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Redetermination of tris(ethyl carbazate-κ^2N,O)cobalt(II) dinitrate

Krishnan Srinivasan,[a] Subbaiah Govindarajan[a] and William T. A. Harrison[b]*

[a]Department of Chemistry, Bharathiar University, Coimbatore 641 046, India, and [b]Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland
Correspondence e-mail: w.harrison@abdn.ac.uk

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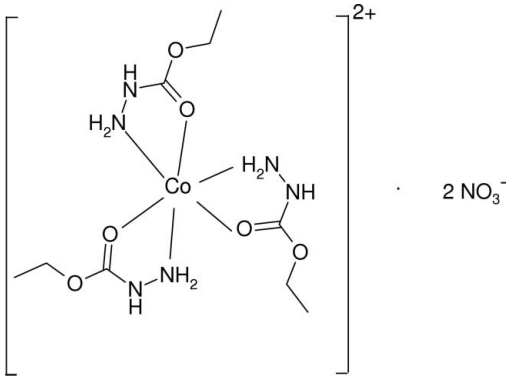
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.037; wR factor = 0.091; data-to-parameter ratio = 16.4.

The present study of the title compound, $[Co(C_3H_8N_2O_2)_3](NO_3)_2$, probably represents a correction to that reported by Zhang, Song, Zhang, Ma & Yu [*Z. Naturforsch. Teil B* (2005), **60**, 505–510] with a doubled *a* axis. As modelled here, there are four independent cations, each built up around a *fac*-CoN_3O_3 octahedron, and eight anions in the asymmetric unit. Two of the cations show disorder in one of their ethyl side chains in ratios of 0.712 (10):0.288 (10) and 0.612 (7):0.388 (8). Numerous cation-to-anion N—H···O hydrogen bonds, many of which are bifurcated, help to establish the crystal packing.

Related literature

For the previous determination of the structure, see: Zhang *et al.* (2005). For background, see: Indira *et al.* (1993).



Experimental

Crystal data

$[Co(C_3H_8N_2O_2)_3](NO_3)_2$
M_r = 495.29
Monoclinic, $P2_1/n$
a = 28.0291 (6) Å
b = 8.6245 (2) Å
c = 35.6763 (7) Å
β = 110.2445 (5)°
V = 8091.5 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 120 (2) K
0.44 × 0.40 × 0.28 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.687, T_{max} = 0.784
86674 measured reflections
18519 independent reflections
14049 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.091
S = 1.04
18519 reflections
1128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O11	2.1005 (15)	Co3—O33	2.0896 (14)
Co1—O15	2.1172 (15)	Co3—O35	2.1062 (14)
Co1—O13	2.1179 (14)	Co3—O31	2.1112 (14)
Co1—N13	2.1236 (17)	Co3—N35	2.1285 (17)
Co1—N15	2.1460 (17)	Co3—N31	2.1515 (16)
Co1—N11	2.1649 (17)	Co3—N33	2.1582 (16)
Co2—O25	2.0853 (14)	Co4—O41	2.1063 (14)
Co2—O23	2.1090 (14)	Co4—O43	2.1064 (14)
Co2—N21	2.1240 (17)	Co4—O45	2.1297 (14)
Co2—O21	2.1270 (14)	Co4—N45	2.1338 (16)
Co2—N25	2.1534 (17)	Co4—N43	2.1450 (17)
Co2—N23	2.1678 (17)	Co4—N41	2.1671 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11*A*···O152	0.92	2.40	3.166 (2)	140
N11—H11*A*···O163	0.92	2.60	3.111 (2)	116
N11—H11*A*···O171	0.92	2.64	3.188 (2)	119
N11—H11*B*···O142	0.92	2.19	3.028 (2)	151
N12—H12···O172	0.88	2.19	2.931 (2)	141
N13—H13*D*···O151	0.92	2.10	2.947 (2)	153
N13—H13*D*···O152	0.92	2.40	3.155 (2)	139
N13—H13*E*···O162	0.92	2.12	3.016 (2)	166
N13—H13*E*···O163	0.92	2.64	3.395 (3)	140
N14—H14···O131^{i}	0.88	2.09	2.939 (2)	161
N14—H14···O132^{i}	0.88	2.33	3.053 (2)	140
N15—H15*C*···O143	0.92	2.14	2.968 (2)	149
N15—H15*C*···O151	0.92	2.45	2.984 (2)	117
N15—H15*D*···O161^{ii}	0.92	2.06	2.982 (2)	176
N15—H15*D*···O163^{ii}	0.92	2.66	3.307 (2)	128
N16—H16···O171^{ii}	0.88	2.09	2.889 (2)	151
N21—H21*A*···O101^{iii}	0.92	2.28	3.013 (2)	137
N21—H21*A*···O103^{iii}	0.92	2.43	3.336 (2)	167
N21—H21*B*···O121	0.92	2.10	2.939 (2)	151
N21—H21*B*···O112^{iii}	0.92	2.44	2.979 (2)	117
N22—H22···O131	0.88	2.05	2.907 (2)	164
N23—H23*D*···O113^{iv}	0.92	2.26	3.166 (2)	169
N23—H23*D*···O111^{iv}	0.92	2.39	3.121 (2)	136
N23—H23*E*···O111^{iii}	0.92	2.34	3.141 (2)	146
N23—H23*E*···O112^{iii}	0.92	2.64	3.496 (2)	156
N24—H24···O122^{iv}	0.88	2.16	2.852 (2)	135
N25—H25*C*···O102	0.92	2.12	3.038 (2)	176
N25—H25*C*···O103	0.92	2.57	3.243 (2)	130
N25—H25*D*···O122	0.92	2.02	2.924 (2)	169
N26—H26···O111	0.88	2.25	3.043 (2)	150
N31—H31*A*···O112	0.92	2.12	2.970 (2)	153
N31—H31*A*···O101	0.92	2.63	3.152 (2)	116
N31—H31*B*···O131^{ii}	0.92	2.16	3.073 (2)	175
N31—H31*B*···O133^{ii}	0.92	2.61	3.303 (3)	133

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D—H···A	D—H	H···A	D···A	D—H···A
N32—H32···O121^{ii}	0.88	2.26	2.992 (2)	141
N32—H32···O123^{ii}	0.88	2.42	3.234 (3)	154
N33—H33*D*···O102	0.92	2.31	3.083 (2)	142
N33—H33*E*···O113	0.92	2.25	3.071 (2)	149
N34—H34···O123	0.88	2.21	2.929 (2)	139
N35—H35*C*···O101	0.92	2.06	2.922 (2)	155
N35—H35*C*···O102	0.92	2.50	3.233 (2)	136
N35—H35*D*···O132	0.92	2.11	3.025 (2)	171
N36—H36···O161^{i}	0.88	2.04	2.896 (2)	164
N36—H36···O162^{i}	0.88	2.46	3.144 (2)	135
N41—H41*A*···O141^{v}	0.92	2.30	3.066 (2)	140
N41—H41*A*···O142^{v}	0.92	2.36	3.255 (2)	165
N41—H41*B*···O141^{iii}	0.92	2.32	3.088 (2)	141
N41—H41*B*···O143^{iii}	0.92	2.60	3.460 (2)	156
N42—H42···O173^{v}	0.88	2.09	2.818 (2)	139
N43—H43*D*···O152	0.92	2.11	3.018 (2)	169
N43—H43*D*···O153	0.92	2.49	3.187 (2)	133
N43—H43*E*···O173	0.92	1.98	2.898 (2)	175
N44—H44···O141	0.88	2.22	3.041 (2)	155
N45—H45*C*···O151^{iii}	0.92	2.30	3.028 (2)	136
N45—H45*C*···O153^{iii}	0.92	2.45	3.358 (2)	169
N45—H45*D*···O171	0.92	2.13	3.012 (2)	159
N46—H46···O161	0.88	2.13	2.991 (2)	165

Symmetry codes: (i) $-x+1,-y+1,-z$; (ii) $x,y-1,z$; (iii) $x,y+1,z$; (iv) $-x+\frac{3}{2},y+\frac{1}{2},-z+\frac{1}{2}$; (v) $-x+\frac{1}{2},y+\frac{1}{2},-z+\frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* (Otwinowski & Minor 1997), *HKL SCALEPACK* and *SORTAV* (Blessing 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2213).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Bruker (2003). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Indira, A., Babu, A. M., Bellad, S. B., Sridhar, M. A., Shashidhara Prasad, J. & Prout, C. K. (1993). *Curr. Sci.* **64**, 247–252.

Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Zhang, T.-L., Song, J.-C., Zhang, J.-G., Ma, G.-X. & Yu, K.-B. (2005). *Z. Naturforsch. Teil B*, **60**, 505–510.

supplementary materials

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Redetermination of tris(ethyl carbazate-κ^2N,O)cobalt(II) dinitrate

K. Srinivasan, S. Govindarajan and W. T. A. Harrison

Comment

The title compound, (I), was recently described by Zhang *et al.* (2005). We inadvertantly prepared the same material, and report here its structure. The cell described here has a doubled *a* axis and doubled volume compared to the Zhang unit cell and its aymmetric unit contains four $[Co(C_3H_8N_2O_2)_3]^{2+}$ cations and eight nitrate anions, compared to two cations and four anions in the Zhang model in the same space group. It is notable that both the cations showed disorder in the Zhang model, and visual comparison of the two structures suggest that they are closely related. It seems that the previous unit cell may have been too small. However, in such a complex system, it is possible that the present structure and the Zhang structure are actually polymorphs, perhaps with different hydrogen bonding motifs.

The four complex cations in (I) are similar (Fig. 1) and are each built up around a slightly distorted *fac*-CoN_3O_3 octahedral core (Table 1). In every case, a five-membered –Co—N—N—C—O– chelate ring arises for the twelve distinct N,*O*-bidentate ligands. In the Co1 and Co2-containing cations, one of the ethyl-carbazate ligands shows disorder of its ethyl side chains.

One feature of the crystal of (I) is a very short nitro-O133···C34 contact of 2.706 (3) Å. The displacement ellipsoid of O133 is suggestive of disorder, but attempts to model this feature with split-site atom schemes were not successful. There is some literature precedent for short O···C contacts arising from nitro groups. For example, in $(C_{14}H_{22}N_2O)_2{\cdot}CuCl(NO_3)_3$ (Indira *et al.*, 1993), an intermolecular nitro-O···C separation of 2.680 (5) Å occurs, which is even shorter than the value reported here.

The crystal packing for (I) is consolidated by a large number of cation-to-anion N—H···O hydrogen bonds (Table 2), a number of which are bifurcated. This helps to generate a structure (Fig. 2) in which [010] columns of cation are present, with the nitrate anions occupying the space between the columns. It is notable that the cores of the columns appear to be made up of the hydrophobic ethyl side chains of the ligands.

Experimental

Ethyl carbazate (0.208 g, 0.002 mol) was added to an aqueous solution (25 ml) containing formic acid (85%, 0.08 ml). To this solution was added cobalt nitrate hexahydrate (0.291 g, 0.001 mol) dissolved in doubly distilled water (50 ml). The resulting pink solution was concentrated over a water bath to about 15 ml and kept for crystallization at room temperature. Pink blocks of (I) obtained after a week were separated and washed with ethanol and air dried.

Refinement

The C18/C19 and C28/C29 ethyl side chains of the ligands are disordered in 0.712 (10):0.288 (10) and 0.612 (7):0.388 (8) ratios, respectively. The H atoms were geometrically placed (N—H = 0.88–0.92 Å, C—H = 0.98–0.99 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(N,*C*) or 1.5U_{eq}(methyl C).

Figures

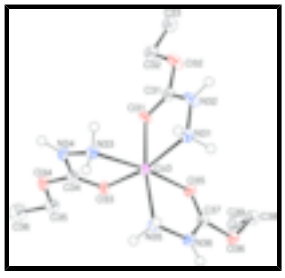

Fig. 1. View of the Co3-containing complex cation in (I) shoiwng 50% displacement ellipsoids (arbitrary spheres for the H atoms). The C-bound H atoms are omitted for clarity.

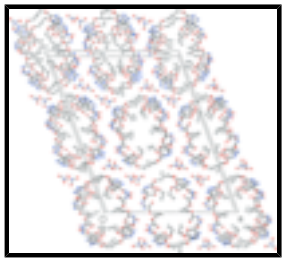

Fig. 2. Unit cell packing in (I) viewed down [010] with H atoms and minor disorder components omitted for clarity.

tris(ethyl carbazate-κ^2*N*,*O*)cobalt(II) dinitrate

Crystal data

$[Co(C_3H_8N_2O_2)_3](NO_3)_2$	F_{000} = 4112
M_r = 495.29	D_x = 1.626 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 19276 reflections
a = 28.0291 (6) Å	θ = 2.9–27.5º
b = 8.6245 (2) Å	μ = 0.92 mm^{-1}
c = 35.6763 (7) Å	T = 120 (2) K
β = 110.2445 (5)º	Block, pink
V = 8091.5 (3) Å^3	0.44 × 0.40 × 0.28 mm
Z = 16	

Data collection

Nonius KappaCCD diffractometer	18519 independent reflections
Radiation source: fine-focus sealed tube	14049 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
T = 120(2) K	θ_{max} = 27.5º
ω and φ scans	θ_{min} = 2.9º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	h = −36→36
T_{min} = 0.687, T_{max} = 0.784	k = −10→11
86674 measured reflections	l = −46→46

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 4.8866P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.003$
18519 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
1128 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.378517 (10)	0.22555 (3)	0.109456 (8)	0.01724 (7)	
C11	0.43324 (8)	0.5019 (2)	0.13542 (7)	0.0232 (5)	
C12	0.49470 (10)	0.6426 (3)	0.11677 (9)	0.0451 (7)	
H12A	0.5016	0.5411	0.1067	0.054*	
H12B	0.5277	0.6931	0.1312	0.054*	
C13	0.46476 (12)	0.7405 (4)	0.08305 (9)	0.0523 (8)	
H13A	0.4845	0.7606	0.0656	0.078*	
H13B	0.4568	0.8390	0.0932	0.078*	
H13C	0.4331	0.6870	0.0679	0.078*	
N11	0.36718 (6)	0.3885 (2)	0.15178 (5)	0.0209 (4)	
H11A	0.3370	0.4408	0.1405	0.025*	
H11B	0.3664	0.3374	0.1742	0.025*	
N12	0.40882 (6)	0.4933 (2)	0.16183 (5)	0.0220 (4)	
H12	0.4180	0.5489	0.1839	0.026*	
O11	0.42745 (5)	0.40812 (17)	0.10801 (4)	0.0234 (3)	
O12	0.46638 (6)	0.61959 (19)	0.14385 (5)	0.0357 (4)	
C14	0.34850 (8)	0.1177 (2)	0.03016 (6)	0.0202 (4)	
C15	0.37987 (9)	−0.0675 (3)	−0.00506 (7)	0.0314 (5)	

H15A	0.3648	−0.1400	−0.0276	0.038*	
H15B	0.3904	−0.1285	0.0200	0.038*	
C16	0.42593 (10)	0.0086 (3)	−0.00952 (9)	0.0456 (7)	
H16A	0.4504	−0.0712	−0.0104	0.068*	
H16B	0.4416	0.0776	0.0132	0.068*	
H16C	0.4157	0.0688	−0.0343	0.068*	
N13	0.31313 (7)	0.3000 (2)	0.06174 (5)	0.0212 (4)	
H13D	0.2844	0.2865	0.0683	0.025*	
H13E	0.3159	0.4035	0.0565	0.025*	
N14	0.30982 (7)	0.2100 (2)	0.02783 (5)	0.0241 (4)	
H14	0.2829	0.2151	0.0059	0.029*	
O13	0.38688 (5)	0.10170 (17)	0.06084 (4)	0.0219 (3)	
O14	0.34184 (6)	0.04539 (18)	−0.00426 (4)	0.0264 (3)	
C17	0.42888 (8)	−0.0037 (3)	0.16649 (6)	0.0237 (5)	
C18A	0.51489 (11)	−0.0781 (6)	0.20164 (14)	0.0274 (12)	0.712 (10)
H18A	0.5224	0.0232	0.1918	0.033*	0.712 (10)
H18B	0.5265	−0.1616	0.1878	0.033*	0.712 (10)
C19A	0.5410 (2)	−0.0904 (9)	0.24591 (15)	0.0488 (16)	0.712 (10)
H19A	0.5779	−0.0896	0.2522	0.073*	0.712 (10)
H19B	0.5310	−0.1874	0.2555	0.073*	0.712 (10)
H19C	0.5312	−0.0024	0.2590	0.073*	0.712 (10)
C18B	0.5134 (3)	−0.0007 (14)	0.2175 (3)	0.023 (3)	0.288 (10)
H18C	0.5268	0.0520	0.1985	0.028*	0.288 (10)
H18D	0.5085	0.0765	0.2363	0.028*	0.288 (10)
C19B	0.5477 (6)	−0.1283 (17)	0.2390 (4)	0.031 (3)*	0.288 (10)
H19D	0.5816	−0.0863	0.2534	0.046*	0.288 (10)
H19E	0.5500	−0.2063	0.2197	0.046*	0.288 (10)
H19F	0.5341	−0.1763	0.2581	0.046*	0.288 (10)
N15	0.34325 (6)	0.03124 (19)	0.12700 (5)	0.0185 (4)	
H15C	0.3199	0.0653	0.1380	0.022*	
H15D	0.3266	−0.0290	0.1051	0.022*	
N16	0.38162 (6)	−0.0566 (2)	0.15541 (5)	0.0221 (4)	
H16	0.3744	−0.1432	0.1653	0.026*	
O15	0.44102 (5)	0.11584 (18)	0.15282 (5)	0.0293 (4)	
O16	0.46121 (6)	−0.0928 (2)	0.19427 (5)	0.0350 (4)	
Co2	0.661707 (10)	0.76084 (3)	0.155900 (8)	0.01657 (7)	
C21	0.66557 (8)	0.6839 (2)	0.08018 (6)	0.0198 (4)	
C22	0.62819 (9)	0.4910 (3)	0.03125 (7)	0.0316 (5)	
H22A	0.6276	0.4297	0.0546	0.038*	
H22B	0.6412	0.4235	0.0145	0.038*	
C23	0.57506 (11)	0.5427 (3)	0.00744 (8)	0.0499 (7)	
H23A	0.5535	0.4516	−0.0025	0.075*	
H23B	0.5757	0.6060	−0.0152	0.075*	
H23C	0.5614	0.6040	0.0245	0.075*	
N21	0.70996 (7)	0.8665 (2)	0.12868 (5)	0.0210 (4)	
H21A	0.7032	0.9710	0.1254	0.025*	
H21B	0.7435	0.8538	0.1446	0.025*	
N22	0.70081 (7)	0.7952 (2)	0.09118 (5)	0.0237 (4)	
H22	0.7177	0.8232	0.0756	0.028*	

O21	0.63925 (5)	0.64307 (16)	0.10010 (4)	0.0201 (3)	
O22	0.66203 (6)	0.62304 (17)	0.04504 (4)	0.0266 (3)	
C24	0.60653 (8)	1.0327 (2)	0.15778 (6)	0.0202 (4)	
C25	0.53594 (8)	1.1650 (3)	0.11072 (7)	0.0299 (5)	
H25A	0.5042	1.2116	0.1120	0.036*	
H25B	0.5276	1.0615	0.0981	0.036*	
C26	0.55730 (10)	1.2659 (3)	0.08614 (7)	0.0361 (6)	
H26A	0.5315	1.2819	0.0597	0.054*	
H26B	0.5871	1.2155	0.0832	0.054*	
H26C	0.5672	1.3662	0.0994	0.054*	
N23	0.68026 (6)	0.9259 (2)	0.20469 (5)	0.0207 (4)	
H23D	0.6828	0.8763	0.2281	0.025*	
H23E	0.7108	0.9734	0.2079	0.025*	
N24	0.64041 (7)	1.0370 (2)	0.19474 (5)	0.0210 (4)	
H24	0.6382	1.1059	0.2123	0.025*	
O23	0.60516 (5)	0.93140 (17)	0.13296 (4)	0.0220 (3)	
O24	0.57298 (6)	1.14897 (19)	0.15107 (5)	0.0301 (4)	
C27	0.63903 (8)	0.5134 (3)	0.19850 (7)	0.0260 (5)	
C28A	0.5735 (2)	0.4775 (7)	0.22683 (19)	0.0322 (13)	0.612 (7)
H28A	0.5835	0.4955	0.2559	0.039*	0.612 (7)
H28B	0.5613	0.5764	0.2127	0.039*	0.612 (7)
C29A	0.53289 (15)	0.3553 (5)	0.21343 (12)	0.0339 (13)	0.612 (7)
H29A	0.5025	0.3908	0.2186	0.051*	0.612 (7)
H29B	0.5453	0.2591	0.2282	0.051*	0.612 (7)
H29C	0.5243	0.3365	0.1848	0.051*	0.612 (7)
C28B	0.5622 (3)	0.4169 (10)	0.2051 (3)	0.048 (2)	0.388 (7)
H28C	0.5450	0.4571	0.1778	0.058*	0.388 (7)
H28D	0.5479	0.3144	0.2081	0.058*	0.388 (7)
C29B	0.5609 (4)	0.5253 (13)	0.2354 (3)	0.057 (3)	0.388 (7)
H29D	0.5255	0.5461	0.2327	0.086*	0.388 (7)
H29E	0.5773	0.6223	0.2323	0.086*	0.388 (7)
H29F	0.5789	0.4814	0.2619	0.086*	0.388 (7)
N25	0.71077 (6)	0.5678 (2)	0.18181 (5)	0.0203 (4)	
H25C	0.7177	0.5127	0.1622	0.024*	
H25D	0.7410	0.6028	0.1999	0.024*	
N26	0.68546 (6)	0.4719 (2)	0.20128 (5)	0.0227 (4)	
H26	0.7000	0.3887	0.2146	0.027*	
O25	0.61747 (5)	0.63310 (18)	0.18129 (5)	0.0263 (3)	
O26	0.61803 (7)	0.4136 (2)	0.21639 (6)	0.0535 (6)	
Co3	0.861768 (10)	0.23284 (3)	0.102066 (8)	0.01656 (7)	
C31	0.92004 (8)	0.0164 (2)	0.15870 (6)	0.0201 (4)	
C32	1.00754 (8)	−0.0041 (3)	0.19841 (7)	0.0286 (5)	
H32A	1.0107	0.0782	0.2185	0.034*	
H32B	1.0155	0.0411	0.1757	0.034*	
C33	1.04293 (9)	−0.1347 (3)	0.21655 (7)	0.0328 (6)	
H33A	1.0778	−0.0954	0.2274	0.049*	
H33B	1.0406	−0.2129	0.1961	0.049*	
H33C	1.0336	−0.1816	0.2381	0.049*	
N31	0.83223 (6)	0.03374 (19)	0.12312 (5)	0.0190 (4)	

H31A	0.8104	0.0645	0.1359	0.023*
H31B	0.8147	−0.0292	0.1020	0.023*
N32	0.87400 (6)	−0.0467 (2)	0.14988 (5)	0.0239 (4)
H32	0.8698	−0.1357	0.1604	0.029*
O31	0.92832 (5)	0.14003 (16)	0.14449 (4)	0.0210 (3)
O32	0.95605 (6)	−0.06886 (18)	0.18456 (5)	0.0290 (4)
C34	0.91254 (7)	0.5176 (2)	0.11969 (6)	0.0185 (4)
C35	0.95894 (9)	0.6621 (3)	0.08829 (7)	0.0277 (5)
H35A	0.9303	0.6579	0.0625	0.033*
H35B	0.9831	0.5780	0.0887	0.033*
C36	0.98499 (12)	0.8170 (3)	0.09326 (8)	0.0489 (8)
H36A	0.9980	0.8333	0.0714	0.073*
H36B	1.0133	0.8195	0.1188	0.073*
H36C	0.9606	0.8991	0.0928	0.073*
N33	0.85559 (6)	0.39863 (19)	0.14547 (5)	0.0185 (4)
H33D	0.8244	0.4471	0.1364	0.022*
H33E	0.8593	0.3502	0.1693	0.022*
N34	0.89534 (6)	0.5077 (2)	0.15053 (5)	0.0185 (4)
H34	0.9078	0.5647	0.1722	0.022*
O33	0.90476 (5)	0.41820 (16)	0.09329 (4)	0.0202 (3)
O34	0.94035 (6)	0.64404 (17)	0.12149 (4)	0.0239 (3)
C37	0.82773 (8)	0.1031 (2)	0.02534 (6)	0.0187 (4)
C38	0.85617 (9)	−0.1023 (3)	−0.00621 (7)	0.0303 (5)
H38A	0.8389	−0.1896	−0.0237	0.036*
H38B	0.8710	−0.1422	0.0214	0.036*
C39	0.89794 (12)	−0.0420 (4)	−0.01941 (9)	0.0538 (8)
H39A	0.9215	−0.1264	−0.0190	0.081*
H39B	0.9163	0.0405	−0.0012	0.081*
H39C	0.8833	−0.0006	−0.0466	0.081*
N35	0.79322 (6)	0.2941 (2)	0.05538 (5)	0.0193 (4)
H35C	0.7659	0.2834	0.0638	0.023*
H35D	0.7946	0.3955	0.0478	0.023*
N36	0.78822 (7)	0.1928 (2)	0.02297 (5)	0.0203 (4)
H36	0.7600	0.1894	0.0021	0.024*
O35	0.86768 (5)	0.09820 (16)	0.05461 (4)	0.0210 (3)
O36	0.81902 (6)	0.01782 (17)	−0.00770 (4)	0.0242 (3)
Co4	0.169396 (10)	0.75473 (3)	0.153429 (8)	0.01597 (6)
C41	0.11708 (8)	1.0333 (2)	0.15505 (6)	0.0182 (4)
C42	0.05033 (8)	1.1801 (3)	0.10802 (7)	0.0281 (5)
H42A	0.0153	1.1967	0.1079	0.034*
H42B	0.0501	1.0893	0.0910	0.034*
C43	0.06818 (10)	1.3211 (3)	0.09203 (8)	0.0358 (6)
H43A	0.0449	1.3425	0.0649	0.054*
H43B	0.1025	1.3027	0.0915	0.054*
H43C	0.0688	1.4102	0.1092	0.054*
N41	0.18798 (7)	0.91604 (19)	0.20300 (5)	0.0202 (4)
H41A	0.1884	0.8659	0.2259	0.024*
H41B	0.2195	0.9590	0.2075	0.024*
N42	0.15002 (7)	1.0330 (2)	0.19243 (5)	0.0208 (4)

H42	0.1483	1.1028	0.2099	0.025*
O41	0.11619 (5)	0.93343 (16)	0.12992 (4)	0.0190 (3)
O42	0.08458 (6)	1.15162 (17)	0.14867 (4)	0.0269 (3)
C44	0.14550 (7)	0.5096 (2)	0.19671 (6)	0.0170 (4)
C45	0.07985 (8)	0.4684 (3)	0.22343 (7)	0.0265 (5)
H45A	0.0837	0.5796	0.2308	0.032*
H45B	0.0757	0.4102	0.2460	0.032*
C46	0.03322 (9)	0.4472 (3)	0.18709 (8)	0.0345 (6)
H46A	0.0033	0.4829	0.1929	0.052*
H46B	0.0292	0.3372	0.1798	0.052*
H46C	0.0367	0.5076	0.1649	0.052*
N43	0.21539 (6)	0.55428 (19)	0.17677 (5)	0.0192 (4)
H43D	0.2205	0.4999	0.1563	0.023*
H43E	0.2466	0.5842	0.1945	0.023*
N44	0.19016 (6)	0.4594 (2)	0.19640 (5)	0.0199 (4)
H44	0.2034	0.3716	0.2078	0.024*
O43	0.12486 (5)	0.63135 (16)	0.18029 (4)	0.0188 (3)
O44	0.12563 (5)	0.41468 (17)	0.21669 (5)	0.0251 (3)
C47	0.17398 (8)	0.6915 (2)	0.07687 (6)	0.0194 (4)
C48	0.13050 (9)	0.5236 (3)	0.02327 (7)	0.0325 (6)
H48A	0.1308	0.4497	0.0446	0.039*
H48B	0.1394	0.4656	0.0027	0.039*
C49	0.07804 (10)	0.5910 (3)	0.00489 (8)	0.0441 (7)
H49A	0.0534	0.5070	−0.0054	0.066*
H49B	0.0772	0.6603	−0.0171	0.066*
H49C	0.0693	0.6495	0.0252	0.066*
N45	0.22220 (6)	0.8546 (2)	0.12932 (5)	0.0199 (4)
H45C	0.2183	0.9606	0.1277	0.024*
H45D	0.2549	0.8324	0.1455	0.024*
N46	0.21268 (7)	0.7915 (2)	0.09073 (5)	0.0230 (4)
H46	0.2315	0.8172	0.0764	0.028*
O45	0.14707 (5)	0.64853 (16)	0.09604 (4)	0.0201 (3)
O46	0.16830 (6)	0.64395 (18)	0.04004 (4)	0.0273 (4)
N101	0.71481 (6)	0.2698 (2)	0.11364 (5)	0.0216 (4)
O101	0.72087 (6)	0.16852 (17)	0.08997 (5)	0.0281 (4)
O102	0.73847 (6)	0.39666 (17)	0.11777 (5)	0.0300 (4)
O103	0.68603 (6)	0.24390 (19)	0.13268 (5)	0.0342 (4)
N111	0.79002 (6)	0.1855 (2)	0.20916 (5)	0.0192 (4)
O111	0.75882 (6)	0.20017 (18)	0.22718 (4)	0.0253 (3)
O112	0.78583 (6)	0.07391 (19)	0.18579 (5)	0.0312 (4)
O113	0.82537 (6)	0.2811 (2)	0.21539 (5)	0.0358 (4)
N121	0.83351 (7)	0.6941 (2)	0.20478 (5)	0.0222 (4)
O121	0.80825 (6)	0.71321 (18)	0.16828 (4)	0.0302 (4)
O122	0.81160 (6)	0.68252 (19)	0.22976 (4)	0.0270 (4)
O123	0.88088 (6)	0.6874 (2)	0.21545 (5)	0.0369 (4)
N131	0.79525 (7)	0.7141 (2)	0.05358 (5)	0.0228 (4)
O131	0.77184 (5)	0.84304 (16)	0.04915 (4)	0.0218 (3)
O132	0.78612 (6)	0.62343 (18)	0.02471 (4)	0.0308 (4)
O133	0.82550 (9)	0.6800 (3)	0.08622 (6)	0.0746 (8)

N141	0.29539 (6)	0.1812 (2)	0.21059 (5)	0.0187 (4)
O141	0.26319 (5)	0.19033 (18)	0.22794 (4)	0.0241 (3)
O142	0.32952 (7)	0.2818 (2)	0.21749 (5)	0.0359 (4)
O143	0.29348 (6)	0.07125 (19)	0.18752 (5)	0.0316 (4)
N151	0.22660 (6)	0.2607 (2)	0.11169 (5)	0.0217 (4)
O151	0.23779 (6)	0.15584 (17)	0.09150 (4)	0.0266 (3)
O152	0.24698 (6)	0.39237 (18)	0.11406 (5)	0.0314 (4)
O153	0.19592 (6)	0.2345 (2)	0.12905 (5)	0.0362 (4)
N161	0.31379 (7)	0.7123 (2)	0.05965 (5)	0.0202 (4)
O161	0.29207 (5)	0.84470 (16)	0.05366 (4)	0.0216 (3)
O162	0.30895 (7)	0.62641 (18)	0.03041 (5)	0.0334 (4)
O163	0.33890 (7)	0.6712 (2)	0.09410 (5)	0.0398 (4)
N171	0.34031 (6)	0.6733 (2)	0.21102 (5)	0.0186 (4)
O171	0.32225 (6)	0.70080 (17)	0.17398 (4)	0.0228 (3)
O172	0.38704 (5)	0.64911 (18)	0.22713 (5)	0.0272 (4)
O173	0.31158 (5)	0.66930 (18)	0.23114 (4)	0.0239 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01957 (14)	0.01827 (15)	0.01411 (13)	0.00035 (11)	0.00613 (11)	0.00113 (11)
C11	0.0215 (11)	0.0184 (11)	0.0289 (12)	0.0006 (9)	0.0078 (9)	0.0016 (9)
C12	0.0348 (14)	0.0362 (16)	0.068 (2)	−0.0076 (12)	0.0232 (14)	0.0034 (14)
C13	0.0545 (18)	0.053 (2)	0.0514 (18)	0.0023 (15)	0.0207 (15)	0.0042 (15)
N11	0.0217 (9)	0.0231 (10)	0.0188 (9)	0.0009 (7)	0.0085 (7)	0.0004 (7)
N12	0.0227 (9)	0.0226 (10)	0.0184 (9)	−0.0007 (7)	0.0043 (7)	−0.0057 (8)
O11	0.0271 (8)	0.0197 (8)	0.0278 (8)	0.0004 (6)	0.0150 (7)	−0.0004 (7)
O12	0.0350 (9)	0.0259 (9)	0.0472 (11)	−0.0083 (7)	0.0156 (8)	−0.0043 (8)
C14	0.0284 (11)	0.0191 (11)	0.0146 (10)	−0.0015 (9)	0.0095 (9)	0.0003 (8)
C15	0.0426 (14)	0.0243 (13)	0.0277 (13)	0.0080 (10)	0.0126 (11)	−0.0060 (10)
C16	0.0452 (16)	0.0494 (18)	0.0501 (17)	0.0040 (13)	0.0266 (14)	−0.0125 (14)
N13	0.0273 (9)	0.0207 (9)	0.0163 (9)	0.0050 (7)	0.0086 (7)	0.0004 (7)
N14	0.0278 (10)	0.0284 (10)	0.0129 (8)	0.0076 (8)	0.0030 (7)	−0.0017 (8)
O13	0.0247 (8)	0.0234 (8)	0.0168 (7)	0.0039 (6)	0.0063 (6)	−0.0015 (6)
O14	0.0341 (9)	0.0275 (9)	0.0172 (7)	0.0061 (7)	0.0085 (7)	−0.0039 (6)
C17	0.0202 (10)	0.0308 (13)	0.0212 (11)	0.0040 (9)	0.0087 (9)	0.0080 (10)
C18A	0.0170 (16)	0.031 (3)	0.032 (2)	0.0015 (14)	0.0066 (14)	0.0084 (19)
C19A	0.034 (3)	0.086 (5)	0.023 (2)	−0.015 (3)	0.005 (2)	−0.004 (3)
C18B	0.016 (4)	0.027 (6)	0.024 (5)	0.002 (3)	0.004 (3)	0.003 (4)
N15	0.0179 (8)	0.0198 (9)	0.0169 (9)	0.0009 (7)	0.0049 (7)	−0.0006 (7)
N16	0.0209 (9)	0.0186 (9)	0.0260 (10)	−0.0001 (7)	0.0073 (8)	0.0073 (8)
O15	0.0204 (8)	0.0339 (9)	0.0309 (9)	−0.0030 (7)	0.0053 (7)	0.0184 (7)
O16	0.0201 (8)	0.0429 (10)	0.0404 (10)	0.0052 (7)	0.0085 (7)	0.0253 (8)
Co2	0.01984 (13)	0.01599 (15)	0.01447 (13)	−0.00063 (11)	0.00670 (11)	0.00120 (11)
C21	0.0254 (11)	0.0186 (11)	0.0151 (10)	0.0022 (8)	0.0066 (9)	0.0006 (8)
C22	0.0488 (15)	0.0228 (12)	0.0281 (13)	−0.0093 (11)	0.0195 (11)	−0.0088 (10)
C23	0.0536 (18)	0.0495 (18)	0.0370 (16)	−0.0132 (14)	0.0034 (13)	−0.0070 (14)
N21	0.0263 (9)	0.0189 (9)	0.0176 (9)	−0.0046 (7)	0.0071 (7)	−0.0005 (7)

N22	0.0319 (10)	0.0252 (10)	0.0181 (9)	−0.0085 (8)	0.0139 (8)	−0.0024 (8)
O21	0.0248 (8)	0.0195 (8)	0.0176 (7)	−0.0040 (6)	0.0093 (6)	−0.0019 (6)
O22	0.0416 (9)	0.0231 (8)	0.0204 (8)	−0.0070 (7)	0.0174 (7)	−0.0054 (7)
C24	0.0231 (11)	0.0212 (11)	0.0205 (11)	0.0018 (9)	0.0130 (9)	0.0036 (9)
C25	0.0248 (12)	0.0350 (14)	0.0286 (12)	0.0097 (10)	0.0074 (10)	0.0053 (11)
C26	0.0399 (14)	0.0395 (15)	0.0305 (13)	0.0094 (12)	0.0144 (11)	0.0105 (11)
N23	0.0239 (9)	0.0209 (9)	0.0166 (9)	−0.0006 (7)	0.0058 (7)	0.0025 (7)
N24	0.0292 (10)	0.0189 (9)	0.0166 (9)	0.0037 (7)	0.0098 (7)	−0.0022 (7)
O23	0.0249 (8)	0.0224 (8)	0.0175 (7)	0.0039 (6)	0.0057 (6)	0.0002 (6)
O24	0.0347 (9)	0.0323 (9)	0.0258 (8)	0.0136 (7)	0.0139 (7)	0.0023 (7)
C27	0.0262 (11)	0.0255 (12)	0.0263 (12)	−0.0016 (9)	0.0091 (9)	0.0097 (10)
C28A	0.037 (3)	0.023 (3)	0.046 (3)	−0.002 (2)	0.026 (3)	0.006 (2)
C29A	0.025 (2)	0.046 (3)	0.030 (2)	0.0026 (19)	0.0090 (17)	0.0064 (19)
C28B	0.048 (5)	0.030 (5)	0.074 (7)	−0.009 (4)	0.032 (5)	0.005 (4)
C29B	0.071 (7)	0.057 (7)	0.056 (6)	0.029 (5)	0.038 (5)	0.027 (5)
N25	0.0202 (9)	0.0184 (9)	0.0237 (9)	−0.0016 (7)	0.0092 (7)	0.0023 (7)
N26	0.0240 (9)	0.0181 (9)	0.0261 (10)	−0.0004 (7)	0.0087 (8)	0.0091 (8)
O25	0.0229 (8)	0.0273 (9)	0.0316 (9)	0.0030 (6)	0.0131 (7)	0.0133 (7)
O26	0.0350 (10)	0.0508 (12)	0.0836 (15)	0.0073 (9)	0.0318 (10)	0.0436 (11)
Co3	0.01981 (14)	0.01586 (15)	0.01406 (13)	−0.00134 (11)	0.00592 (11)	−0.00030 (11)
C31	0.0242 (11)	0.0177 (11)	0.0210 (11)	0.0031 (8)	0.0112 (9)	0.0008 (9)
C32	0.0232 (11)	0.0263 (13)	0.0364 (13)	0.0019 (9)	0.0105 (10)	0.0029 (11)
C33	0.0281 (12)	0.0290 (13)	0.0385 (14)	0.0047 (10)	0.0080 (11)	0.0036 (11)
N31	0.0192 (9)	0.0170 (9)	0.0218 (9)	−0.0017 (7)	0.0083 (7)	−0.0024 (7)
N32	0.0228 (9)	0.0165 (9)	0.0338 (11)	0.0016 (7)	0.0114 (8)	0.0106 (8)
O31	0.0218 (7)	0.0174 (8)	0.0230 (8)	−0.0014 (6)	0.0069 (6)	0.0045 (6)
O32	0.0230 (8)	0.0228 (8)	0.0405 (10)	0.0044 (6)	0.0102 (7)	0.0129 (7)
C34	0.0184 (10)	0.0177 (11)	0.0179 (10)	−0.0009 (8)	0.0044 (8)	0.0021 (8)
C35	0.0322 (12)	0.0294 (13)	0.0249 (12)	−0.0066 (10)	0.0143 (10)	−0.0018 (10)
C36	0.067 (2)	0.0451 (17)	0.0442 (16)	−0.0283 (15)	0.0321 (15)	−0.0064 (14)
N33	0.0190 (9)	0.0198 (9)	0.0175 (9)	−0.0005 (7)	0.0073 (7)	0.0001 (7)
N34	0.0207 (9)	0.0196 (9)	0.0151 (8)	−0.0043 (7)	0.0060 (7)	−0.0039 (7)
O33	0.0271 (8)	0.0171 (8)	0.0185 (7)	−0.0030 (6)	0.0106 (6)	−0.0023 (6)
O34	0.0301 (8)	0.0211 (8)	0.0238 (8)	−0.0081 (6)	0.0134 (7)	−0.0030 (6)
C37	0.0279 (11)	0.0140 (10)	0.0159 (10)	−0.0005 (8)	0.0098 (9)	0.0019 (8)
C38	0.0444 (14)	0.0210 (12)	0.0224 (12)	0.0116 (10)	0.0076 (10)	−0.0051 (9)
C39	0.066 (2)	0.0546 (19)	0.0579 (19)	0.0287 (16)	0.0427 (17)	0.0135 (15)
N35	0.0253 (9)	0.0170 (9)	0.0158 (9)	0.0012 (7)	0.0075 (7)	−0.0023 (7)
N36	0.0268 (9)	0.0194 (9)	0.0124 (8)	0.0020 (7)	0.0037 (7)	−0.0020 (7)
O35	0.0242 (8)	0.0211 (8)	0.0165 (7)	0.0015 (6)	0.0058 (6)	−0.0020 (6)
O36	0.0343 (8)	0.0216 (8)	0.0156 (7)	0.0056 (7)	0.0073 (6)	−0.0033 (6)
Co4	0.01871 (13)	0.01439 (14)	0.01511 (13)	−0.00110 (11)	0.00620 (10)	0.00028 (11)
C41	0.0229 (10)	0.0155 (11)	0.0195 (10)	−0.0011 (8)	0.0113 (9)	0.0016 (8)
C42	0.0270 (12)	0.0254 (12)	0.0272 (12)	0.0035 (9)	0.0033 (10)	0.0038 (10)
C43	0.0398 (14)	0.0334 (14)	0.0353 (14)	−0.0003 (11)	0.0144 (12)	0.0069 (11)
N41	0.0251 (9)	0.0184 (9)	0.0151 (8)	−0.0022 (7)	0.0045 (7)	0.0022 (7)
N42	0.0294 (10)	0.0174 (9)	0.0158 (9)	0.0024 (7)	0.0082 (7)	−0.0015 (7)
O41	0.0227 (7)	0.0165 (7)	0.0161 (7)	0.0007 (6)	0.0046 (6)	−0.0012 (6)
O42	0.0320 (9)	0.0224 (8)	0.0251 (8)	0.0077 (7)	0.0083 (7)	0.0000 (7)

C44	0.0220 (10)	0.0149 (10)	0.0136 (9)	−0.0015 (8)	0.0056 (8)	−0.0002 (8)
C45	0.0306 (12)	0.0251 (12)	0.0313 (12)	0.0074 (10)	0.0202 (10)	0.0103 (10)
C46	0.0279 (12)	0.0335 (14)	0.0456 (15)	−0.0024 (10)	0.0172 (11)	0.0005 (12)
N43	0.0164 (8)	0.0188 (9)	0.0229 (9)	−0.0025 (7)	0.0076 (7)	0.0004 (7)
N44	0.0197 (9)	0.0144 (9)	0.0256 (9)	0.0021 (7)	0.0079 (7)	0.0058 (7)
O43	0.0207 (7)	0.0153 (7)	0.0223 (7)	0.0026 (6)	0.0098 (6)	0.0037 (6)
O44	0.0262 (8)	0.0223 (8)	0.0320 (9)	0.0065 (6)	0.0165 (7)	0.0109 (7)
C47	0.0260 (11)	0.0146 (10)	0.0185 (10)	0.0017 (8)	0.0089 (9)	0.0014 (8)
C48	0.0501 (15)	0.0251 (13)	0.0299 (13)	−0.0159 (11)	0.0235 (12)	−0.0142 (10)
C49	0.0446 (16)	0.0543 (18)	0.0306 (14)	−0.0140 (14)	0.0093 (12)	−0.0127 (13)
N45	0.0215 (9)	0.0202 (9)	0.0168 (9)	−0.0043 (7)	0.0051 (7)	−0.0002 (7)
N46	0.0272 (10)	0.0261 (10)	0.0200 (9)	−0.0076 (8)	0.0135 (8)	−0.0017 (8)
O45	0.0244 (8)	0.0197 (8)	0.0184 (7)	−0.0039 (6)	0.0102 (6)	−0.0022 (6)
O46	0.0390 (9)	0.0257 (9)	0.0227 (8)	−0.0103 (7)	0.0175 (7)	−0.0076 (7)
N101	0.0186 (9)	0.0213 (10)	0.0221 (9)	0.0010 (7)	0.0036 (7)	0.0032 (8)
O101	0.0393 (9)	0.0202 (8)	0.0258 (8)	−0.0026 (7)	0.0127 (7)	−0.0041 (7)
O102	0.0286 (8)	0.0193 (8)	0.0440 (10)	−0.0059 (7)	0.0150 (8)	−0.0070 (7)
O103	0.0349 (9)	0.0356 (10)	0.0398 (10)	−0.0036 (8)	0.0228 (8)	0.0024 (8)
N111	0.0209 (9)	0.0216 (10)	0.0143 (8)	0.0002 (7)	0.0051 (7)	−0.0002 (7)
O111	0.0265 (8)	0.0320 (9)	0.0222 (8)	0.0034 (7)	0.0145 (7)	0.0000 (7)
O112	0.0393 (9)	0.0294 (9)	0.0262 (8)	−0.0013 (7)	0.0130 (7)	−0.0135 (7)
O113	0.0379 (10)	0.0431 (11)	0.0301 (9)	−0.0222 (8)	0.0164 (8)	−0.0077 (8)
N121	0.0283 (10)	0.0165 (9)	0.0255 (10)	−0.0026 (7)	0.0142 (8)	−0.0016 (8)
O121	0.0461 (10)	0.0280 (9)	0.0185 (8)	0.0046 (7)	0.0136 (7)	0.0045 (7)
O122	0.0283 (8)	0.0366 (9)	0.0201 (8)	−0.0070 (7)	0.0136 (7)	0.0014 (7)
O123	0.0242 (9)	0.0488 (11)	0.0411 (10)	−0.0059 (8)	0.0154 (8)	−0.0184 (9)
N131	0.0255 (9)	0.0242 (10)	0.0180 (9)	0.0040 (8)	0.0066 (8)	0.0015 (8)
O131	0.0254 (8)	0.0154 (8)	0.0249 (8)	0.0017 (6)	0.0091 (6)	0.0040 (6)
O132	0.0447 (10)	0.0223 (9)	0.0217 (8)	0.0014 (7)	0.0067 (7)	−0.0039 (7)
O133	0.0900 (17)	0.0707 (15)	0.0281 (11)	0.0559 (13)	−0.0240 (10)	−0.0135 (10)
N141	0.0210 (9)	0.0200 (9)	0.0140 (8)	0.0010 (7)	0.0045 (7)	−0.0004 (7)
O141	0.0264 (8)	0.0287 (9)	0.0214 (8)	0.0017 (7)	0.0135 (6)	−0.0008 (7)
O142	0.0413 (10)	0.0381 (10)	0.0332 (9)	−0.0223 (8)	0.0193 (8)	−0.0081 (8)
O143	0.0399 (9)	0.0294 (9)	0.0274 (9)	0.0006 (7)	0.0143 (7)	−0.0142 (7)
N151	0.0185 (8)	0.0210 (10)	0.0230 (9)	−0.0002 (7)	0.0039 (7)	0.0024 (8)
O151	0.0333 (9)	0.0206 (8)	0.0263 (8)	0.0001 (7)	0.0109 (7)	−0.0049 (7)
O152	0.0359 (9)	0.0189 (8)	0.0461 (10)	−0.0046 (7)	0.0226 (8)	−0.0044 (7)
O153	0.0350 (9)	0.0375 (10)	0.0450 (11)	−0.0077 (8)	0.0251 (8)	−0.0014 (8)
N161	0.0249 (9)	0.0199 (9)	0.0176 (9)	0.0018 (7)	0.0094 (7)	0.0007 (7)
O161	0.0263 (8)	0.0163 (8)	0.0206 (8)	0.0040 (6)	0.0062 (6)	−0.0006 (6)
O162	0.0542 (11)	0.0238 (9)	0.0220 (8)	0.0071 (8)	0.0130 (8)	−0.0060 (7)
O163	0.0557 (11)	0.0338 (10)	0.0195 (8)	0.0171 (9)	−0.0002 (8)	0.0043 (7)
N171	0.0213 (9)	0.0169 (9)	0.0180 (9)	−0.0040 (7)	0.0073 (7)	−0.0002 (7)
O171	0.0301 (8)	0.0249 (8)	0.0159 (7)	0.0016 (6)	0.0110 (6)	0.0056 (6)
O172	0.0189 (8)	0.0310 (9)	0.0282 (8)	−0.0003 (7)	0.0036 (6)	−0.0057 (7)
O173	0.0251 (8)	0.0311 (9)	0.0185 (7)	−0.0063 (7)	0.0114 (6)	−0.0001 (7)

Geometric parameters (Å, °)

Co1—O11	2.1005 (15)	Co3—N33	2.1582 (16)
Co1—O15	2.1172 (15)	C31—O31	1.237 (2)
Co1—O13	2.1179 (14)	C31—O32	1.329 (2)
Co1—N13	2.1236 (17)	C31—N32	1.334 (3)
Co1—N15	2.1460 (17)	C32—O32	1.465 (3)
Co1—N11	2.1649 (17)	C32—C33	1.492 (3)
C11—O11	1.236 (3)	C32—H32A	0.9900
C11—O12	1.338 (3)	C32—H32B	0.9900
C11—N12	1.345 (3)	C33—H33A	0.9800
C12—O12	1.461 (3)	C33—H33B	0.9800
C12—C13	1.471 (4)	C33—H33C	0.9800
C12—H12A	0.9900	N31—N32	1.411 (2)
C12—H12B	0.9900	N31—H31A	0.9200
C13—H13A	0.9800	N31—H31B	0.9200
C13—H13B	0.9800	N32—H32	0.8800
C13—H13C	0.9800	C34—O33	1.236 (2)
N11—N12	1.421 (2)	C34—O34	1.329 (2)
N11—H11A	0.9200	C34—N34	1.348 (2)
N11—H11B	0.9200	C35—O34	1.458 (2)
N12—H12	0.8800	C35—C36	1.503 (3)
C14—O13	1.249 (2)	C35—H35A	0.9900
C14—N14	1.324 (3)	C35—H35B	0.9900
C14—O14	1.332 (2)	C36—H36A	0.9800
C15—O14	1.451 (3)	C36—H36B	0.9800
C15—C16	1.505 (3)	C36—H36C	0.9800
C15—H15A	0.9900	N33—N34	1.421 (2)
C15—H15B	0.9900	N33—H33D	0.9200
C16—H16A	0.9800	N33—H33E	0.9200
C16—H16B	0.9800	N34—H34	0.8800
C16—H16C	0.9800	C37—O35	1.240 (2)
N13—N14	1.413 (2)	C37—N36	1.329 (3)
N13—H13D	0.9200	C37—O36	1.338 (2)
N13—H13E	0.9200	C38—O36	1.457 (2)
N14—H14	0.8800	C38—C39	1.498 (4)
C17—O15	1.238 (3)	C38—H38A	0.9900
C17—N16	1.326 (3)	C38—H38B	0.9900
C17—O16	1.331 (2)	C39—H39A	0.9800
C18A—O16	1.441 (3)	C39—H39B	0.9800
C18A—C19A	1.497 (7)	C39—H39C	0.9800
C18A—H18A	0.9900	N35—N36	1.417 (2)
C18A—H18B	0.9900	N35—H35C	0.9200
C19A—H19A	0.9800	N35—H35D	0.9200
C19A—H19B	0.9800	N36—H36	0.8800
C19A—H19C	0.9800	Co4—O41	2.1063 (14)
C18B—C19B	1.488 (17)	Co4—O43	2.1064 (14)
C18B—O16	1.619 (9)	Co4—O45	2.1297 (14)

C18B—H18C	0.9900	Co4—N45	2.1338 (16)
C18B—H18D	0.9900	Co4—N43	2.1450 (17)
C19B—H19D	0.9800	Co4—N41	2.1671 (17)
C19B—H19E	0.9800	C41—O41	1.237 (2)
C19B—H19F	0.9800	C41—N42	1.334 (3)
N15—N16	1.416 (2)	C41—O42	1.334 (2)
N15—H15C	0.9200	C42—O42	1.457 (3)
N15—H15D	0.9200	C42—C43	1.501 (3)
N16—H16	0.8800	C42—H42A	0.9900
Co2—O25	2.0853 (14)	C42—H42B	0.9900
Co2—O23	2.1090 (14)	C43—H43A	0.9800
Co2—N21	2.1240 (17)	C43—H43B	0.9800
Co2—O21	2.1270 (14)	C43—H43C	0.9800
Co2—N25	2.1534 (17)	N41—N42	1.420 (2)
Co2—N23	2.1678 (17)	N41—H41A	0.9200
C21—O21	1.239 (2)	N41—H41B	0.9200
C21—O22	1.331 (2)	N42—H42	0.8800
C21—N22	1.335 (3)	C44—O43	1.243 (2)
C22—O22	1.455 (3)	C44—O44	1.328 (2)
C22—C23	1.504 (4)	C44—N44	1.328 (3)
C22—H22A	0.9900	C45—O44	1.460 (2)
C22—H22B	0.9900	C45—C46	1.500 (3)
C23—H23A	0.9800	C45—H45A	0.9900
C23—H23B	0.9800	C45—H45B	0.9900
C23—H23C	0.9800	C46—H46A	0.9800
N21—N22	1.413 (2)	C46—H46B	0.9800
N21—H21A	0.9200	C46—H46C	0.9800
N21—H21B	0.9200	N43—N44	1.415 (2)
N22—H22	0.8800	N43—H43D	0.9200
C24—O23	1.235 (2)	N43—H43E	0.9200
C24—N24	1.332 (3)	N44—H44	0.8800
C24—O24	1.338 (2)	C47—O45	1.237 (2)
C25—O24	1.461 (3)	C47—O46	1.332 (2)
C25—C26	1.499 (3)	C47—N46	1.340 (3)
C25—H25A	0.9900	C48—O46	1.456 (3)
C25—H25B	0.9900	C48—C49	1.504 (4)
C26—H26A	0.9800	C48—H48A	0.9900
C26—H26B	0.9800	C48—H48B	0.9900
C26—H26C	0.9800	C49—H49A	0.9800
N23—N24	1.421 (2)	C49—H49B	0.9800
N23—H23D	0.9200	C49—H49C	0.9800
N23—H23E	0.9200	N45—N46	1.417 (2)
N24—H24	0.8800	N45—H45C	0.9200
C27—O25	1.246 (3)	N45—H45D	0.9200
C27—N26	1.320 (3)	N46—H46	0.8800
C27—O26	1.324 (3)	N101—O103	1.241 (2)
C28A—C29A	1.502 (7)	N101—O102	1.261 (2)
C28A—O26	1.524 (6)	N101—O101	1.267 (2)
C28A—H28A	0.9900	N111—O113	1.248 (2)

C28A—H28B	0.9900	N111—O112	1.252 (2)
C29A—H29A	0.9800	N111—O111	1.258 (2)
C29A—H29B	0.9800	N121—O122	1.249 (2)
C29A—H29C	0.9800	N121—O123	1.250 (2)
C28B—C29B	1.440 (14)	N121—O121	1.260 (2)
C28B—O26	1.476 (8)	N131—O133	1.216 (2)
C28B—H28C	0.9900	N131—O132	1.247 (2)
C28B—H28D	0.9900	N131—O131	1.273 (2)
C29B—H29D	0.9800	N141—O143	1.245 (2)
C29B—H29E	0.9800	N141—O142	1.251 (2)
C29B—H29F	0.9800	N141—O141	1.261 (2)
N25—N26	1.418 (2)	N151—O153	1.242 (2)
N25—H25C	0.9200	N151—O152	1.261 (2)
N25—H25D	0.9200	N151—O151	1.261 (2)
N26—H26	0.8800	N161—O163	1.238 (2)
Co3—O33	2.0896 (14)	N161—O162	1.248 (2)
Co3—O35	2.1062 (14)	N161—O161	1.277 (2)
Co3—O31	2.1112 (14)	N171—O173	1.251 (2)
Co3—N35	2.1285 (17)	N171—O172	1.252 (2)
Co3—N31	2.1515 (16)	N171—O171	1.263 (2)
O11—Co1—O15	88.32 (6)	O35—Co3—N31	89.28 (6)
O11—Co1—O13	95.73 (6)	O31—Co3—N31	78.37 (6)
O15—Co1—O13	94.30 (6)	N35—Co3—N31	96.84 (7)
O11—Co1—N13	98.24 (6)	O33—Co3—N33	78.13 (6)
O15—Co1—N13	170.86 (7)	O35—Co3—N33	171.95 (6)
O13—Co1—N13	78.78 (6)	O31—Co3—N33	90.41 (6)
O11—Co1—N15	164.39 (6)	N35—Co3—N33	97.01 (6)
O15—Co1—N15	77.65 (6)	N31—Co3—N33	98.17 (6)
O13—Co1—N15	92.16 (6)	O31—C31—O32	123.81 (19)
N13—Co1—N15	96.49 (7)	O31—C31—N32	123.95 (19)
O11—Co1—N11	77.60 (6)	O32—C31—N32	112.24 (18)
O15—Co1—N11	93.69 (7)	O32—C32—C33	106.73 (18)
O13—Co1—N11	169.43 (6)	O32—C32—H32A	110.4
N13—Co1—N11	93.93 (6)	C33—C32—H32A	110.4
N15—Co1—N11	96.30 (6)	O32—C32—H32B	110.4
O11—C11—O12	124.4 (2)	C33—C32—H32B	110.4
O11—C11—N12	123.98 (19)	H32A—C32—H32B	108.6
O12—C11—N12	111.50 (19)	C32—C33—H33A	109.5
O12—C12—C13	109.4 (2)	C32—C33—H33B	109.5
O12—C12—H12A	109.8	H33A—C33—H33B	109.5
C13—C12—H12A	109.8	C32—C33—H33C	109.5
O12—C12—H12B	109.8	H33A—C33—H33C	109.5
C13—C12—H12B	109.8	H33B—C33—H33C	109.5
H12A—C12—H12B	108.2	N32—N31—Co3	107.42 (11)
C12—C13—H13A	109.5	N32—N31—H31A	110.2
C12—C13—H13B	109.5	Co3—N31—H31A	110.2
H13A—C13—H13B	109.5	N32—N31—H31B	110.2
C12—C13—H13C	109.5	Co3—N31—H31B	110.2
H13A—C13—H13C	109.5	H31A—N31—H31B	108.5

H13B—C13—H13C	109.5	C31—N32—N31	117.87 (17)
N12—N11—Co1	106.45 (11)	C31—N32—H32	121.1
N12—N11—H11A	110.4	N31—N32—H32	121.1
Co1—N11—H11A	110.4	C31—O31—Co3	112.10 (13)
N12—N11—H11B	110.4	C31—O32—C32	116.51 (17)
Co1—N11—H11B	110.4	O33—C34—O34	123.49 (18)
H11A—N11—H11B	108.6	O33—C34—N34	124.04 (18)
C11—N12—N11	115.54 (17)	O34—C34—N34	112.44 (17)
C11—N12—H12	122.2	O34—C35—C36	107.14 (18)
N11—N12—H12	122.2	O34—C35—H35A	110.3
C11—O11—Co1	112.30 (13)	C36—C35—H35A	110.3
C11—O12—C12	116.64 (19)	O34—C35—H35B	110.3
O13—C14—N14	124.03 (19)	C36—C35—H35B	110.3
O13—C14—O14	124.05 (19)	H35A—C35—H35B	108.5
N14—C14—O14	111.92 (18)	C35—C36—H36A	109.5
O14—C15—C16	111.8 (2)	C35—C36—H36B	109.5
O14—C15—H15A	109.2	H36A—C36—H36B	109.5
C16—C15—H15A	109.2	C35—C36—H36C	109.5
O14—C15—H15B	109.2	H36A—C36—H36C	109.5
C16—C15—H15B	109.2	H36B—C36—H36C	109.5
H15A—C15—H15B	107.9	N34—N33—Co3	106.00 (11)
C15—C16—H16A	109.5	N34—N33—H33D	110.5
C15—C16—H16B	109.5	Co3—N33—H33D	110.5
H16A—C16—H16B	109.5	N34—N33—H33E	110.5
C15—C16—H16C	109.5	Co3—N33—H33E	110.5
H16A—C16—H16C	109.5	H33D—N33—H33E	108.7
H16B—C16—H16C	109.5	C34—N34—N33	115.09 (16)
N14—N13—Co1	107.63 (12)	C34—N34—H34	122.5
N14—N13—H13D	110.2	N33—N34—H34	122.5
Co1—N13—H13D	110.2	C34—O33—Co3	112.04 (13)
N14—N13—H13E	110.2	C34—O34—C35	114.64 (16)
Co1—N13—H13E	110.2	O35—C37—N36	124.28 (18)
H13D—N13—H13E	108.5	O35—C37—O36	124.02 (18)
C14—N14—N13	117.82 (17)	N36—C37—O36	111.71 (17)
C14—N14—H14	121.1	O36—C38—C39	111.58 (19)
N13—N14—H14	121.1	O36—C38—H38A	109.3
C14—O13—Co1	110.88 (13)	C39—C38—H38A	109.3
C14—O14—C15	117.57 (17)	O36—C38—H38B	109.3
O15—C17—N16	123.5 (2)	C39—C38—H38B	109.3
O15—C17—O16	124.41 (19)	H38A—C38—H38B	108.0
N16—C17—O16	112.09 (19)	C38—C39—H39A	109.5
O16—C18A—C19A	106.6 (4)	C38—C39—H39B	109.5
O16—C18A—H18A	110.4	H39A—C39—H39B	109.5
C19A—C18A—H18A	110.4	C38—C39—H39C	109.5
O16—C18A—H18B	110.4	H39A—C39—H39C	109.5
C19A—C18A—H18B	110.4	H39B—C39—H39C	109.5
H18A—C18A—H18B	108.6	N36—N35—Co3	107.03 (12)
C19B—C18B—O16	102.1 (9)	N36—N35—H35C	110.3
C19B—C18B—H18C	111.3	Co3—N35—H35C	110.3

O16—C18B—H18C	111.3	N36—N35—H35D	110.3
C19B—C18B—H18D	111.3	Co3—N35—H35D	110.3
O16—C18B—H18D	111.3	H35C—N35—H35D	108.6
H18C—C18B—H18D	109.2	C37—N36—N35	117.52 (16)
C18B—C19B—H19D	109.5	C37—N36—H36	121.2
C18B—C19B—H19E	109.5	N35—N36—H36	121.2
H19D—C19B—H19E	109.5	C37—O35—Co3	111.03 (13)
C18B—C19B—H19F	109.5	C37—O36—C38	116.65 (16)
H19D—C19B—H19F	109.5	O41—Co4—O43	95.82 (5)
H19E—C19B—H19F	109.5	O41—Co4—O45	90.00 (5)
N16—N15—Co1	108.32 (11)	O43—Co4—O45	101.36 (5)
N16—N15—H15C	110.0	O41—Co4—N45	92.21 (6)
Co1—N15—H15C	110.0	O43—Co4—N45	171.97 (6)
N16—N15—H15D	110.0	O45—Co4—N45	78.47 (6)
Co1—N15—H15D	110.0	O41—Co4—N43	172.67 (6)
H15C—N15—H15D	108.4	O43—Co4—N43	77.72 (6)
C17—N16—N15	117.57 (17)	O45—Co4—N43	87.92 (6)
C17—N16—H16	121.2	N45—Co4—N43	94.26 (6)
N15—N16—H16	121.2	O41—Co4—N41	78.01 (6)
C17—O15—Co1	112.92 (13)	O43—Co4—N41	88.05 (6)
C17—O16—C18A	118.95 (19)	O45—Co4—N41	165.52 (6)
C17—O16—C18B	111.1 (3)	N45—Co4—N41	93.75 (6)
C18A—O16—C18B	32.9 (3)	N43—Co4—N41	104.96 (6)
O25—Co2—O23	93.27 (6)	O41—C41—N42	123.83 (19)
O25—Co2—N21	173.50 (7)	O41—C41—O42	124.59 (19)
O23—Co2—N21	92.03 (6)	N42—C41—O42	111.56 (17)
O25—Co2—O21	97.26 (6)	O42—C42—C43	108.87 (19)
O23—Co2—O21	91.76 (6)	O42—C42—H42A	109.9
N21—Co2—O21	78.81 (6)	C43—C42—H42A	109.9
O25—Co2—N25	78.02 (6)	O42—C42—H42B	109.9
O23—Co2—N25	171.23 (6)	C43—C42—H42B	109.9
N21—Co2—N25	96.59 (7)	H42A—C42—H42B	108.3
O21—Co2—N25	88.33 (6)	C42—C43—H43A	109.5
O25—Co2—N23	90.66 (6)	C42—C43—H43B	109.5
O23—Co2—N23	78.05 (6)	H43A—C43—H43B	109.5
N21—Co2—N23	94.11 (7)	C42—C43—H43C	109.5
O21—Co2—N23	167.46 (6)	H43A—C43—H43C	109.5
N25—Co2—N23	102.87 (7)	H43B—C43—H43C	109.5
O21—C21—O22	124.25 (19)	N42—N41—Co4	107.05 (11)
O21—C21—N22	124.23 (19)	N42—N41—H41A	110.3
O22—C21—N22	111.52 (18)	Co4—N41—H41A	110.3
O22—C22—C23	111.2 (2)	N42—N41—H41B	110.3
O22—C22—H22A	109.4	Co4—N41—H41B	110.3
C23—C22—H22A	109.4	H41A—N41—H41B	108.6
O22—C22—H22B	109.4	C41—N42—N41	117.56 (16)
C23—C22—H22B	109.4	C41—N42—H42	121.2
H22A—C22—H22B	108.0	N41—N42—H42	121.2
C22—C23—H23A	109.5	C41—O41—Co4	112.77 (13)
C22—C23—H23B	109.5	C41—O42—C42	118.33 (17)

H23A—C23—H23B	109.5	O43—C44—O44	124.08 (18)
C22—C23—H23C	109.5	O43—C44—N44	123.88 (18)
H23A—C23—H23C	109.5	O44—C44—N44	112.04 (17)
H23B—C23—H23C	109.5	O44—C45—C46	111.80 (18)
N22—N21—Co2	108.10 (12)	O44—C45—H45A	109.3
N22—N21—H21A	110.1	C46—C45—H45A	109.3
Co2—N21—H21A	110.1	O44—C45—H45B	109.3
N22—N21—H21B	110.1	C46—C45—H45B	109.3
Co2—N21—H21B	110.1	H45A—C45—H45B	107.9
H21A—N21—H21B	108.4	C45—C46—H46A	109.5
C21—N22—N21	117.67 (16)	C45—C46—H46B	109.5
C21—N22—H22	121.2	H46A—C46—H46B	109.5
N21—N22—H22	121.2	C45—C46—H46C	109.5
C21—O21—Co2	111.03 (13)	H46A—C46—H46C	109.5
C21—O22—C22	117.05 (16)	H46B—C46—H46C	109.5
O23—C24—N24	124.32 (19)	N44—N43—Co4	108.77 (11)
O23—C24—O24	123.81 (19)	N44—N43—H43D	109.9
N24—C24—O24	111.84 (18)	Co4—N43—H43D	109.9
O24—C25—C26	109.86 (19)	N44—N43—H43E	109.9
O24—C25—H25A	109.7	Co4—N43—H43E	109.9
C26—C25—H25A	109.7	H43D—N43—H43E	108.3
O24—C25—H25B	109.7	C44—N44—N43	116.73 (16)
C26—C25—H25B	109.7	C44—N44—H44	121.6
H25A—C25—H25B	108.2	N43—N44—H44	121.6
C25—C26—H26A	109.5	C44—O43—Co4	112.87 (12)
C25—C26—H26B	109.5	C44—O44—C45	116.64 (16)
H26A—C26—H26B	109.5	O45—C47—O46	124.43 (19)
C25—C26—H26C	109.5	O45—C47—N46	124.01 (19)
H26A—C26—H26C	109.5	O46—C47—N46	111.57 (18)
H26B—C26—H26C	109.5	O46—C48—C49	111.5 (2)
N24—N23—Co2	107.04 (11)	O46—C48—H48A	109.3
N24—N23—H23D	110.3	C49—C48—H48A	109.3
Co2—N23—H23D	110.3	O46—C48—H48B	109.3
N24—N23—H23E	110.3	C49—C48—H48B	109.3
Co2—N23—H23E	110.3	H48A—C48—H48B	108.0
H23D—N23—H23E	108.6	C48—C49—H49A	109.5
C24—N24—N23	117.26 (16)	C48—C49—H49B	109.5
C24—N24—H24	121.4	H49A—C49—H49B	109.5
N23—N24—H24	121.4	C48—C49—H49C	109.5
C24—O23—Co2	112.50 (13)	H49A—C49—H49C	109.5
C24—O24—C25	117.56 (17)	H49B—C49—H49C	109.5
O25—C27—N26	124.0 (2)	N46—N45—Co4	108.25 (11)
O25—C27—O26	123.7 (2)	N46—N45—H45C	110.0
N26—C27—O26	112.28 (19)	Co4—N45—H45C	110.0
C29A—C28A—O26	105.3 (4)	N46—N45—H45D	110.0
C29A—C28A—H28A	110.7	Co4—N45—H45D	110.0
O26—C28A—H28A	110.7	H45C—N45—H45D	108.4
C29A—C28A—H28B	110.7	C47—N46—N45	117.52 (16)
O26—C28A—H28B	110.7	C47—N46—H46	121.2

H28A—C28A—H28B	108.8	N45—N46—H46	121.2
C29B—C28B—O26	96.2 (7)	C47—O45—Co4	111.73 (13)
C29B—C28B—H28C	112.5	C47—O46—C48	116.51 (16)
O26—C28B—H28C	112.5	O103—N101—O102	120.49 (18)
C29B—C28B—H28D	112.5	O103—N101—O101	120.18 (18)
O26—C28B—H28D	112.5	O102—N101—O101	119.32 (17)
H28C—C28B—H28D	110.0	O113—N111—O112	120.81 (17)
N26—N25—Co2	107.93 (12)	O113—N111—O111	119.44 (17)
N26—N25—H25C	110.1	O112—N111—O111	119.74 (17)
Co2—N25—H25C	110.1	O122—N121—O123	120.79 (18)
N26—N25—H25D	110.1	O122—N121—O121	120.60 (18)
Co2—N25—H25D	110.1	O123—N121—O121	118.61 (18)
H25C—N25—H25D	108.4	O133—N131—O132	121.02 (19)
C27—N26—N25	116.92 (17)	O133—N131—O131	119.27 (18)
C27—N26—H26	121.5	O132—N131—O131	119.70 (17)
N25—N26—H26	121.5	O143—N141—O142	120.88 (17)
C27—O25—Co2	113.10 (13)	O143—N141—O141	119.85 (17)
C27—O26—C28B	117.6 (4)	O142—N141—O141	119.26 (17)
C27—O26—C28A	114.9 (3)	O153—N151—O152	120.41 (18)
C28B—O26—C28A	34.7 (4)	O153—N151—O151	120.42 (18)
O33—Co3—O35	95.25 (5)	O152—N151—O151	119.17 (17)
O33—Co3—O31	89.16 (5)	O163—N161—O162	121.33 (18)
O35—Co3—O31	94.10 (5)	O163—N161—O161	119.76 (17)
O33—Co3—N35	95.97 (6)	O162—N161—O161	118.91 (17)
O35—Co3—N35	78.98 (6)	O173—N171—O172	120.72 (17)
O31—Co3—N35	171.71 (6)	O173—N171—O171	120.05 (16)
O33—Co3—N31	167.01 (6)	O172—N171—O171	119.23 (16)
O11—Co1—N11—N12	−16.86 (11)	O25—C27—O26—C28A	−19.3 (4)
O15—Co1—N11—N12	70.60 (12)	N26—C27—O26—C28A	160.2 (3)
O13—Co1—N11—N12	−68.5 (4)	C29B—C28B—O26—C27	−91.4 (7)
N13—Co1—N11—N12	−114.45 (12)	C29B—C28B—O26—C28A	3.3 (6)
N15—Co1—N11—N12	148.57 (12)	C29A—C28A—O26—C27	133.8 (3)
O11—C11—N12—N11	−13.1 (3)	C29A—C28A—O26—C28B	30.7 (6)
O12—C11—N12—N11	170.23 (16)	O33—Co3—N31—N32	−20.7 (3)
Co1—N11—N12—C11	21.0 (2)	O35—Co3—N31—N32	89.93 (12)
O12—C11—O11—Co1	172.74 (16)	O31—Co3—N31—N32	−4.40 (12)
N12—C11—O11—Co1	−3.6 (3)	N35—Co3—N31—N32	168.74 (12)
O15—Co1—O11—C11	−82.34 (15)	N33—Co3—N31—N32	−93.13 (13)
O13—Co1—O11—C11	−176.49 (14)	O31—C31—N32—N31	−0.8 (3)
N13—Co1—O11—C11	104.05 (15)	O32—C31—N32—N31	179.09 (17)
N15—Co1—O11—C11	−56.5 (3)	Co3—N31—N32—C31	4.4 (2)
N11—Co1—O11—C11	11.81 (14)	O32—C31—O31—Co3	176.67 (16)
O11—C11—O12—C12	4.3 (3)	N32—C31—O31—Co3	−3.4 (3)
N12—C11—O12—C12	−178.97 (19)	O33—Co3—O31—C31	−179.30 (14)
C13—C12—O12—C11	86.4 (3)	O35—Co3—O31—C31	−84.10 (14)
O11—Co1—N13—N14	102.08 (13)	N31—Co3—O31—C31	4.32 (14)
O13—Co1—N13—N14	7.83 (12)	N33—Co3—O31—C31	102.58 (14)
N15—Co1—N13—N14	−83.09 (13)	O31—C31—O32—C32	4.2 (3)
N11—Co1—N13—N14	−179.90 (13)	N32—C31—O32—C32	−175.75 (18)

O13—C14—N14—N13	2.4 (3)	C33—C32—O32—C31	−163.38 (19)
O14—C14—N14—N13	−176.86 (17)	O33—Co3—N33—N34	−17.32 (11)
Co1—N13—N14—C14	−8.2 (2)	O31—Co3—N33—N34	71.73 (12)
N14—C14—O13—Co1	5.1 (3)	N35—Co3—N33—N34	−111.98 (12)
O14—C14—O13—Co1	−175.76 (16)	N31—Co3—N33—N34	150.03 (11)
O11—Co1—O13—C14	−104.45 (14)	O33—C34—N34—N33	−17.1 (3)
O15—Co1—O13—C14	166.81 (14)	O34—C34—N34—N33	164.95 (16)
N13—Co1—O13—C14	−7.15 (14)	Co3—N33—N34—C34	23.07 (19)
N15—Co1—O13—C14	89.04 (14)	O34—C34—O33—Co3	177.68 (15)
N11—Co1—O13—C14	−54.2 (4)	N34—C34—O33—Co3	0.0 (2)
O13—C14—O14—C15	4.9 (3)	O35—Co3—O33—C34	−174.28 (13)
N14—C14—O14—C15	−175.89 (18)	O31—Co3—O33—C34	−80.24 (14)
C16—C15—O14—C14	−80.9 (2)	N35—Co3—O33—C34	106.29 (14)
O11—Co1—N15—N16	−28.4 (3)	N31—Co3—O33—C34	−64.3 (3)
O15—Co1—N15—N16	−1.97 (12)	N33—Co3—O33—C34	10.36 (13)
O13—Co1—N15—N16	91.97 (12)	O33—C34—O34—C35	3.4 (3)
N13—Co1—N15—N16	170.92 (12)	N34—C34—O34—C35	−178.67 (17)
N11—Co1—N15—N16	−94.38 (13)	C36—C35—O34—C34	174.7 (2)
O15—C17—N16—N15	−1.3 (3)	O33—Co3—N35—N36	103.27 (12)
O16—C17—N16—N15	177.74 (17)	O35—Co3—N35—N36	9.06 (12)
Co1—N15—N16—C17	2.4 (2)	N31—Co3—N35—N36	−78.86 (12)
N16—C17—O15—Co1	−0.6 (3)	N33—Co3—N35—N36	−178.01 (12)
O16—C17—O15—Co1	−179.56 (17)	O35—C37—N36—N35	2.9 (3)
O11—Co1—O15—C17	174.60 (16)	O36—C37—N36—N35	−177.45 (16)
O13—Co1—O15—C17	−89.78 (16)	Co3—N35—N36—C37	−9.5 (2)
N15—Co1—O15—C17	1.49 (15)	N36—C37—O35—Co3	5.8 (2)
N11—Co1—O15—C17	97.14 (16)	O36—C37—O35—Co3	−173.81 (15)
O15—C17—O16—C18A	−17.9 (4)	O33—Co3—O35—C37	−103.34 (14)
N16—C17—O16—C18A	163.1 (3)	O31—Co3—O35—C37	167.13 (13)
O15—C17—O16—C18B	17.6 (6)	N35—Co3—O35—C37	−8.27 (13)
N16—C17—O16—C18B	−161.5 (5)	N31—Co3—O35—C37	88.85 (14)
C19A—C18A—O16—C17	140.5 (4)	O35—C37—O36—C38	8.9 (3)
C19A—C18A—O16—C18B	56.0 (7)	N36—C37—O36—C38	−170.72 (17)
C19B—C18B—O16—C17	−166.6 (8)	C39—C38—O36—C37	−89.8 (2)
C19B—C18B—O16—C18A	−55.6 (9)	O41—Co4—N41—N42	7.45 (11)
O23—Co2—N21—N22	−93.57 (13)	O43—Co4—N41—N42	−88.92 (12)
O21—Co2—N21—N22	−2.18 (12)	O45—Co4—N41—N42	42.1 (3)
N25—Co2—N21—N22	84.79 (13)	N45—Co4—N41—N42	98.91 (12)
N23—Co2—N21—N22	−171.73 (13)	N43—Co4—N41—N42	−165.67 (11)
O21—C21—N22—N21	2.6 (3)	O41—C41—N42—N41	3.9 (3)
O22—C21—N22—N21	−177.79 (17)	O42—C41—N42—N41	−177.95 (16)
Co2—N21—N22—C21	0.8 (2)	Co4—N41—N42—C41	−8.5 (2)
O22—C21—O21—Co2	175.97 (16)	N42—C41—O41—Co4	3.5 (2)
N22—C21—O21—Co2	−4.5 (3)	O42—C41—O41—Co4	−174.43 (15)
O25—Co2—O21—C21	−171.25 (14)	O43—Co4—O41—C41	80.55 (14)
O23—Co2—O21—C21	95.22 (14)	O45—Co4—O41—C41	−178.03 (13)
N21—Co2—O21—C21	3.50 (14)	N45—Co4—O41—C41	−99.58 (14)
N25—Co2—O21—C21	−93.55 (14)	N41—Co4—O41—C41	−6.21 (13)
N23—Co2—O21—C21	60.0 (3)	O41—C41—O42—C42	−9.6 (3)

O21—C21—O22—C22	−5.7 (3)	N42—C41—O42—C42	172.28 (17)
N22—C21—O22—C22	174.70 (18)	C43—C42—O42—C41	−106.3 (2)
C23—C22—O22—C21	89.1 (2)	O43—Co4—N43—N44	−0.61 (12)
O25—Co2—N23—N24	−85.66 (12)	O45—Co4—N43—N44	−102.70 (12)
O23—Co2—N23—N24	7.55 (11)	N45—Co4—N43—N44	179.03 (12)
N21—Co2—N23—N24	98.75 (12)	N41—Co4—N43—N44	83.99 (13)
O21—Co2—N23—N24	43.7 (3)	O43—C44—N44—N43	1.4 (3)
N25—Co2—N23—N24	−163.52 (12)	O44—C44—N44—N43	−178.36 (16)
O23—C24—N24—N23	6.2 (3)	Co4—N43—N44—C44	−0.1 (2)
O24—C24—N24—N23	−175.75 (16)	O44—C44—O43—Co4	177.82 (15)
Co2—N23—N24—C24	−9.6 (2)	N44—C44—O43—Co4	−2.0 (2)
N24—C24—O23—Co2	1.4 (3)	O41—Co4—O43—C44	177.81 (13)
O24—C24—O23—Co2	−176.45 (15)	O45—Co4—O43—C44	86.64 (13)
O25—Co2—O23—C24	84.79 (14)	N43—Co4—O43—C44	1.32 (13)
N21—Co2—O23—C24	−98.98 (14)	N41—Co4—O43—C44	−104.45 (14)
O21—Co2—O23—C24	−177.84 (14)	O43—C44—O44—C45	−7.6 (3)
N23—Co2—O23—C24	−5.20 (14)	N44—C44—O44—C45	172.22 (17)
O23—C24—O24—C25	−6.5 (3)	C46—C45—O44—C44	79.3 (2)
N24—C24—O24—C25	175.49 (18)	O41—Co4—N45—N46	−90.76 (13)
C26—C25—O24—C24	−88.9 (2)	O45—Co4—N45—N46	−1.21 (12)
O25—Co2—N25—N26	−1.47 (12)	N43—Co4—N45—N46	85.79 (13)
N21—Co2—N25—N26	−177.79 (12)	N41—Co4—N45—N46	−168.88 (13)
O21—Co2—N25—N26	−99.25 (13)	O45—C47—N46—N45	−1.7 (3)
N23—Co2—N25—N26	86.45 (13)	O46—C47—N46—N45	178.43 (17)
O25—C27—N26—N25	−2.8 (3)	Co4—N45—N46—C47	1.9 (2)
O26—C27—N26—N25	177.69 (19)	O46—C47—O45—Co4	−179.68 (16)
Co2—N25—N26—C27	2.6 (2)	N46—C47—O45—Co4	0.5 (3)
N26—C27—O25—Co2	1.3 (3)	O41—Co4—O45—C47	92.72 (14)
O26—C27—O25—Co2	−179.3 (2)	O43—Co4—O45—C47	−171.34 (14)
O23—Co2—O25—C27	179.18 (16)	N45—Co4—O45—C47	0.47 (14)
O21—Co2—O25—C27	86.99 (16)	N43—Co4—O45—C47	−94.30 (14)
N25—Co2—O25—C27	0.26 (16)	N41—Co4—O45—C47	58.9 (3)
N23—Co2—O25—C27	−102.76 (16)	O45—C47—O46—C48	−5.5 (3)
O25—C27—O26—C28B	19.5 (6)	N46—C47—O46—C48	174.34 (18)
N26—C27—O26—C28B	−161.0 (5)	C49—C48—O46—C47	84.0 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11A···O152	0.92	2.40	3.166 (2)	140
N11—H11A···O163	0.92	2.60	3.111 (2)	116
N11—H11A···O171	0.92	2.64	3.188 (2)	119
N11—H11B···O142	0.92	2.19	3.028 (2)	151
N12—H12···O172	0.88	2.19	2.931 (2)	141
N13—H13D···O151	0.92	2.10	2.947 (2)	153
N13—H13D···O152	0.92	2.40	3.155 (2)	139
N13—H13E···O162	0.92	2.12	3.016 (2)	166
N13—H13E···O163	0.92	2.64	3.395 (3)	140
N14—H14···O131^{i}	0.88	2.09	2.939 (2)	161

N14—H14···O132^{i}	0.88	2.33	3.053 (2)	140
N15—H15C···O143	0.92	2.14	2.968 (2)	149
N15—H15C···O151	0.92	2.45	2.984 (2)	117
N15—H15D···O161^{ii}	0.92	2.06	2.982 (2)	176
N15—H15D···O163^{ii}	0.92	2.66	3.307 (2)	128
N16—H16···O171^{ii}	0.88	2.09	2.889 (2)	151
N21—H21A···O101^{iii}	0.92	2.28	3.013 (2)	137
N21—H21A···O103^{iii}	0.92	2.43	3.336 (2)	167
N21—H21B···O121	0.92	2.10	2.939 (2)	151
N21—H21B···O112^{iii}	0.92	2.44	2.979 (2)	117
N22—H22···O131	0.88	2.05	2.907 (2)	164
N23—H23D···O113^{iv}	0.92	2.26	3.166 (2)	169
N23—H23D···O111^{iv}	0.92	2.39	3.121 (2)	136
N23—H23E···O111^{iii}	0.92	2.34	3.141 (2)	146
N23—H23E···O112^{iii}	0.92	2.64	3.496 (2)	156
N24—H24···O122^{iv}	0.88	2.16	2.852 (2)	135
N25—H25C···O102	0.92	2.12	3.038 (2)	176
N25—H25C···O103	0.92	2.57	3.243 (2)	130
N25—H25D···O122	0.92	2.02	2.924 (2)	169
N26—H26···O111	0.88	2.25	3.043 (2)	150
N31—H31A···O112	0.92	2.12	2.970 (2)	153
N31—H31A···O101	0.92	2.63	3.152 (2)	116
N31—H31B···O131^{ii}	0.92	2.16	3.073 (2)	175
N31—H31B···O133^{ii}	0.92	2.61	3.303 (3)	133
N32—H32···O121^{ii}	0.88	2.26	2.992 (2)	141
N32—H32···O123^{ii}	0.88	2.42	3.234 (3)	154
N33—H33D···O102	0.92	2.31	3.083 (2)	142
N33—H33E···O113	0.92	2.25	3.071 (2)	149
N34—H34···O123	0.88	2.21	2.929 (2)	139
N35—H35C···O101	0.92	2.06	2.922 (2)	155
N35—H35C···O102	0.92	2.50	3.233 (2)	136
N35—H35D···O132	0.92	2.11	3.025 (2)	171
N36—H36···O161^{i}	0.88	2.04	2.896 (2)	164
N36—H36···O162^{i}	0.88	2.46	3.144 (2)	135
N41—H41A···O141^{v}	0.92	2.30	3.066 (2)	140
N41—H41A···O142^{v}	0.92	2.36	3.255 (2)	165
N41—H41B···O141^{iii}	0.92	2.32	3.088 (2)	141
N41—H41B···O143^{iii}	0.92	2.60	3.460 (2)	156
N42—H42···O173^{v}	0.88	2.09	2.818 (2)	139
N43—H43D···O152	0.92	2.11	3.018 (2)	169
N43—H43D···O153	0.92	2.49	3.187 (2)	133
N43—H43E···O173	0.92	1.98	2.898 (2)	175
N44—H44···O141	0.88	2.22	3.041 (2)	155
N45—H45C···O151^{iii}	0.92	2.30	3.028 (2)	136

N45—H45C···O153^{iii}	0.92	2.45	3.358 (2)	169
N45—H45D···O171	0.92	2.13	3.012 (2)	159
N46—H46···O161	0.88	2.13	2.991 (2)	165

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) *x*, *y*−1, *z*; (iii) *x*, *y*+1, *z*; (iv) −*x*+3/2, *y*+1/2, −*z*+1/2; (v) −*x*+1/2, *y*+1/2, −*z*+1/2.

Fig. 1

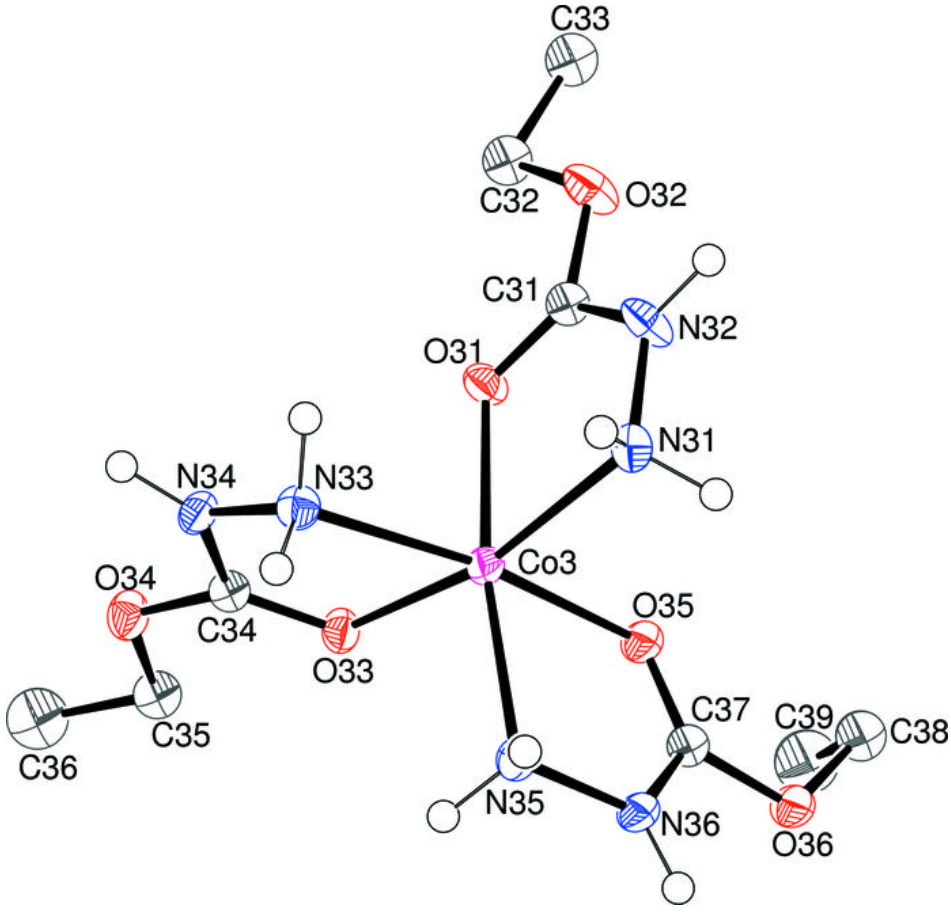
C33
C32
O32
C31
N32
O31
N31
N34
N33
Co3
O34
C34
O35
O33
C37
C39
C38
C35
C36
N35
N36
O36

Fig. 2