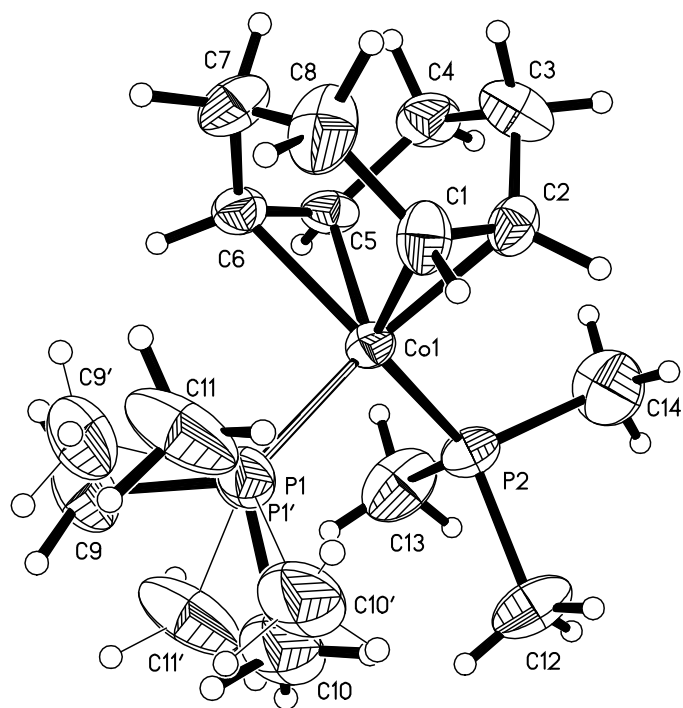
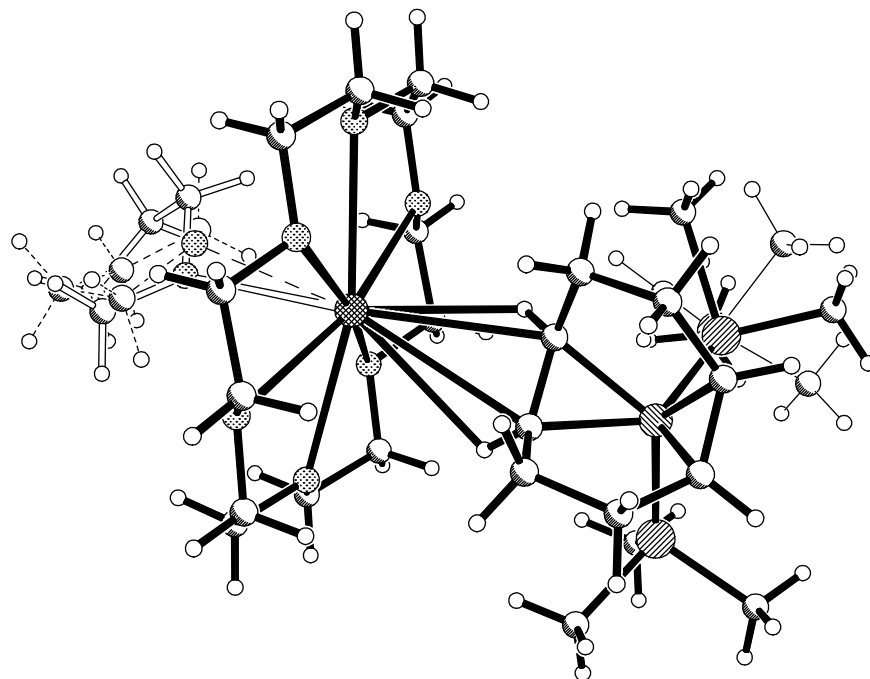
$$R_{\text{int}} = \Sigma |F_o|^2 - \langle F_o^2 \rangle / \Sigma |F_o|^2$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

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

where $w = 1 / [\sigma^2(F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$

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



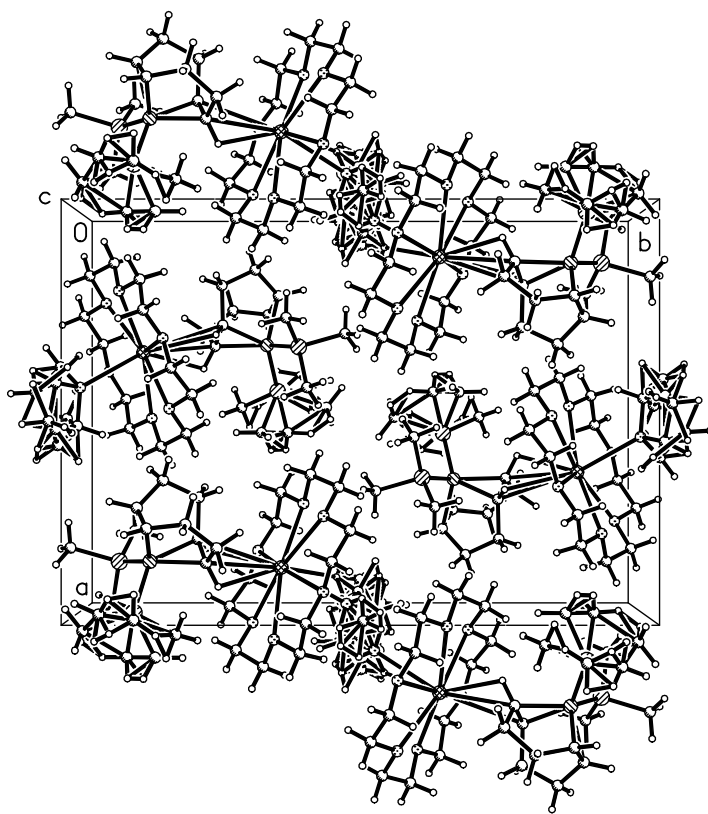
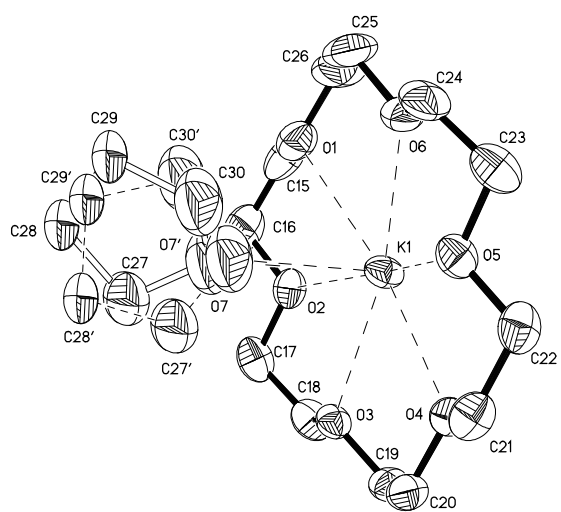


Table 1. Crystal data and structure refinement for 04349.

Identification code	04349	
Empirical formula	C ₂₈ H ₅₈ Co K O _{6.50} P ₂	
Formula weight	658.71	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	<i>P</i> 2 ₁ 2 ₁ 2	
Unit cell dimensions	<i>a</i> = 15.884(2) Å	$\alpha = 90^\circ$
	<i>b</i> = 22.297(3) Å	$\beta = 90^\circ$
	<i>c</i> = 9.8714(13) Å	$\gamma = 90^\circ$
Volume	3496.0(8) Å ³	
<i>Z</i>	4	
Density (calculated)	1.251 Mg/m ³	
Absorption coefficient	0.738 mm ⁻¹	
<i>F</i> (000)	1416	
Crystal color, morphology	red, block	
Crystal size	0.24 x 0.20 x 0.20 mm ³	
Theta range for data collection	1.57 to 25.05°	
Index ranges	-18 ≤ <i>h</i> ≤ 18, -24 ≤ <i>k</i> ≤ 26, -11 ≤ <i>l</i> ≤ 9	
Reflections collected	21212	
Independent reflections	6194 [<i>R</i> (int) = 0.0649]	
Observed reflections	4916	
Completeness to theta = 25.05°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8664 and 0.8428	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	6194 / 43 / 395	
Goodness-of-fit on <i>F</i> ²	1.040	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0429, <i>wR</i> 2 = 0.0926	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0657, <i>wR</i> 2 = 0.1037	
Absolute structure parameter	-0.026(18)	
Largest diff. peak and hole	0.395 and -0.318 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04349. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Co1	1633(1)	8379(1)	3338(1)	28(1)
C1	1608(3)	7474(2)	3527(4)	42(1)
C2	2102(3)	7638(2)	2416(4)	36(1)
C3	3058(3)	7620(2)	2457(5)	53(1)
C4	3459(2)	8182(2)	3014(5)	45(1)
C5	2855(2)	8569(2)	3807(4)	33(1)
C6	2422(2)	8370(2)	4963(4)	34(1)
C7	2534(3)	7736(2)	5521(5)	49(1)
C8	1984(4)	7268(2)	4840(5)	63(2)
P1	533(3)	8590(30)	4450(20)	44(2)
C9	574(7)	9075(5)	5862(11)	91(4)
C10	-500(5)	8731(5)	3756(11)	73(3)
C11	117(7)	7889(4)	5549(14)	86(3)
P1'	519(3)	8550(30)	4450(20)	44(2)
C9'	471(7)	8518(6)	6230(9)	91(4)
C10'	-497(6)	8274(5)	3915(12)	73(3)
C11'	122(7)	9406(4)	4379(14)	86(3)
P2	1562(1)	8949(1)	1635(1)	38(1)
C12	586(3)	9100(2)	675(5)	61(2)
C13	1887(3)	9738(2)	1836(6)	67(2)
C14	2224(4)	8756(3)	152(5)	73(2)
K1	1435(1)	6293(1)	1939(1)	37(1)
O1	86(2)	6791(2)	356(3)	52(1)
C15	410(3)	7201(2)	-608(5)	63(2)
C16	1029(3)	6889(3)	-1481(5)	63(1)
O2	1727(2)	6723(1)	-677(3)	46(1)
C17	2367(3)	6429(2)	-1426(4)	50(1)
C18	3104(3)	6335(2)	-515(4)	49(1)
O3	2869(2)	5943(1)	549(3)	37(1)
C19	3559(2)	5820(2)	1429(5)	44(1)
C20	3292(3)	5354(2)	2417(4)	45(1)

O4	2654(2)	5593(1)	3266(3)	38(1)
C21	2363(3)	5164(2)	4231(5)	47(1)
C22	1690(3)	5450(2)	5072(4)	48(1)
O5	993(2)	5591(1)	4232(3)	42(1)
C23	319(3)	5859(2)	4959(5)	55(1)
C24	-400(3)	5967(2)	4005(5)	56(1)
O6	-150(2)	6394(1)	3023(3)	46(1)
C25	-825(3)	6586(3)	2189(6)	76(2)
C26	-509(3)	7050(3)	1244(6)	76(2)
O7	581(19)	5310(20)	260(30)	94(5)
C27	688(18)	4970(20)	-980(40)	84(7)
C28	-207(19)	4880(30)	-1540(30)	96(7)
C29	-774(17)	4960(30)	-280(30)	96(7)
C30	-150(20)	5050(30)	900(20)	94(5)
O7'	545(10)	5231(12)	787(15)	94(5)
C27'	1056(10)	5010(12)	-310(20)	84(7)
C28'	461(10)	4651(11)	-1230(20)	96(7)
C29'	-389(12)	4967(14)	-1030(20)	96(7)
C30'	-327(11)	5251(13)	387(18)	94(5)

Table 3. Bond lengths [Å] and angles [°] for 04349.

Co(1)-C(1)	2.028(4)	C(9)-H(9C)	0.9800
Co(1)-C(2)	2.029(4)	C(10)-H(10A)	0.9800
Co(1)-C(6)	2.035(4)	C(10)-H(10B)	0.9800
Co(1)-C(5)	2.039(4)	C(10)-H(10C)	0.9800
Co(1)-P(2)	2.1095(12)	C(11)-H(11A)	0.9800
Co(1)-P(1')	2.114(2)	C(11)-H(11B)	0.9800
Co(1)-P(1)	2.114(3)	C(11)-H(11C)	0.9800
C(1)-C(2)	1.398(6)	P(1')-C(9')	1.76(3)
C(1)-C(8)	1.499(6)	P(1')-C(10')	1.80(2)
C(1)-K(1)	3.077(4)	P(1')-C(11')	2.02(7)
C(1)-H(1)	1.0000	C(9')-H(9'A)	0.9800
C(2)-C(3)	1.520(6)	C(9')-H(9'B)	0.9800
C(2)-K(1)	3.216(4)	C(9')-H(9'C)	0.9800
C(2)-H(2)	1.0000	C(10')-H(10D)	0.9800
C(3)-C(4)	1.509(6)	C(10')-H(10E)	0.9800
C(3)-H(3A)	0.9900	C(10')-H(10F)	0.9800
C(3)-H(3B)	0.9900	C(11')-H(11D)	0.9800
C(4)-C(5)	1.509(6)	C(11')-H(11E)	0.9800
C(4)-H(4A)	0.9900	C(11')-H(11F)	0.9800
C(4)-H(4B)	0.9900	P(2)-C(13)	1.845(5)
C(5)-C(6)	1.404(6)	P(2)-C(12)	1.849(5)
C(5)-H(5)	1.0000	P(2)-C(14)	1.853(5)
C(6)-C(7)	1.529(6)	C(12)-H(12A)	0.9800
C(6)-H(6)	1.0000	C(12)-H(12B)	0.9800
C(7)-C(8)	1.517(6)	C(12)-H(12C)	0.9800
C(7)-H(7A)	0.9900	C(13)-H(13A)	0.9800
C(7)-H(7B)	0.9900	C(13)-H(13B)	0.9800
C(8)-H(8A)	0.9900	C(13)-H(13C)	0.9800
C(8)-H(8B)	0.9900	C(14)-H(14A)	0.9800
P(1)-C(9)	1.77(3)	C(14)-H(14B)	0.9800
P(1)-C(10)	1.81(2)	C(14)-H(14C)	0.9800
P(1)-C(11)	2.01(7)	K(1)-O(6)	2.745(3)
C(9)-H(9A)	0.9800	K(1)-O(3)	2.771(3)
C(9)-H(9B)	0.9800	K(1)-O(2)	2.793(3)

K(1)-O(4)	2.810(3)	C(23)-H(23A)	0.9900
K(1)-O(5)	2.840(3)	C(23)-H(23B)	0.9900
K(1)-O(1)	2.876(3)	C(24)-O(6)	1.415(6)
K(1)-O(7')	2.98(2)	C(24)-H(24A)	0.9900
K(1)-O(7)	3.07(3)	C(24)-H(24B)	0.9900
O(1)-C(26)	1.412(6)	O(6)-C(25)	1.418(6)
O(1)-C(15)	1.417(6)	C(25)-C(26)	1.479(8)
C(15)-C(16)	1.480(7)	C(25)-H(25A)	0.9900
C(15)-H(15A)	0.9900	C(25)-H(25B)	0.9900
C(15)-H(15B)	0.9900	C(26)-H(26A)	0.9900
C(16)-O(2)	1.414(5)	C(26)-H(26B)	0.9900
C(16)-H(16A)	0.9900	O(7)-C(27)	1.442(5)
C(16)-H(16B)	0.9900	O(7)-C(30)	1.443(5)
O(2)-C(17)	1.418(5)	C(27)-C(28)	1.539(5)
C(17)-C(18)	1.491(6)	C(27)-H(27A)	0.9900
C(17)-H(17A)	0.9900	C(27)-H(27B)	0.9900
C(17)-H(17B)	0.9900	C(28)-C(29)	1.540(5)
C(18)-O(3)	1.415(5)	C(28)-H(28A)	0.9900
C(18)-H(18A)	0.9900	C(28)-H(28B)	0.9900
C(18)-H(18B)	0.9900	C(29)-C(30)	1.539(5)
O(3)-C(19)	1.424(5)	C(29)-H(29A)	0.9900
C(19)-C(20)	1.488(6)	C(29)-H(29B)	0.9900
C(19)-H(19A)	0.9900	C(30)-H(30A)	0.9900
C(19)-H(19B)	0.9900	C(30)-H(30B)	0.9900
C(20)-O(4)	1.420(5)	O(7')-C(27')	1.437(5)
C(20)-H(20A)	0.9900	O(7')-C(30')	1.441(5)
C(20)-H(20B)	0.9900	C(27')-C(28')	1.538(5)
O(4)-C(21)	1.427(5)	C(27')-H(27C)	0.9900
C(21)-C(22)	1.495(6)	C(27')-H(27D)	0.9900
C(21)-H(21A)	0.9900	C(28')-C(29')	1.534(5)
C(21)-H(21B)	0.9900	C(28')-H(28C)	0.9900
C(22)-O(5)	1.418(5)	C(28')-H(28D)	0.9900
C(22)-H(22A)	0.9900	C(29')-C(30')	1.537(5)
C(22)-H(22B)	0.9900	C(29')-H(29C)	0.9900
O(5)-C(23)	1.420(5)	C(29')-H(29D)	0.9900
C(23)-C(24)	1.500(7)	C(30')-H(30C)	0.9900

C(30')-H(30D)	0.9900	C(3)-C(2)-K(1)	108.0(3)
C(1)-Co(1)-C(2)	40.31(16)	Co(1)-C(2)-K(1)	134.80(18)
C(1)-Co(1)-C(6)	85.96(17)	C(1)-C(2)-H(2)	114.9
C(2)-Co(1)-C(6)	96.87(17)	C(3)-C(2)-H(2)	114.9
C(1)-Co(1)-C(5)	101.79(17)	Co(1)-C(2)-H(2)	114.9
C(2)-Co(1)-C(5)	85.51(16)	K(1)-C(2)-H(2)	62.9
C(6)-Co(1)-C(5)	40.32(16)	C(4)-C(3)-C(2)	114.1(4)
C(1)-Co(1)-P(2)	132.16(12)	C(4)-C(3)-H(3A)	108.7
C(2)-Co(1)-P(2)	98.74(12)	C(2)-C(3)-H(3A)	108.7
C(6)-Co(1)-P(2)	131.83(12)	C(4)-C(3)-H(3B)	108.7
C(5)-Co(1)-P(2)	96.13(12)	C(2)-C(3)-H(3B)	108.7
C(1)-Co(1)-P(1')	96(2)	H(3A)-C(3)-H(3B)	107.6
C(2)-Co(1)-P(1')	133.1(18)	C(3)-C(4)-C(5)	113.3(3)
C(6)-Co(1)-P(1')	96.3(5)	C(3)-C(4)-H(4A)	108.9
C(5)-Co(1)-P(1')	130.0(5)	C(5)-C(4)-H(4A)	108.9
P(2)-Co(1)-P(1')	105.2(17)	C(3)-C(4)-H(4B)	108.9
C(1)-Co(1)-P(1)	99(2)	C(5)-C(4)-H(4B)	108.9
C(2)-Co(1)-P(1)	135.7(18)	H(4A)-C(4)-H(4B)	107.7
C(6)-Co(1)-P(1)	95.8(5)	C(6)-C(5)-C(4)	123.5(4)
C(5)-Co(1)-P(1)	128.5(5)	C(6)-C(5)-Co(1)	69.7(2)
P(2)-Co(1)-P(1)	103.7(17)	C(4)-C(5)-Co(1)	111.6(3)
P(1')-Co(1)-P(1)	3(4)	C(6)-C(5)-H(5)	114.6
C(2)-C(1)-C(8)	122.4(4)	C(4)-C(5)-H(5)	114.6
C(2)-C(1)-Co(1)	69.9(2)	Co(1)-C(5)-H(5)	114.6
C(8)-C(1)-Co(1)	112.1(3)	C(5)-C(6)-C(7)	121.9(4)
C(2)-C(1)-K(1)	82.8(2)	C(5)-C(6)-Co(1)	70.0(2)
C(8)-C(1)-K(1)	102.4(3)	C(7)-C(6)-Co(1)	111.4(3)
Co(1)-C(1)-K(1)	143.80(18)	C(5)-C(6)-H(6)	115.1
C(2)-C(1)-H(1)	114.8	C(7)-C(6)-H(6)	115.1
C(8)-C(1)-H(1)	114.8	Co(1)-C(6)-H(6)	115.1
Co(1)-C(1)-H(1)	114.8	C(8)-C(7)-C(6)	114.1(4)
K(1)-C(1)-H(1)	55.9	C(8)-C(7)-H(7A)	108.7
C(1)-C(2)-C(3)	122.2(4)	C(6)-C(7)-H(7A)	108.7
C(1)-C(2)-Co(1)	69.8(2)	C(8)-C(7)-H(7B)	108.7
C(3)-C(2)-Co(1)	112.1(3)	C(6)-C(7)-H(7B)	108.7
C(1)-C(2)-K(1)	71.7(2)	H(7A)-C(7)-H(7B)	107.6

C(1)-C(8)-C(7)	113.7(4)	P(2)-C(14)-H(14A)	109.5
C(1)-C(8)-H(8A)	108.8	P(2)-C(14)-H(14B)	109.5
C(7)-C(8)-H(8A)	108.8	H(14A)-C(14)-H(14B)	109.5
C(1)-C(8)-H(8B)	108.8	P(2)-C(14)-H(14C)	109.5
C(7)-C(8)-H(8B)	108.8	H(14A)-C(14)-H(14C)	109.5
H(8A)-C(8)-H(8B)	107.7	H(14B)-C(14)-H(14C)	109.5
C(9)-P(1)-C(10)	102.9(18)	O(6)-K(1)-O(3)	165.95(9)
C(9)-P(1)-C(11)	93.5(16)	O(6)-K(1)-O(2)	118.97(9)
C(10)-P(1)-C(11)	92.4(17)	O(3)-K(1)-O(2)	60.15(9)
C(9)-P(1)-Co(1)	121.0(13)	O(6)-K(1)-O(4)	119.69(9)
C(10)-P(1)-Co(1)	126.4(11)	O(3)-K(1)-O(4)	60.57(8)
C(11)-P(1)-Co(1)	112(3)	O(2)-K(1)-O(4)	120.49(9)
C(9')-P(1')-C(10')	103.8(19)	O(6)-K(1)-O(5)	60.50(9)
C(9')-P(1')-C(11')	93.1(16)	O(3)-K(1)-O(5)	116.30(9)
C(10')-P(1')-C(11')	91.8(17)	O(2)-K(1)-O(5)	165.23(9)
C(9')-P(1')-Co(1)	123.1(14)	O(4)-K(1)-O(5)	59.51(8)
C(10')-P(1')-Co(1)	122.6(11)	O(6)-K(1)-O(1)	59.76(9)
C(11')-P(1')-Co(1)	114(3)	O(3)-K(1)-O(1)	116.89(9)
C(13)-P(2)-C(12)	96.6(2)	O(2)-K(1)-O(1)	59.25(9)
C(13)-P(2)-C(14)	98.5(3)	O(4)-K(1)-O(1)	168.83(9)
C(12)-P(2)-C(14)	96.5(3)	O(5)-K(1)-O(1)	117.49(9)
C(13)-P(2)-Co(1)	118.24(18)	O(6)-K(1)-O(7')	77.2(3)
C(12)-P(2)-Co(1)	124.30(17)	O(3)-K(1)-O(7')	88.7(3)
C(14)-P(2)-Co(1)	117.41(18)	O(2)-K(1)-O(7')	89.9(4)
P(2)-C(12)-H(12A)	109.5	O(4)-K(1)-O(7')	93.6(4)
P(2)-C(12)-H(12B)	109.5	O(5)-K(1)-O(7')	75.5(4)
H(12A)-C(12)-H(12B)	109.5	O(1)-K(1)-O(7')	75.3(5)
P(2)-C(12)-H(12C)	109.5	O(6)-K(1)-O(7)	82.2(6)
H(12A)-C(12)-H(12C)	109.5	O(3)-K(1)-O(7)	83.9(6)
H(12B)-C(12)-H(12C)	109.5	O(2)-K(1)-O(7)	79.6(6)
P(2)-C(13)-H(13A)	109.5	O(4)-K(1)-O(7)	99.1(8)
P(2)-C(13)-H(13B)	109.5	O(5)-K(1)-O(7)	85.8(6)
H(13A)-C(13)-H(13B)	109.5	O(1)-K(1)-O(7)	69.8(9)
P(2)-C(13)-H(13C)	109.5	O(7')-K(1)-O(7)	10.3(9)
H(13A)-C(13)-H(13C)	109.5	O(6)-K(1)-C(1)	79.22(11)
H(13B)-C(13)-H(13C)	109.5	O(3)-K(1)-C(1)	114.81(11)

O(2)-K(1)-C(1)	99.36(10)	O(2)-C(17)-H(17B)	110.0
O(4)-K(1)-C(1)	100.18(10)	C(18)-C(17)-H(17B)	110.0
O(5)-K(1)-C(1)	95.02(10)	H(17A)-C(17)-H(17B)	108.4
O(1)-K(1)-C(1)	90.72(11)	O(3)-C(18)-C(17)	109.1(4)
O(7')-K(1)-C(1)	156.3(3)	O(3)-C(18)-H(18A)	109.9
O(7)-K(1)-C(1)	158.1(8)	C(17)-C(18)-H(18A)	109.9
O(6)-K(1)-C(2)	99.70(10)	O(3)-C(18)-H(18B)	109.9
O(3)-K(1)-C(2)	93.68(10)	C(17)-C(18)-H(18B)	109.9
O(2)-K(1)-C(2)	76.15(10)	H(18A)-C(18)-H(18B)	108.3
O(4)-K(1)-C(2)	102.91(10)	C(18)-O(3)-C(19)	111.6(3)
O(5)-K(1)-C(2)	118.60(10)	C(18)-O(3)-K(1)	114.2(2)
O(1)-K(1)-C(2)	87.97(10)	C(19)-O(3)-K(1)	112.6(2)
O(7')-K(1)-C(2)	162.2(5)	O(3)-C(19)-C(20)	108.4(3)
O(7)-K(1)-C(2)	153.2(8)	O(3)-C(19)-H(19A)	110.0
C(1)-K(1)-C(2)	25.54(10)	C(20)-C(19)-H(19A)	110.0
C(26)-O(1)-C(15)	113.4(4)	O(3)-C(19)-H(19B)	110.0
C(26)-O(1)-K(1)	108.6(3)	C(20)-C(19)-H(19B)	110.0
C(15)-O(1)-K(1)	110.1(3)	H(19A)-C(19)-H(19B)	108.4
O(1)-C(15)-C(16)	109.2(4)	O(4)-C(20)-C(19)	109.1(3)
O(1)-C(15)-H(15A)	109.8	O(4)-C(20)-H(20A)	109.9
C(16)-C(15)-H(15A)	109.8	C(19)-C(20)-H(20A)	109.9
O(1)-C(15)-H(15B)	109.8	O(4)-C(20)-H(20B)	109.9
C(16)-C(15)-H(15B)	109.8	C(19)-C(20)-H(20B)	109.9
H(15A)-C(15)-H(15B)	108.3	H(20A)-C(20)-H(20B)	108.3
O(2)-C(16)-C(15)	108.5(4)	C(20)-O(4)-C(21)	112.0(3)
O(2)-C(16)-H(16A)	110.0	C(20)-O(4)-K(1)	115.2(2)
C(15)-C(16)-H(16A)	110.0	C(21)-O(4)-K(1)	117.4(2)
O(2)-C(16)-H(16B)	110.0	O(4)-C(21)-C(22)	108.5(4)
C(15)-C(16)-H(16B)	110.0	O(4)-C(21)-H(21A)	110.0
H(16A)-C(16)-H(16B)	108.4	C(22)-C(21)-H(21A)	110.0
C(16)-O(2)-C(17)	113.0(3)	O(4)-C(21)-H(21B)	110.0
C(16)-O(2)-K(1)	118.7(3)	C(22)-C(21)-H(21B)	110.0
C(17)-O(2)-K(1)	116.3(2)	H(21A)-C(21)-H(21B)	108.4
O(2)-C(17)-C(18)	108.3(3)	O(5)-C(22)-C(21)	109.2(3)
O(2)-C(17)-H(17A)	110.0	O(5)-C(22)-H(22A)	109.8
C(18)-C(17)-H(17A)	110.0	C(21)-C(22)-H(22A)	109.8

O(5)-C(22)-H(22B)	109.8	O(7)-C(27)-C(28)	105.2(16)
C(21)-C(22)-H(22B)	109.8	O(7)-C(27)-H(27A)	110.7
H(22A)-C(22)-H(22B)	108.3	C(28)-C(27)-H(27A)	110.7
C(22)-O(5)-C(23)	112.8(3)	O(7)-C(27)-H(27B)	110.7
C(22)-O(5)-K(1)	113.3(2)	C(28)-C(27)-H(27B)	110.7
C(23)-O(5)-K(1)	110.9(2)	H(27A)-C(27)-H(27B)	108.8
O(5)-C(23)-C(24)	109.0(4)	C(27)-C(28)-C(29)	103.8(12)
O(5)-C(23)-H(23A)	109.9	C(27)-C(28)-H(28A)	111.0
C(24)-C(23)-H(23A)	109.9	C(29)-C(28)-H(28A)	111.0
O(5)-C(23)-H(23B)	109.9	C(27)-C(28)-H(28B)	111.0
C(24)-C(23)-H(23B)	109.9	C(29)-C(28)-H(28B)	111.0
H(23A)-C(23)-H(23B)	108.3	H(28A)-C(28)-H(28B)	109.0
O(6)-C(24)-C(23)	108.9(4)	C(30)-C(29)-C(28)	104.3(12)
O(6)-C(24)-H(24A)	109.9	C(30)-C(29)-H(29A)	110.9
C(23)-C(24)-H(24A)	109.9	C(28)-C(29)-H(29A)	110.9
O(6)-C(24)-H(24B)	109.9	C(30)-C(29)-H(29B)	110.9
C(23)-C(24)-H(24B)	109.9	C(28)-C(29)-H(29B)	110.9
H(24A)-C(24)-H(24B)	108.3	H(29A)-C(29)-H(29B)	108.9
C(24)-O(6)-C(25)	112.8(4)	O(7)-C(30)-C(29)	103.9(19)
C(24)-O(6)-K(1)	118.0(2)	O(7)-C(30)-H(30A)	111.0
C(25)-O(6)-K(1)	119.5(3)	C(29)-C(30)-H(30A)	111.0
O(6)-C(25)-C(26)	108.7(4)	O(7)-C(30)-H(30B)	111.0
O(6)-C(25)-H(25A)	109.9	C(29)-C(30)-H(30B)	111.0
C(26)-C(25)-H(25A)	109.9	H(30A)-C(30)-H(30B)	109.0
O(6)-C(25)-H(25B)	109.9	C(27')-O(7')-C(30')	110.4(14)
C(26)-C(25)-H(25B)	109.9	C(27')-O(7')-K(1)	106.9(13)
H(25A)-C(25)-H(25B)	108.3	C(30')-O(7')-K(1)	122.3(18)
O(1)-C(26)-C(25)	109.4(5)	O(7')-C(27')-C(28')	106.0(12)
O(1)-C(26)-H(26A)	109.8	O(7')-C(27')-H(27C)	110.5
C(25)-C(26)-H(26A)	109.8	C(28')-C(27')-H(27C)	110.5
O(1)-C(26)-H(26B)	109.8	O(7')-C(27')-H(27D)	110.5
C(25)-C(26)-H(26B)	109.8	C(28')-C(27')-H(27D)	110.5
H(26A)-C(26)-H(26B)	108.2	H(27C)-C(27')-H(27D)	108.7
C(27)-O(7)-C(30)	105(2)	C(29')-C(28')-C(27')	103.0(11)
C(27)-O(7)-K(1)	140.8(19)	C(29')-C(28')-H(28C)	111.2
C(30)-O(7)-K(1)	114.0(18)	C(27')-C(28')-H(28C)	111.2

C(29')-C(28')-H(28D)	111.2	H(29C)-C(29')-H(29D)	108.9
C(27')-C(28')-H(28D)	111.2	O(7')-C(30')-C(29')	107.2(12)
H(28C)-C(28')-H(28D)	109.1	O(7')-C(30')-H(30C)	110.3
C(28')-C(29')-C(30')	104.6(11)	C(29')-C(30')-H(30C)	110.3
C(28')-C(29')-H(29C)	110.8	O(7')-C(30')-H(30D)	110.3
C(30')-C(29')-H(29C)	110.8	C(29')-C(30')-H(30D)	110.3
C(28')-C(29')-H(29D)	110.8	H(30C)-C(30')-H(30D)	108.5
C(30')-C(29')-H(29D)	110.8		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04349. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	25(1)	30(1)	29(1)	1(1)	-2(1)	0(1)
C1	52(2)	37(2)	37(2)	-8(2)	0(2)	-11(2)
C2	48(3)	27(2)	32(2)	-1(2)	-8(2)	-5(2)
C3	43(3)	41(3)	75(4)	-4(3)	11(2)	7(2)
C4	27(2)	57(3)	52(3)	2(2)	-3(2)	0(2)
C5	23(2)	27(2)	48(3)	-2(2)	-7(2)	-1(2)
C6	32(2)	31(2)	39(2)	-3(2)	-8(2)	2(2)
C7	56(3)	44(3)	46(3)	16(2)	-14(2)	-3(2)
C8	109(5)	36(3)	44(3)	10(2)	-4(3)	-9(3)
P1	29(1)	61(7)	43(1)	-13(1)	3(1)	0(1)
C9	62(5)	152(12)	60(6)	-12(7)	25(4)	28(8)
C10	33(3)	94(8)	90(6)	-18(7)	7(3)	-2(6)
C11	66(5)	61(5)	130(8)	23(5)	56(6)	18(4)
P1'	29(1)	61(7)	43(1)	-13(1)	3(1)	0(1)
C9'	62(5)	152(12)	60(6)	-12(7)	25(4)	28(8)
C10'	33(3)	94(8)	90(6)	-18(7)	7(3)	-2(6)
C11'	66(5)	61(5)	130(8)	23(5)	56(6)	18(4)
P2	38(1)	37(1)	38(1)	9(1)	-6(1)	0(1)
C12	61(3)	62(4)	60(3)	26(3)	-24(3)	-5(3)
C13	85(4)	52(3)	64(4)	22(3)	-17(3)	-16(3)
C14	92(4)	82(4)	45(3)	24(3)	16(3)	11(3)
K1	36(1)	40(1)	33(1)	6(1)	9(1)	8(1)
O1	47(2)	60(2)	48(2)	5(2)	-10(2)	7(2)
C15	60(3)	70(4)	57(3)	20(3)	-31(3)	1(3)
C16	70(3)	79(4)	39(3)	15(3)	-11(3)	-5(3)
O2	54(2)	59(2)	25(2)	3(1)	-5(1)	4(2)
C17	70(3)	52(3)	29(3)	4(2)	13(2)	-5(2)
C18	54(3)	53(3)	40(3)	5(2)	21(2)	-5(2)
O3	34(2)	41(2)	34(2)	-2(1)	8(1)	-1(1)
C19	29(2)	48(3)	55(3)	-4(2)	5(2)	-1(2)
C20	38(2)	44(3)	52(3)	-2(2)	-5(2)	6(2)

O4	40(2)	37(2)	37(2)	5(2)	1(2)	1(1)
C21	53(3)	40(3)	47(3)	12(2)	-7(2)	-3(2)
C22	58(3)	56(3)	30(2)	10(2)	1(2)	-5(3)
O5	47(2)	46(2)	33(2)	3(2)	8(1)	-1(1)
C23	60(3)	63(3)	42(3)	6(2)	26(3)	-3(3)
C24	38(3)	70(4)	61(3)	-9(3)	22(2)	-4(2)
O6	32(2)	61(2)	45(2)	0(2)	7(1)	3(1)
C25	31(2)	133(6)	64(3)	3(4)	0(2)	21(3)
C26	53(3)	104(5)	72(4)	9(4)	-4(3)	37(3)
O7	93(7)	128(11)	62(9)	-31(10)	13(7)	-26(6)
C27	70(16)	75(12)	110(20)	-39(15)	-3(12)	-10(13)
C28	76(12)	127(17)	85(12)	-69(11)	-36(10)	28(11)
C29	76(12)	127(17)	85(12)	-69(11)	-36(10)	28(11)
C30	93(7)	128(11)	62(9)	-31(10)	13(7)	-26(6)
O7'	93(7)	128(11)	62(9)	-31(10)	13(7)	-26(6)
C27'	70(16)	75(12)	110(20)	-39(15)	-3(12)	-10(13)
C28'	76(12)	127(17)	85(12)	-69(11)	-36(10)	28(11)
C29'	76(12)	127(17)	85(12)	-69(11)	-36(10)	28(11)
C30'	93(7)	128(11)	62(9)	-31(10)	13(7)	-26(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 04349.

	x	y	z	U(eq)
H1	1058	7283	3291	50
H2	1849	7546	1512	43
H3A	3236	7275	3019	64
H3B	3271	7552	1527	64
H4A	3690	8420	2253	55
H4B	3934	8068	3609	55
H5	2996	9006	3809	39
H6	2308	8686	5659	40
H7A	3131	7617	5415	58
H7B	2406	7740	6503	58
H8A	2325	6905	4670	76
H8B	1523	7156	5466	76
H9A	6	9125	6235	137
H9B	794	9466	5579	137
H9C	944	8903	6555	137
H10A	-923	8688	4472	109
H10B	-617	8444	3030	109
H10C	-521	9140	3391	109
H11A	-368	8015	6095	128
H11B	568	7749	6148	128
H11C	-52	7564	4941	128
H9'A	192	8879	6572	137
H9'B	1042	8495	6600	137
H9'C	151	8163	6509	137
H10D	-933	8433	4519	109
H10E	-502	7835	3953	109
H10F	-609	8405	2985	109
H11D	-260	9483	5139	128
H11E	-174	9478	3524	128
H11F	608	9676	4442	128

H12A	710	9373	-77	92
H12B	169	9286	1276	92
H12C	361	8723	317	92
H13A	1835	9946	966	101
H13B	2474	9754	2141	101
H13C	1526	9933	2509	101
H14A	2130	9050	-571	109
H14B	2073	8355	-175	109
H14C	2818	8761	416	109
H15A	686	7541	-138	75
H15B	-54	7363	-1169	75
H16A	769	6528	-1889	75
H16B	1213	7158	-2222	75
H17A	2534	6677	-2213	61
H17B	2159	6038	-1765	61
H18A	3577	6159	-1033	59
H18B	3291	6724	-137	59
H19A	3727	6190	1914	53
H19B	4047	5676	898	53
H20A	3076	4998	1929	54
H20B	3780	5227	2973	54
H21A	2834	5034	4817	56
H21B	2135	4807	3760	56
H22A	1511	5171	5798	57
H22B	1910	5819	5500	57
H23A	506	6244	5360	66
H23B	138	5591	5703	66
H24A	-561	5588	3556	68
H24B	-894	6119	4513	68
H25A	-1282	6754	2755	92
H25B	-1053	6242	1673	92
H26A	-984	7218	716	91
H26B	-244	7380	1761	91
H27A	962	4582	-800	101
H27B	1038	5200	-1631	101
H28A	-273	4476	-1931	115

H28B	-342	5185	-2236	115
H29A	-1145	5313	-383	115
H29B	-1126	4599	-135	115
H30A	-387	5323	1588	113
H30B	-14	4660	1332	113
H27C	1511	4749	46	101
H27D	1314	5347	-810	101
H28C	644	4672	-2187	115
H28D	431	4226	-948	115
H29C	-858	4675	-1069	115
H29D	-477	5278	-1730	115
H30C	-528	5672	360	113
H30D	-678	5026	1040	113

Table 6. Torsion angles [°] for 04349.

C6-Co1-C1-C2	-105.6(3)	P1-Co1-C2-C3	-147.9(15)
C5-Co1-C1-C2	-68.3(3)	C1-Co1-C2-K1	33.1(2)
P2-Co1-C1-C2	41.3(3)	C6-Co1-C2-K1	108.6(2)
P1'-Co1-C1-C2	158.6(5)	C5-Co1-C2-K1	147.3(3)
P1-Co1-C1-C2	159.1(5)	P2-Co1-C2-K1	-117.2(2)
C2-Co1-C1-C8	117.8(5)	P1'-Co1-C2-K1	3.3(14)
C6-Co1-C1-C8	12.2(4)	P1-Co1-C2-K1	2.9(15)
C5-Co1-C1-C8	49.5(4)	C1-C2-C3-C4	-86.3(5)
P2-Co1-C1-C8	159.2(3)	Co1-C2-C3-C4	-6.9(5)
P1'-Co1-C1-C8	-83.6(5)	K1-C2-C3-C4	-165.5(3)
P1-Co1-C1-C8	-83.1(5)	C2-C3-C4-C5	17.7(6)
C2-Co1-C1-K1	-43.4(3)	C3-C4-C5-C6	59.2(5)
C6-Co1-C1-K1	-148.9(3)	C3-C4-C5-Co1	-20.0(5)
C5-Co1-C1-K1	-111.7(3)	C1-Co1-C5-C6	-69.1(3)
P2-Co1-C1-K1	-2.0(4)	C2-Co1-C5-C6	-106.1(3)
P1'-Co1-C1-K1	115.2(5)	P2-Co1-C5-C6	155.5(2)
P1-Co1-C1-K1	115.8(5)	P1'-Co1-C5-C6	40(3)
C8-C1-C2-C3	0.0(6)	P1-Co1-C5-C6	43(3)
Co1-C1-C2-C3	104.0(4)	C1-Co1-C5-C4	50.0(3)
K1-C1-C2-C3	-100.1(4)	C2-Co1-C5-C4	13.0(3)
C8-C1-C2-Co1	-104.0(4)	C6-Co1-C5-C4	119.1(4)
K1-C1-C2-Co1	155.87(15)	P2-Co1-C5-C4	-85.4(3)
C8-C1-C2-K1	100.1(4)	P1'-Co1-C5-C4	159(3)
Co1-C1-C2-K1	-155.87(15)	P1-Co1-C5-C4	162(3)
C6-Co1-C2-C1	75.4(3)	C4-C5-C6-C7	0.4(6)
C5-Co1-C2-C1	114.2(3)	Co1-C5-C6-C7	103.4(4)
P2-Co1-C2-C1	-150.3(2)	C4-C5-C6-Co1	-103.0(4)
P1'-Co1-C2-C1	-29.9(14)	C1-Co1-C6-C5	113.6(3)
P1-Co1-C2-C1	-30.3(15)	C2-Co1-C6-C5	74.7(3)
C1-Co1-C2-C3	-117.6(4)	P2-Co1-C6-C5	-33.6(3)
C6-Co1-C2-C3	-42.2(3)	P1'-Co1-C6-C5	-150(2)
C5-Co1-C2-C3	-3.4(3)	P1-Co1-C6-C5	-148(2)
P2-Co1-C2-C3	92.1(3)	C1-Co1-C6-C7	-3.9(3)
P1'-Co1-C2-C3	-147.5(14)	C2-Co1-C6-C7	-42.8(3)

C5-Co1-C6-C7	-117.5(4)	C6-Co1-P1'-C10'	-149(4)
P2-Co1-C6-C7	-151.0(2)	C5-Co1-P1'-C10'	-174(2)
P1'-Co1-C6-C7	92(2)	P2-Co1-P1'-C10'	74(4)
P1-Co1-C6-C7	95(2)	P1-Co1-P1'-C10'	130(40)
C5-C6-C7-C8	-84.3(5)	C1-Co1-P1'-C11'	-171.7(5)
Co1-C6-C7-C8	-5.2(5)	C2-Co1-P1'-C11'	-152.8(9)
C2-C1-C8-C7	61.3(6)	C6-Co1-P1'-C11'	101.6(6)
Co1-C1-C8-C7	-18.2(6)	C5-Co1-P1'-C11'	77.0(19)
K1-C1-C8-C7	150.6(4)	P2-Co1-P1'-C11'	-34.8(6)
C6-C7-C8-C1	15.3(6)	P1-Co1-P1'-C11'	21(36)
C1-Co1-P1-C9	123(4)	C1-Co1-P2-C13	-164.0(3)
C2-Co1-P1-C9	142(3)	C2-Co1-P2-C13	-138.4(2)
C6-Co1-P1-C9	36(4)	C6-Co1-P2-C13	-30.9(3)
C5-Co1-P1-C9	10(5)	C5-Co1-P2-C13	-52.0(2)
P2-Co1-P1-C9	-100(4)	P1'-Co1-P2-C13	82.3(12)
P1'-Co1-P1-C9	135(40)	P1-Co1-P2-C13	80.1(11)
C1-Co1-P1-C10	-97(4)	C1-Co1-P2-C12	74.4(3)
C2-Co1-P1-C10	-78(5)	C2-Co1-P2-C12	100.0(3)
C6-Co1-P1-C10	176(4)	C6-Co1-P2-C12	-152.6(3)
C5-Co1-P1-C10	150(3)	C5-Co1-P2-C12	-173.7(3)
P2-Co1-P1-C10	40(5)	P1'-Co1-P2-C12	-39.3(12)
P1'-Co1-P1-C10	-85(32)	P1-Co1-P2-C12	-41.6(12)
C1-Co1-P1-C11	13.9(6)	C1-Co1-P2-C14	-46.2(3)
C2-Co1-P1-C11	33.1(10)	C2-Co1-P2-C14	-20.5(3)
C6-Co1-P1-C11	-73.0(7)	C6-Co1-P2-C14	86.9(3)
C5-Co1-P1-C11	-99.1(18)	C5-Co1-P2-C14	65.8(3)
P2-Co1-P1-C11	151.4(5)	P1'-Co1-P2-C14	-159.9(12)
P1'-Co1-P1-C11	26(36)	P1-Co1-P2-C14	-162.1(12)
C1-Co1-P1'-C9'	77(4)	C2-C1-K1-O6	-142.8(3)
C2-Co1-P1'-C9'	96(3)	C8-C1-K1-O6	95.6(3)
C6-Co1-P1'-C9'	-10(4)	Co1-C1-K1-O6	-102.2(3)
C5-Co1-P1'-C9'	-34(6)	C2-C1-K1-O3	36.5(3)
P2-Co1-P1'-C9'	-146(4)	C8-C1-K1-O3	-85.1(3)
P1-Co1-P1'-C9'	-91(32)	Co1-C1-K1-O3	77.0(3)
C1-Co1-P1'-C10'	-62(4)	C2-C1-K1-O2	-24.8(3)
C2-Co1-P1'-C10'	-44(5)	C8-C1-K1-O2	-146.5(3)

Co1-C1-K1-O2	15.7(4)	C1-C2-K1-O7'	115.4(10)
C2-C1-K1-O4	98.7(2)	C3-C2-K1-O7'	-125.7(10)
C8-C1-K1-O4	-23.0(3)	Co1-C2-K1-O7'	82.7(10)
Co1-C1-K1-O4	139.2(3)	C1-C2-K1-O7	128.9(13)
C2-C1-K1-O5	158.6(2)	C3-C2-K1-O7	-112.2(13)
C8-C1-K1-O5	36.9(3)	Co1-C2-K1-O7	96.2(13)
Co1-C1-K1-O5	-160.9(3)	C3-C2-K1-C1	118.9(4)
C2-C1-K1-O1	-83.8(3)	Co1-C2-K1-C1	-32.7(2)
C8-C1-K1-O1	154.6(3)	O6-K1-O1-C26	27.1(3)
Co1-C1-K1-O1	-43.2(3)	O3-K1-O1-C26	-168.4(3)
C2-C1-K1-O7'	-136.7(11)	O2-K1-O1-C26	-150.4(4)
C8-C1-K1-O7'	101.7(11)	O4-K1-O1-C26	117.6(5)
Co1-C1-K1-O7'	-96.1(11)	O5-K1-O1-C26	46.1(4)
C2-C1-K1-O7	-110.3(17)	O7'-K1-O1-C26	110.7(5)
C8-C1-K1-O7	128.0(17)	O7-K1-O1-C26	119.8(6)
Co1-C1-K1-O7	-69.8(17)	C1-K1-O1-C26	-49.9(4)
C8-C1-K1-C2	-121.6(4)	C2-K1-O1-C26	-75.3(4)
Co1-C1-K1-C2	40.5(3)	O6-K1-O1-C15	151.8(3)
C1-C2-K1-O6	37.1(3)	O3-K1-O1-C15	-43.7(3)
C3-C2-K1-O6	156.0(3)	O2-K1-O1-C15	-25.7(3)
Co1-C2-K1-O6	4.4(3)	O4-K1-O1-C15	-117.7(5)
C1-C2-K1-O3	-147.2(3)	O5-K1-O1-C15	170.8(3)
C3-C2-K1-O3	-28.4(3)	O7'-K1-O1-C15	-124.6(4)
Co1-C2-K1-O3	-180.0(2)	O7-K1-O1-C15	-115.5(6)
C1-C2-K1-O2	154.7(3)	C1-K1-O1-C15	74.8(3)
C3-C2-K1-O2	-86.4(3)	C2-K1-O1-C15	49.4(3)
Co1-C2-K1-O2	122.0(3)	C26-O1-C15-C16	179.7(4)
C1-C2-K1-O4	-86.6(3)	K1-O1-C15-C16	57.8(4)
C3-C2-K1-O4	32.3(3)	O1-C15-C16-O2	-65.9(5)
Co1-C2-K1-O4	-119.3(2)	C15-C16-O2-C17	-178.9(4)
C1-C2-K1-O5	-24.5(3)	C15-C16-O2-K1	39.8(5)
C3-C2-K1-O5	94.4(3)	O6-K1-O2-C16	-10.7(4)
Co1-C2-K1-O5	-57.2(3)	O3-K1-O2-C16	153.2(4)
C1-C2-K1-O1	95.9(3)	O4-K1-O2-C16	158.7(3)
C3-C2-K1-O1	-145.2(3)	O5-K1-O2-C16	73.1(5)
Co1-C2-K1-O1	63.2(2)	O1-K1-O2-C16	-8.3(3)

O7'-K1-O2-C16	64.6(5)	C18-O3-C19-C20	-173.4(3)
O7-K1-O2-C16	64.2(8)	K1-O3-C19-C20	56.5(4)
C1-K1-O2-C16	-93.5(3)	O3-C19-C20-O4	-65.9(4)
C2-K1-O2-C16	-104.3(3)	C19-C20-O4-C21	179.4(3)
O6-K1-O2-C17	-150.8(3)	C19-C20-O4-K1	41.7(4)
O3-K1-O2-C17	13.1(3)	O6-K1-O4-C20	153.9(2)
O4-K1-O2-C17	18.6(3)	O3-K1-O4-C20	-10.0(2)
O5-K1-O2-C17	-67.0(5)	O2-K1-O4-C20	-15.5(3)
O1-K1-O2-C17	-148.4(3)	O5-K1-O4-C20	147.3(3)
O7'-K1-O2-C17	-75.5(5)	O1-K1-O4-C20	69.9(6)
O7-K1-O2-C17	-75.8(8)	O7'-K1-O4-C20	76.5(4)
C1-K1-O2-C17	126.4(3)	O7-K1-O4-C20	67.7(6)
C2-K1-O2-C17	115.6(3)	C1-K1-O4-C20	-122.8(3)
C16-O2-C17-C18	173.9(4)	C2-K1-O4-C20	-96.9(3)
K1-O2-C17-C18	-43.8(4)	O6-K1-O4-C21	18.6(3)
O2-C17-C18-O3	64.0(5)	O3-K1-O4-C21	-145.2(3)
C17-C18-O3-C19	178.0(3)	O2-K1-O4-C21	-150.8(3)
C17-C18-O3-K1	-52.8(4)	O5-K1-O4-C21	12.1(3)
O6-K1-O3-C18	111.8(4)	O1-K1-O4-C21	-65.4(6)
O2-K1-O3-C18	21.3(3)	O7'-K1-O4-C21	-58.8(4)
O4-K1-O3-C18	-153.2(3)	O7-K1-O4-C21	-67.5(6)
O5-K1-O3-C18	-174.9(3)	C1-K1-O4-C21	101.9(3)
O1-K1-O3-C18	39.2(3)	C2-K1-O4-C21	127.8(3)
O7'-K1-O3-C18	111.9(5)	C20-O4-C21-C22	-179.6(3)
O7-K1-O3-C18	102.8(8)	K1-O4-C21-C22	-42.9(4)
C1-K1-O3-C18	-65.3(3)	O4-C21-C22-O5	64.1(5)
C2-K1-O3-C18	-50.4(3)	C21-C22-O5-C23	179.3(4)
O6-K1-O3-C19	-119.6(4)	C21-C22-O5-K1	-53.6(4)
O2-K1-O3-C19	150.0(3)	O6-K1-O5-C22	-151.3(3)
O4-K1-O3-C19	-24.5(2)	O3-K1-O5-C22	44.2(3)
O5-K1-O3-C19	-46.3(3)	O2-K1-O5-C22	116.6(4)
O1-K1-O3-C19	167.9(2)	O4-K1-O5-C22	22.2(3)
O7'-K1-O3-C19	-119.4(5)	O1-K1-O5-C22	-170.1(3)
O7-K1-O3-C19	-128.5(8)	O7'-K1-O5-C22	125.4(5)
C1-K1-O3-C19	63.4(3)	O7-K1-O5-C22	125.3(8)
C2-K1-O3-C19	78.3(3)	C1-K1-O5-C22	-76.7(3)

C2-K1-O5-C22	-66.3(3)	K1-O1-C26-C25	-58.5(5)
O6-K1-O5-C23	-23.3(3)	O6-C25-C26-O1	65.1(6)
O3-K1-O5-C23	172.2(3)	O6-K1-O7-C27	160(5)
O2-K1-O5-C23	-115.4(4)	O3-K1-O7-C27	-22(5)
O4-K1-O5-C23	150.2(3)	O2-K1-O7-C27	38(5)
O1-K1-O5-C23	-42.1(3)	O4-K1-O7-C27	-81(5)
O7'-K1-O5-C23	-106.6(5)	O5-K1-O7-C27	-139(5)
O7-K1-O5-C23	-106.7(8)	O1-K1-O7-C27	99(5)
C1-K1-O5-C23	51.3(3)	O7'-K1-O7-C27	-140(9)
C2-K1-O5-C23	61.7(3)	C1-K1-O7-C27	128(4)
C22-O5-C23-C24	-177.5(4)	C2-K1-O7-C27	64(5)
K1-O5-C23-C24	54.2(4)	O6-K1-O7-C30	-25(3)
O5-C23-C24-O6	-64.8(5)	O3-K1-O7-C30	153(3)
C23-C24-O6-C25	-171.9(4)	O2-K1-O7-C30	-146(3)
C23-C24-O6-K1	42.1(5)	O4-K1-O7-C30	94(3)
O3-K1-O6-C24	69.7(5)	O5-K1-O7-C30	36(3)
O2-K1-O6-C24	152.2(3)	O1-K1-O7-C30	-85(3)
O4-K1-O6-C24	-17.4(3)	O7'-K1-O7-C30	36(4)
O5-K1-O6-C24	-10.9(3)	C1-K1-O7-C30	-57(4)
O1-K1-O6-C24	149.8(3)	C2-K1-O7-C30	-121(3)
O7'-K1-O6-C24	69.5(5)	C30-O7-C27-C28	40(4)
O7-K1-O6-C24	78.6(9)	K1-O7-C27-C28	-144(4)
C1-K1-O6-C24	-113.0(3)	O7-C27-C28-C29	-22(6)
C2-K1-O6-C24	-128.4(3)	C27-C28-C29-C30	-3(6)
O3-K1-O6-C25	-74.0(6)	C27-O7-C30-C29	-42(4)
O2-K1-O6-C25	8.5(4)	K1-O7-C30-C29	141(4)
O4-K1-O6-C25	-161.0(4)	C28-C29-C30-O7	27(6)
O5-K1-O6-C25	-154.6(4)	O6-K1-O7'-C27'	165.4(17)
O1-K1-O6-C25	6.1(4)	O3-K1-O7'-C27'	-14.5(16)
O7'-K1-O6-C25	-74.2(6)	O2-K1-O7'-C27'	45.6(16)
O7-K1-O6-C25	-65.0(9)	O4-K1-O7'-C27'	-74.9(16)
C1-K1-O6-C25	103.3(4)	O5-K1-O7'-C27'	-132.1(17)
C2-K1-O6-C25	87.9(4)	O1-K1-O7'-C27'	103.7(17)
C24-O6-C25-C26	177.4(4)	O7-K1-O7'-C27'	48(5)
K1-O6-C25-C26	-37.2(6)	C1-K1-O7'-C27'	159.3(13)
C15-O1-C26-C25	178.8(4)	C2-K1-O7'-C27'	84(2)

O6-K1-O7'-C30'	36.9(18)	C2-K1-O7'-C30'	-45(2)
O3-K1-O7'-C30'	-143.1(19)	C30'-O7'-C27'-C28'	-22(3)
O2-K1-O7'-C30'	-82.9(19)	K1-O7'-C27'-C28'	-157.5(16)
O4-K1-O7'-C30'	156.5(18)	O7'-C27'-C28'-C29'	30(3)
O5-K1-O7'-C30'	99.3(18)	C27'-C28'-C29'-C30'	-26(3)
O1-K1-O7'-C30'	-24.8(18)	C27'-O7'-C30'-C29'	6(4)
O7-K1-O7'-C30'	-81(6)	K1-O7'-C30'-C29'	132.5(19)
C1-K1-O7'-C30'	31(3)	C28'-C29'-C30'-O7'	13(4)

Symmetry transformations used to generate equivalent atoms: