

μ_2 -Chlorido-chlorido(μ_2 -4-{[2-(diethylamino)ethyl]imino}pent-2-en-2-olato)bis(tetrahydrofuran- κ O)cobalt(II)lithium

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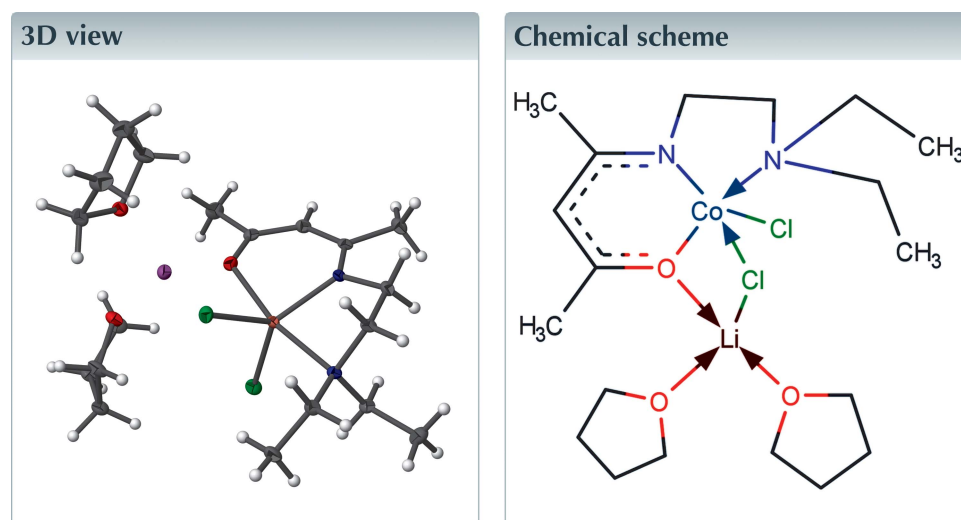
Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; β -ketoiminato ligand; cobalt; coordination compound; lithium.

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Structural data: full structural data are available from iucrdata.iucr.org

The crystal structure of the title compound, $[\text{CoLi}(\text{C}_{11}\text{H}_{21}\text{N}_2\text{O})\text{Cl}_2(\text{C}_4\text{H}_8\text{O})_2]$, has monoclinic symmetry and comprises one heterometallic binuclear complex molecule in the asymmetric unit. The Co^{2+} cation is bonded to one oxygen and two nitrogen atoms of a β -ketoiminato ligand and to two chlorido ligands, leading to a distorted trigonal-bipyramidal coordination sphere. One of the Cl ligands and the oxygen atom of the β -ketoiminato ligand are bridging to a Li^+ cation, which is further bonded to oxygen atoms of two THF molecules. The resulting coordination sphere is distorted tetrahedral. In the crystal, weak intermolecular $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds are identified that link the complex molecules into a three-dimensional network structure.



Structure description

Interest in cobalt complexes for solar harvesting devices such as dye-sensitized solar cells (DSSCs) stems from their application as alternative redox mediators to iodide/triiodide electrolytes (Hamann, 2012). Several synthetic approaches based on organic (Sauvage, 2014), inorganic (Bergeron *et al.*, 2005; Burschka *et al.*, 2012; Carli *et al.*, 2013), or organometallic compounds (Carli *et al.*, 2016; Spokoiny *et al.*, 2010; Sun *et al.*, 2015; Magni *et al.*, 2016) have been reported with $[\text{Co}(\text{bpy})_3]^{2+/3+}$ and $[\text{Co}(\text{phen})_3]^{2+/3+}$ (where bpy = 2,2'-bipyridine and phen = 1,10-phenanthroline) as redox couples. Notably, DSSCs using cobalt redox pairs mostly tether to pyridine-type ligands with complex formal charge (2+/3+) (Ben Aribia *et al.*, 2013; Lee *et al.*, 2015; Bella *et al.*, 2016; Kashif *et al.*, 2013; Pashaei *et al.*, 2015; Giribabu *et al.*, 2015), displaying few structural deviations mainly by varying the ligand backbone with groups of different donating/withdrawing

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.013 (3)	O1—Li1	1.879 (6)
Co1—O1	2.074 (2)	Cl1—Li1	2.371 (6)
Co1—N2	2.258 (3)	O2—Li1	1.936 (6)
Co1—Cl2	2.3026 (8)	O3—Li1	1.909 (6)
Co1—Cl1	2.3773 (8)		
N1—Co1—O1	88.14 (10)	N2—Co1—Cl1	94.13 (7)
N1—Co1—N2	80.51 (10)	Cl2—Co1—Cl1	113.01 (3)
O1—Co1—N2	166.65 (9)	O1—Li1—O3	118.9 (3)
N1—Co1—Cl2	121.87 (8)	O1—Li1—O2	120.4 (3)
O1—Co1—Cl2	95.82 (7)	O3—Li1—O2	102.6 (3)
N2—Co1—Cl2	96.14 (7)	O1—Li1—Cl1	91.4 (2)
N1—Co1—Cl1	125.12 (8)	O3—Li1—Cl1	110.7 (3)
O1—Co1—Cl1	86.63 (7)	O2—Li1—Cl1	112.7 (3)

ability (Pashaei *et al.*, 2015; Xu *et al.*, 2013), and without non-neutral ligands in the coordination sphere.

As part of our work on the synthesis and properties of redox couples in DSSCs (Flores-Díaz *et al.*, 2018; Vinocour, 2016), we herein report on the preparation and crystal structure determination of a cobalt complex bearing a monoanionic β -ketoiminate scaffold of chemical composition [Co(C₁₁H₂₁ON₂)Cl(μ -Cl)Li(THF)₂]. The coordination chemistry of this ligand gives an electronic situation resembling that of a formal neutral/monocationic (0/+)[−] charge in Co^{II/III} complexes.

The molecular structure consists of a central Co²⁺ cation which is penta-coordinated by one oxygen and two nitrogen atoms from the 4-(2-diethylamino-ethylamino)-pent-3-en-2-one pendant arm, as well as two chlorido ligands. Bond lengths and angles are collated in Table 1. Calculation of the angular structural index for five-coordinate complexes (τ_5) as a descriptor of trigonality (Addison *et al.*, 1984) suggests that the Co²⁺ cation adopts a distorted trigonal-bipyramidal coordination sphere ($\tau_5 = 0.69$; $\tau_5 = 0$ for an ideal square pyramid and 1 for an ideal trigonal bipyramid). One of the

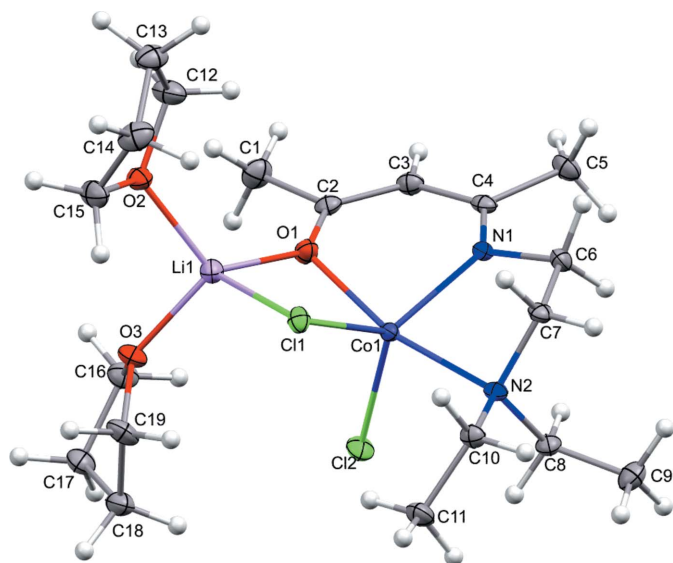


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C5—H00H...Cl1 ⁱ	0.98	2.80	3.770 (3)	172
C6—H6...Cl1 ⁱ	0.99	2.96	3.924 (3)	166
C8—H00L...Cl2	0.99	2.86	3.365 (3)	113
C10—H00I...Cl1	0.99	2.80	3.357 (3)	117
C13—H017...Cl2 ⁱⁱ	0.99	2.89	3.608 (3)	130
C19—H00X...Cl1	0.99	2.91	3.635 (3)	131

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x + 1, y, z$.

chlorido ligand (Cl1) and the oxygen atom of the ligand backbone (O1) bridge the Co²⁺ cation to a Li⁺ cation, whose distorted tetrahedral coordination sphere is completed by two THF molecules (Fig. 1, Table 1). The corresponding τ_4 and τ_4' geometric parameters for four-coordinated central atoms (Yang *et al.*, 2007; Okuniewski *et al.*, 2015; Rosiak *et al.*, 2018) are 0.86 and 0.85, respectively. They indicate that Li1 has a distorted tetrahedral coordination sphere ($\tau_4 = 0$ for an ideal square and 1 for an ideal tetrahedron). As such, the title compound has six-, five-, and four-membered rings around the two metal cations. The resulting coordination environment of Co²⁺ in the title compound is associated with insufficient crowding that prevents the elimination of chloride as a lithium salt by-product. The tendency of forming metal-halogen-lithium fragments was previously reported in many cases where

β -ketoiminate or β -diketiminato ligands have been employed (Yang *et al.*, 2012; Eckert *et al.*, 2004; Panda *et al.*, 2002).

In the crystal structure, weak C—H...Cl hydrogen-bonding contacts are observed between the molecules (Table 2 and Fig. 2), leading to the formation of a three-dimensional network structure.

The title compound is isostructural with other previously reported transition metal complexes, *viz.* the manganese(II) analogue (Lesikar *et al.*, 2008) and the iron(II) analogue where Cl is additionally substituted by Br ligands [Lugo (né Gushwa) & Richards, 2010].

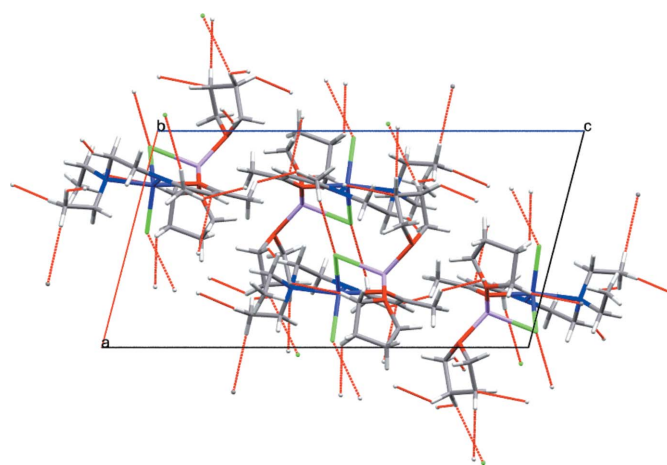


Figure 2
Packing of the molecules viewed along the *b*-axis direction. C—H...Cl hydrogen-bonding interactions are shown as red dashed lines.

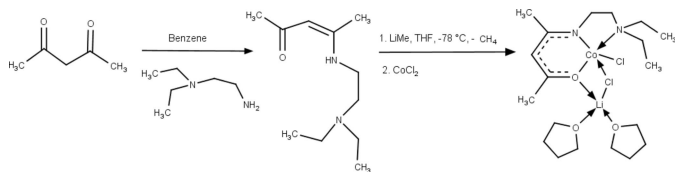


Figure 3
Synthetic scheme for the preparation of the title compound.

Synthesis and crystallization

All manipulations were carried out using standard Schlenk techniques or in a glovebox (Lab MBraun workstation) under nitrogen atmosphere. All reagents and solvents were procured from commercial sources. Anhydrous solvents were dried using MBraun Solvent Purification Systems (MB-SPS).

The ligand 4-(2-diethylamino-ethylamino)-pent-3-en-2-one was synthesized according to a literature procedure (Neculai *et al.*, 2002; Neculai, 2003) (Fig. 3). In short, a solution of *N,N*-diethyldiamine (42 ml, 0.29 mol) and acetylacetone (30 ml, 0.29 mol) was refluxed for 2 d in benzene (250 ml). Then, the solvent was removed, and the remaining crude product was purified by vacuum distillation to furnish a pale-yellow oil. ^1H NMR (400 MHz, CDCl_3 , 25 °C): δ 10.63 (*s*, 1 H), 4.79 (*s*, 1H), 3.15 (*q*, 2 H), 2.45 (*t*, 2 H), 2.40 (*q*, 4 H), 1.83 (*s*, 3 H), 1.78 (*s*, 3 H), 0.88 (*t*, 6 H).

Synthesis of the title compound (Fig. 3): In a 100 ml Schlenk flask 5.06 g (25 mmol) of the ligand were dissolved in dry tetrahydrofuran and cooled to 195 K before a solution of methyl lithium (11 ml, 1.6 M, 18 mmol) was added dropwise. The reaction mixture was stirred for 2 h, until the evolution of methane ceased, then 2.22 g (17 mmol) of anhydrous cobalt chloride in tetrahydrofuran were transferred *via* a syringe; the reaction mixture was stirred overnight at ambient temperature, and kept at 258 K until a green precipitate formed. The product was filtered under nitrogen protection, washed with anhydrous diethyl ether, and dried under vacuum. Yield 6.26 g (77%). ICP-AES: Co (11.9 ± 0.3) % *m/m* (Theoretical 12.3%). FTIR (cm^{-1}): 3386 (*m*, broad), 2968 (*m*), 2873 (*m*), 1607 (*w*), 1510 (*m*, *sh*) 1440 (*m*), 1402 (*w*), 1047 (*s*), 901 (*s*), 737(*sh*). UV-vis (MeCN): (304 nm, 1015 $L \text{ mol}^{-1} \text{ cm}^{-1}$; 634 nm, 351 $L \text{ mol}^{-1} \text{ cm}^{-1}$; 666 nm, 391 $L \text{ mol}^{-1} \text{ cm}^{-1}$; 693 nm, 373 $L \text{ mol}^{-1} \text{ cm}^{-1}$). Single crystals suitable for X-ray diffraction analysis were grown from a saturated THF solution kept at 258 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Acknowledgements

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Table 3

Experimental details.

Crystal data	[CoLi(C ₁₁ H ₂₁ N ₂ O)Cl ₂ (C ₄ H ₈ O) ₂]
Chemical formula	478.27
<i>M_r</i>	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Crystal system, space group	100
Temperature (K)	10.0535 (12), 12.3705 (14), 19.236 (2)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	104.476 (3)
β (°)	2316.4 (5)
<i>V</i> (Å ³)	4
<i>Z</i>	Mo <i>K</i> α
Radiation type	0.99
μ (mm ⁻¹)	0.50 × 0.40 × 0.30
Crystal size (mm)	
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.669, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	165035, 6723, 5903
<i>R_{int}</i>	0.051
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.705
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.052, 0.140, 1.23
No. of reflections	6723
No. of parameters	257
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	1.46, -0.75

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015a), *SHELXL2014/7* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2018). 3, x181577 [https://doi.org/10.1107/S2414314618015778]

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μ_2 -Chlorido-chlorido(μ_2 -4-{[2-(diethylamino)ethyl]imino}pent-2-en-2-olato)bis(tetrahydrofuran- κ O)cobalt(II)lithium

Crystal data

[CoLi(C₁₁H₂₁N₂O)Cl₂(C₄H₈O)₂]

$M_r = 478.27$

Monoclinic, $P2_1/n$

$a = 10.0535$ (12) Å

$b = 12.3705$ (14) Å

$c = 19.236$ (2) Å

$\beta = 104.476$ (3)°

$V = 2316.4$ (5) Å³

$Z = 4$

$F(000) = 1012$

$D_x = 1.371$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 141 reflections

$\theta = 4.1$ – 21.7 °

$\mu = 0.99$ mm⁻¹

$T = 100$ K

Block, translucent light green

$0.50 \times 0.40 \times 0.30$ mm

Data collection

Bruker D8 Venture
diffractometer

Radiation source: Incoatec Microsource

Mirrors monochromator

Detector resolution: 10.4167 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2015)

$T_{\min} = 0.669$, $T_{\max} = 0.746$

165035 measured reflections

6723 independent reflections

5903 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 30.1$ °, $\theta_{\min} = 2.6$ °

$h = -14 \rightarrow 14$

$k = -17 \rightarrow 16$

$l = -26 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.140$

$S = 1.23$

6723 reflections

257 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2 + 11.0438P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.46$ e Å⁻³

$\Delta\rho_{\min} = -0.75$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.25048 (4)	0.65764 (3)	0.47738 (2)	0.01112 (10)
N1	0.2825 (3)	0.4991 (2)	0.46436 (14)	0.0121 (4)
O1	0.2577 (2)	0.68095 (18)	0.37162 (12)	0.0162 (4)
Cl1	0.42565 (7)	0.79101 (6)	0.50801 (4)	0.01488 (14)
Cl2	0.03316 (7)	0.72744 (6)	0.46380 (4)	0.01811 (15)
N2	0.2776 (2)	0.6011 (2)	0.59167 (13)	0.0121 (4)
O2	0.4784 (2)	0.85707 (19)	0.33491 (13)	0.0170 (4)
O3	0.2200 (2)	0.94302 (19)	0.36576 (12)	0.0169 (4)
C1	0.1864 (4)	0.6494 (3)	0.24640 (17)	0.0228 (7)
H00T	0.1747	0.5879	0.2133	0.034*
H00U	0.2619	0.6951	0.2397	0.034*
H00V	0.1014	0.6918	0.2367	0.034*
C2	0.2191 (3)	0.6085 (3)	0.32249 (16)	0.0145 (5)
C3	0.2061 (3)	0.4996 (3)	0.33519 (17)	0.0157 (6)
H00E	0.1711	0.4552	0.2944	0.019*
C4	0.2399 (3)	0.4471 (2)	0.40325 (17)	0.0139 (5)
C5	0.2270 (3)	0.3254 (3)	0.40296 (19)	0.0194 (6)
H00F	0.1871	0.3003	0.3538	0.029*
H00G	0.1674	0.3038	0.4338	0.029*
H00H	0.3181	0.2931	0.421	0.029*
C6	0.3299 (3)	0.4361 (2)	0.53076 (17)	0.0161 (6)
H6	0.4052	0.3868	0.5267	0.019*
H00B	0.2536	0.3921	0.5397	0.019*
C7	0.3804 (3)	0.5155 (3)	0.59168 (16)	0.0143 (5)
H00C	0.3998	0.4764	0.638	0.017*
H00D	0.467	0.5491	0.5869	0.017*
C8	0.1461 (3)	0.5544 (3)	0.60083 (17)	0.0153 (5)
H00K	0.1099	0.5042	0.5605	0.018*
H00L	0.0788	0.6139	0.5971	0.018*
C9	0.1543 (3)	0.4939 (3)	0.67086 (18)	0.0216 (6)
H014	0.0649	0.4613	0.6696	0.032*
H015	0.179	0.5446	0.7112	0.032*
H016	0.2242	0.4372	0.6768	0.032*
C10	0.3376 (3)	0.6792 (2)	0.64914 (16)	0.0147 (5)
H00I	0.4269	0.7044	0.6424	0.018*
H00J	0.3554	0.6417	0.696	0.018*
C11	0.2476 (4)	0.7762 (3)	0.65123 (19)	0.0209 (6)
H00M	0.2241	0.8112	0.604	0.031*
H00N	0.297	0.8275	0.6874	0.031*

H00O	0.1632	0.7529	0.6636	0.031*
C12	0.5612 (3)	0.7755 (3)	0.3118 (2)	0.0233 (7)
H012	0.5412	0.774	0.2587	0.028*
H013	0.5412	0.7033	0.3288	0.028*
C13	0.7108 (3)	0.8055 (3)	0.34383 (19)	0.0224 (7)
H017	0.7656	0.7412	0.3641	0.027*
H018	0.7519	0.8391	0.3074	0.027*
C14	0.7028 (4)	0.8858 (3)	0.4025 (2)	0.0259 (7)
H00R	0.7014	0.8485	0.4479	0.031*
H00S	0.7806	0.9373	0.4116	0.031*
C15	0.5679 (4)	0.9420 (3)	0.3705 (2)	0.0234 (7)
H019	0.5312	0.976	0.4085	0.028*
H01A	0.5791	0.9984	0.3359	0.028*
C16	0.0872 (3)	0.9337 (3)	0.31570 (18)	0.0204 (6)
H00P	0.0431	0.8642	0.3222	0.024*
H00Q	0.0957	0.9384	0.2656	0.024*
C17	0.0046 (3)	1.0280 (3)	0.33303 (19)	0.0214 (6)
H010	-0.0951	1.0124	0.3194	0.026*
H011	0.0226	1.095	0.3087	0.026*
C18	0.0590 (4)	1.0365 (3)	0.41409 (19)	0.0215 (6)
H00Y	0.0431	1.1095	0.4316	0.026*
H00Z	0.016	0.9819	0.4392	0.026*
C19	0.2101 (3)	1.0146 (3)	0.42389 (19)	0.0209 (6)
H00W	0.2604	1.0827	0.4215	0.025*
H00X	0.2493	0.9798	0.4709	0.025*
Li1	0.3372 (6)	0.8193 (5)	0.3830 (3)	0.0172 (10)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01081 (17)	0.00929 (18)	0.01389 (19)	0.00048 (13)	0.00425 (13)	-0.00067 (14)
N1	0.0124 (11)	0.0099 (11)	0.0153 (11)	0.0018 (8)	0.0058 (9)	0.0001 (9)
O1	0.0209 (11)	0.0145 (10)	0.0147 (10)	-0.0025 (8)	0.0070 (8)	-0.0014 (8)
Cl1	0.0135 (3)	0.0135 (3)	0.0171 (3)	-0.0019 (2)	0.0027 (2)	0.0010 (2)
Cl2	0.0127 (3)	0.0193 (3)	0.0215 (3)	0.0045 (3)	0.0028 (3)	0.0024 (3)
N2	0.0097 (10)	0.0127 (11)	0.0141 (11)	0.0005 (9)	0.0035 (8)	-0.0018 (9)
O2	0.0144 (10)	0.0159 (11)	0.0222 (11)	-0.0004 (8)	0.0076 (8)	-0.0011 (9)
O3	0.0136 (10)	0.0164 (10)	0.0199 (11)	0.0036 (8)	0.0027 (8)	-0.0030 (8)
C1	0.0263 (16)	0.0270 (17)	0.0141 (14)	-0.0006 (14)	0.0034 (12)	-0.0010 (13)
C2	0.0103 (12)	0.0185 (14)	0.0158 (13)	-0.0007 (10)	0.0053 (10)	-0.0013 (11)
C3	0.0152 (13)	0.0167 (14)	0.0156 (14)	-0.0011 (11)	0.0042 (10)	-0.0036 (11)
C4	0.0102 (12)	0.0144 (13)	0.0182 (14)	0.0013 (10)	0.0058 (10)	-0.0032 (11)
C5	0.0197 (15)	0.0134 (14)	0.0243 (16)	-0.0003 (11)	0.0040 (12)	-0.0042 (12)
C6	0.0201 (14)	0.0119 (13)	0.0171 (14)	0.0042 (11)	0.0059 (11)	0.0015 (11)
C7	0.0112 (12)	0.0156 (14)	0.0164 (13)	0.0045 (10)	0.0042 (10)	0.0005 (11)
C8	0.0115 (12)	0.0172 (14)	0.0182 (14)	0.0006 (10)	0.0053 (10)	0.0004 (11)
C9	0.0187 (15)	0.0266 (17)	0.0211 (15)	-0.0030 (13)	0.0080 (12)	0.0025 (13)
C10	0.0151 (13)	0.0142 (13)	0.0144 (13)	-0.0015 (10)	0.0031 (10)	-0.0029 (10)

C11	0.0273 (16)	0.0150 (14)	0.0217 (15)	0.0043 (12)	0.0084 (13)	-0.0036 (12)
C12	0.0187 (15)	0.0230 (16)	0.0295 (17)	0.0016 (12)	0.0083 (13)	-0.0075 (14)
C13	0.0161 (14)	0.0308 (18)	0.0200 (15)	0.0057 (13)	0.0043 (12)	0.0021 (13)
C14	0.0193 (15)	0.0328 (19)	0.0261 (17)	-0.0063 (14)	0.0065 (13)	-0.0062 (15)
C15	0.0233 (16)	0.0142 (14)	0.0359 (19)	-0.0049 (12)	0.0134 (14)	-0.0057 (13)
C16	0.0163 (14)	0.0232 (16)	0.0202 (15)	0.0026 (12)	0.0018 (11)	-0.0018 (12)
C17	0.0179 (14)	0.0210 (16)	0.0252 (16)	0.0064 (12)	0.0051 (12)	0.0022 (13)
C18	0.0213 (15)	0.0189 (15)	0.0266 (17)	0.0032 (12)	0.0103 (13)	-0.0018 (13)
C19	0.0212 (15)	0.0167 (15)	0.0228 (16)	0.0050 (12)	0.0018 (12)	-0.0068 (12)
Li1	0.018 (2)	0.015 (3)	0.020 (3)	0.002 (2)	0.008 (2)	0.003 (2)

Geometric parameters (Å, °)

Co1—N1	2.013 (3)	C7—H00D	0.99
Co1—O1	2.074 (2)	C8—C9	1.525 (4)
Co1—N2	2.258 (3)	C8—H00K	0.99
Co1—C12	2.3026 (8)	C8—H00L	0.99
Co1—C11	2.3773 (8)	C9—H014	0.98
Co1—Li1	2.974 (6)	C9—H015	0.98
N1—C4	1.314 (4)	C9—H016	0.98
N1—C6	1.470 (4)	C10—C11	1.510 (4)
O1—C2	1.290 (4)	C10—H00I	0.99
O1—Li1	1.879 (6)	C10—H00J	0.99
C11—Li1	2.371 (6)	C11—H00M	0.98
N2—C10	1.478 (4)	C11—H00N	0.98
N2—C7	1.479 (4)	C11—H00O	0.98
N2—C8	1.493 (4)	C12—C13	1.522 (5)
O2—C15	1.441 (4)	C12—H012	0.99
O2—C12	1.447 (4)	C12—H013	0.99
O2—Li1	1.936 (6)	C13—C14	1.522 (5)
O3—C16	1.442 (4)	C13—H017	0.99
O3—C19	1.449 (4)	C13—H018	0.99
O3—Li1	1.909 (6)	C14—C15	1.512 (5)
C1—C2	1.505 (4)	C14—H00R	0.99
C1—H00T	0.98	C14—H00S	0.99
C1—H00U	0.98	C15—H019	0.99
C1—H00V	0.98	C15—H01A	0.99
C2—C3	1.381 (4)	C16—C17	1.516 (5)
C3—C4	1.424 (4)	C16—H00P	0.99
C3—H00E	0.95	C16—H00Q	0.99
C4—C5	1.511 (4)	C17—C18	1.522 (5)
C5—H00F	0.98	C17—H010	0.99
C5—H00G	0.98	C17—H011	0.99
C5—H00H	0.98	C18—C19	1.508 (5)
C6—C7	1.517 (4)	C18—H00Y	0.99
C6—H6	0.99	C18—H00Z	0.99
C6—H00B	0.99	C19—H00W	0.99
C7—H00C	0.99	C19—H00X	0.99

N1—Co1—O1	88.14 (10)	H014—C9—H015	109.5
N1—Co1—N2	80.51 (10)	C8—C9—H016	109.5
O1—Co1—N2	166.65 (9)	H014—C9—H016	109.5
N1—Co1—Cl2	121.87 (8)	H015—C9—H016	109.5
O1—Co1—Cl2	95.82 (7)	N2—C10—C11	113.9 (3)
N2—Co1—Cl2	96.14 (7)	N2—C10—H00I	108.8
N1—Co1—Cl1	125.12 (8)	C11—C10—H00I	108.8
O1—Co1—Cl1	86.63 (7)	N2—C10—H00J	108.8
N2—Co1—Cl1	94.13 (7)	C11—C10—H00J	108.8
Cl2—Co1—Cl1	113.01 (3)	H00I—C10—H00J	107.7
N1—Co1—Li1	119.92 (13)	C10—C11—H00M	109.5
O1—Co1—Li1	38.78 (13)	C10—C11—H00N	109.5
N2—Co1—Li1	145.09 (13)	H00M—C11—H00N	109.5
Cl2—Co1—Li1	95.35 (11)	C10—C11—H00O	109.5
Cl1—Co1—Li1	51.13 (11)	H00M—C11—H00O	109.5
C4—N1—C6	118.7 (3)	H00N—C11—H00O	109.5
C4—N1—Co1	124.2 (2)	O2—C12—C13	107.0 (3)
C6—N1—Co1	115.84 (19)	O2—C12—H012	110.3
C2—O1—Li1	139.5 (3)	C13—C12—H012	110.3
C2—O1—Co1	123.0 (2)	O2—C12—H013	110.3
Li1—O1—Co1	97.5 (2)	C13—C12—H013	110.3
Li1—Cl1—Co1	77.56 (14)	H012—C12—H013	108.6
C10—N2—C7	108.3 (2)	C14—C13—C12	103.3 (3)
C10—N2—C8	111.8 (2)	C14—C13—H017	111.1
C7—N2—C8	111.2 (2)	C12—C13—H017	111.1
C10—N2—Co1	116.94 (19)	C14—C13—H018	111.1
C7—N2—Co1	97.83 (17)	C12—C13—H018	111.1
C8—N2—Co1	109.87 (18)	H017—C13—H018	109.1
C15—O2—C12	108.4 (2)	C15—C14—C13	101.9 (3)
C15—O2—Li1	113.2 (3)	C15—C14—H00R	111.4
C12—O2—Li1	121.7 (3)	C13—C14—H00R	111.4
C16—O3—C19	109.5 (2)	C15—C14—H00S	111.4
C16—O3—Li1	118.7 (3)	C13—C14—H00S	111.4
C19—O3—Li1	120.9 (3)	H00R—C14—H00S	109.2
C2—C1—H00T	109.5	O2—C15—C14	104.4 (3)
C2—C1—H00U	109.5	O2—C15—H019	110.9
H00T—C1—H00U	109.5	C14—C15—H019	110.9
C2—C1—H00V	109.5	O2—C15—H01A	110.9
H00T—C1—H00V	109.5	C14—C15—H01A	110.9
H00U—C1—H00V	109.5	H019—C15—H01A	108.9
O1—C2—C3	124.9 (3)	O3—C16—C17	104.9 (3)
O1—C2—C1	115.6 (3)	O3—C16—H00P	110.8
C3—C2—C1	119.5 (3)	C17—C16—H00P	110.8
C2—C3—C4	126.6 (3)	O3—C16—H00Q	110.8
C2—C3—H00E	116.7	C17—C16—H00Q	110.8
C4—C3—H00E	116.7	H00P—C16—H00Q	108.8
N1—C4—C3	123.3 (3)	C16—C17—C18	101.7 (3)

N1—C4—C5	120.0 (3)	C16—C17—H010	111.4
C3—C4—C5	116.8 (3)	C18—C17—H010	111.4
C4—C5—H00F	109.5	C16—C17—H011	111.4
C4—C5—H00G	109.5	C18—C17—H011	111.4
H00F—C5—H00G	109.5	H010—C17—H011	109.3
C4—C5—H00H	109.5	C19—C18—C17	102.0 (3)
H00F—C5—H00H	109.5	C19—C18—H00Y	111.4
H00G—C5—H00H	109.5	C17—C18—H00Y	111.4
N1—C6—C7	107.5 (2)	C19—C18—H00Z	111.4
N1—C6—H6	110.2	C17—C18—H00Z	111.4
C7—C6—H6	110.2	H00Y—C18—H00Z	109.2
N1—C6—H00B	110.2	O3—C19—C18	106.0 (3)
C7—C6—H00B	110.2	O3—C19—H00W	110.5
H6—C6—H00B	108.5	C18—C19—H00W	110.5
N2—C7—C6	111.4 (2)	O3—C19—H00X	110.5
N2—C7—H00C	109.3	C18—C19—H00X	110.5
C6—C7—H00C	109.3	H00W—C19—H00X	108.7
N2—C7—H00D	109.3	O1—Li1—O3	118.9 (3)
C6—C7—H00D	109.3	O1—Li1—O2	120.4 (3)
H00C—C7—H00D	108.0	O3—Li1—O2	102.6 (3)
N2—C8—C9	116.1 (3)	O1—Li1—Cl1	91.4 (2)
N2—C8—H00K	108.3	O3—Li1—Cl1	110.7 (3)
C9—C8—H00K	108.3	O2—Li1—Cl1	112.7 (3)
N2—C8—H00L	108.3	O1—Li1—Co1	43.74 (13)
C9—C8—H00L	108.3	O3—Li1—Co1	112.5 (2)
H00K—C8—H00L	107.4	O2—Li1—Co1	144.7 (3)
C8—C9—H014	109.5	Cl1—Li1—Co1	51.31 (11)
C8—C9—H015	109.5		
Li1—O1—C2—C3	156.6 (4)	Co1—N2—C10—C11	66.0 (3)
Co1—O1—C2—C3	-19.4 (4)	C15—O2—C12—C13	7.8 (4)
Li1—O1—C2—C1	-23.5 (5)	Li1—O2—C12—C13	-126.2 (3)
Co1—O1—C2—C1	160.4 (2)	O2—C12—C13—C14	16.6 (4)
O1—C2—C3—C4	-3.9 (5)	C12—C13—C14—C15	-33.3 (4)
C1—C2—C3—C4	176.3 (3)	C12—O2—C15—C14	-29.5 (4)
C6—N1—C4—C3	-172.9 (3)	Li1—O2—C15—C14	108.8 (3)
Co1—N1—C4—C3	20.9 (4)	C13—C14—C15—O2	38.8 (3)
C6—N1—C4—C5	6.0 (4)	C19—O3—C16—C17	16.7 (4)
Co1—N1—C4—C5	-160.2 (2)	Li1—O3—C16—C17	161.3 (3)
C2—C3—C4—N1	3.6 (5)	O3—C16—C17—C18	-34.8 (3)
C2—C3—C4—C5	-175.4 (3)	C16—C17—C18—C19	39.2 (3)
C4—N1—C6—C7	176.8 (3)	C16—O3—C19—C18	8.6 (4)
Co1—N1—C6—C7	-15.9 (3)	Li1—O3—C19—C18	-135.0 (3)
C10—N2—C7—C6	-176.2 (2)	C17—C18—C19—O3	-30.1 (3)
C8—N2—C7—C6	60.5 (3)	C2—O1—Li1—O3	90.2 (5)
Co1—N2—C7—C6	-54.4 (2)	Co1—O1—Li1—O3	-93.2 (3)
N1—C6—C7—N2	50.6 (3)	C2—O1—Li1—O2	-37.6 (6)
C10—N2—C8—C9	-59.3 (3)	Co1—O1—Li1—O2	139.1 (3)

C7—N2—C8—C9	61.9 (3)	C2—O1—Li1—Cl1	-155.1 (3)
Co1—N2—C8—C9	169.1 (2)	Co1—O1—Li1—Cl1	21.53 (18)
C7—N2—C10—C11	175.2 (3)	C2—O1—Li1—Co1	-176.6 (4)
C8—N2—C10—C11	-61.9 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C5—H00H...C11 ⁱ	0.98	2.80	3.770 (3)	172
C6—H6...C11 ⁱ	0.99	2.96	3.924 (3)	166
C8—H00L...C12	0.99	2.86	3.365 (3)	113
C10—H00I...C11	0.99	2.80	3.357 (3)	117
C13—H017...C12 ⁱⁱ	0.99	2.89	3.608 (3)	130
C19—H00X...C11	0.99	2.91	3.635 (3)	131

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$.