

Di- μ_2 -acetato-bis[μ_2 -1,1'-[propane-1,3-diylbis(nitrilomethylidyne)]di-2-naphtholato}tricobalt(II)

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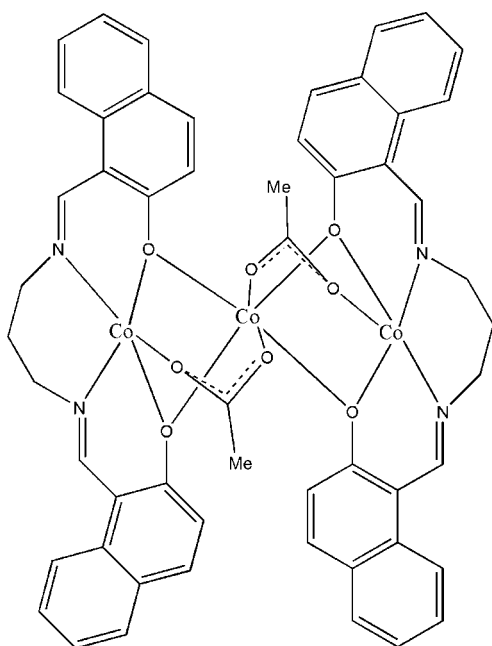
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.041; wR factor = 0.083; data-to-parameter ratio = 12.5.

The title compound, $[\text{Co}_3(\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_2)_2(\text{C}_2\text{H}_3\text{O}_2)_2]$, is an acetate- and phenolate-bridged trinuclear cobalt(II) complex. The central Co atom, lying on an inversion centre, is in an octahedral geometry. Each terminal Co atom is in a square-pyramidal geometry.

Related literature

For related literature, see: Diao (2007*a*, 2007*b*); Dohlakiya & Patel (2005); El-Beahry, Khalil, Ishak & Abd El-Halim (1997); Escuer *et al.* (2000); Eshel *et al.* (2000); Jiang *et al.* (2005); Manhas *et al.* (2005); Salem (2005).



Experimental

Crystal data

$[\text{Co}_3(\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_2)_2(\text{C}_2\text{H}_3\text{O}_2)_2]$
 $M_r = 1055.74$
 Monoclinic, $P2_1/n$
 $a = 11.770$ (3) Å
 $b = 11.765$ (4) Å
 $c = 16.137$ (3) Å
 $\beta = 90.61$ (2)°

$V = 2234.4$ (10) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.17$ mm⁻¹
 $T = 293$ (2) K
 $0.37 \times 0.33 \times 0.32$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.672$, $T_{\max} = 0.707$
 7988 measured reflections
 3927 independent reflections
 2604 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.083$
 $S = 0.86$
 3927 reflections
 313 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2376).

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supplementary materials

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Di- μ_2 -acetato-bis{ μ_2 -1,1'-[propane-1,3-diylbis(nitrilomethylidyne)]di-2-naphtholato}tricobalt(II)

Y.-P. Diao, S.-S. Huang, H.-L. Zhang, S. Deng and K.-X. Liu

Comment

Polynuclear complexes play an important role in the development of coordination chemistry related to magnetism and molecular architectures (Eshel *et al.*, 2000; Jiang *et al.*, 2005; Escuer *et al.*, 2000; El-Behairy *et al.*, 1997; Manhas *et al.*, 2005). The prime strategy for designing these molecular materials is to use suitable bridging ligands that determine the nature of the magnetic interactions (Salem, 2005; Dohlakiya & Patel, 2005). We have recently reported a few polynuclear transition metal complexes (Diao, 2007a,b). As an extension of the work on the polynuclear complexes, we report herein the crystal structure of the title complex, (I).

Compound (I) is an acetate and phenolate bridged trinuclear cobalt(II) complex. The central Co atom, lying on the inversion centre, is coordinated by four O atoms from two Schiff base ligands and two O atoms from two acetate groups, forming an octahedral geometry. Each terminal Co atom is coordinated by two O and two N atoms from one Schiff base ligand and one O atom of an acetate group, forming a square pyramidal geometry.

Experimental

N,N'-1,3-Propanediamine (0.1 mmol, 7.5 mg), 2-hydroxy-1-naphthaldehyde (0.2 mmol, 34.3 mg), and cobalt acetate (0.2 mmol, 50.0 mg) were dissolved in a methanol solution (20 ml). The mixture was stirred for half an hour at room temperature, giving a red solution. After allowing the solution to stand in dark for a week, brown block-like crystals were formed.

Refinement

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å, and with $U_{\text{iso}}(\text{H})$ values were fixed at 0.08 Å².

Figures

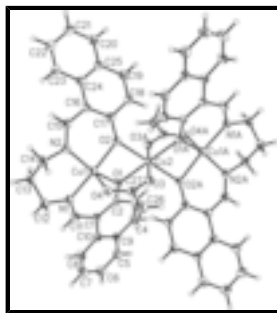


Fig. 1. Molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Symmetry operator (A): $2 - x, -y, -z$.

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Crystal data

$[\text{Co}_3(\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_2)_2(\text{C}_2\text{H}_3\text{O}_2)_2]$	$F_{000} = 1086$
$M_r = 1055.74$	$D_x = 1.569 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 11.770 (3) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 11.765 (4) \text{ \AA}$	Cell parameters from 2321 reflections
$c = 16.137 (3) \text{ \AA}$	$\theta = 2.2\text{--}25.0^\circ$
$\beta = 90.61 (2)^\circ$	$\mu = 1.17 \text{ mm}^{-1}$
$V = 2234.4 (10) \text{ \AA}^3$	$T = 293 (2) \text{ K}$
$Z = 2$	Block, brown
	$0.37 \times 0.33 \times 0.32 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	3927 independent reflections
Radiation source: fine-focus sealed tube	2604 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.032$
$T = 293(2) \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
ω scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -14 \rightarrow 11$
$T_{\text{min}} = 0.672$, $T_{\text{max}} = 0.707$	$k = -14 \rightarrow 12$
7988 measured reflections	$l = -18 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2]$
$S = 0.86$	where $P = (F_o^2 + 2F_c^2)/3$
3927 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
313 parameters	$\Delta\rho_{\text{max}} = 0.45 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
	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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.98733 (4)	0.16208 (3)	0.14688 (3)	0.04044 (15)
Co2	1.0000	0.0000	0.0000	0.03656 (18)
O1	0.94380 (18)	0.00047 (16)	0.12547 (12)	0.0409 (6)
O2	0.96231 (18)	0.17133 (16)	0.02205 (12)	0.0397 (6)
O3	1.16502 (19)	0.03277 (18)	0.03765 (13)	0.0451 (6)
O4	1.15744 (19)	0.14127 (18)	0.15148 (13)	0.0455 (6)
N1	0.9624 (2)	0.1354 (2)	0.27103 (16)	0.0404 (7)
N2	0.9711 (2)	0.3328 (2)	0.15027 (16)	0.0388 (7)
C1	0.9099 (3)	-0.0671 (3)	0.2633 (2)	0.0367 (8)
C2	0.9091 (3)	-0.0797 (3)	0.1763 (2)	0.0354 (8)
C3	0.8677 (3)	-0.1826 (3)	0.1412 (2)	0.0418 (9)
H3A	0.8624	-0.1889	0.0819	0.080*
C4	0.8370 (3)	-0.2703 (3)	0.1894 (2)	0.0459 (9)
H4A	0.8077	-0.3379	0.1637	0.080*
C5	0.8134 (3)	-0.3600 (3)	0.3257 (2)	0.0491 (10)
H5A	0.7868	-0.4276	0.2985	0.080*
C6	0.8199 (3)	-0.3570 (3)	0.4096 (2)	0.0544 (10)
H6A	0.7960	-0.4211	0.4419	0.080*
C7	0.8608 (3)	-0.2584 (3)	0.4477 (2)	0.0568 (11)
H7A	0.8680	-0.2565	0.5070	0.080*
C8	0.8907 (3)	-0.1649 (3)	0.4025 (2)	0.0488 (9)
H8A	0.9195	-0.0988	0.4305	0.080*
C9	0.8441 (3)	-0.2658 (3)	0.2771 (2)	0.0391 (8)
C10	0.8816 (3)	-0.1639 (3)	0.3151 (2)	0.0388 (8)
C11	0.9360 (3)	0.0383 (3)	0.3032 (2)	0.0419 (9)
H11	0.9336	0.0369	0.3608	0.050*
C12	0.9865 (3)	0.2281 (3)	0.3306 (2)	0.0497 (10)
H12A	1.0675	0.2322	0.3374	0.080*
H12B	0.9546	0.2095	0.3835	0.080*
C13	0.9476 (3)	0.3436 (3)	0.3019 (2)	0.0488 (9)
H13A	0.9546	0.3965	0.3469	0.080*
H13B	0.8685	0.3371	0.2876	0.080*
C14	1.0077 (3)	0.3899 (3)	0.2268 (2)	0.0473 (9)
H14A	0.9952	0.4702	0.2217	0.080*
H14B	1.0876	0.3773	0.2347	0.080*
C15	0.9328 (3)	0.3953 (3)	0.0914 (2)	0.0410 (9)
H15	0.9318	0.4730	0.1019	0.049*
C16	0.8909 (3)	0.3609 (2)	0.0109 (2)	0.0366 (8)

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C17	0.9088 (3)	0.2510 (3)	-0.0204 (2)	0.0368 (8)
C18	0.8683 (3)	0.2252 (3)	-0.10198 (19)	0.0415 (9)
H18A	0.8832	0.1512	-0.1244	0.080*
C19	0.8109 (3)	0.3032 (3)	-0.1478 (2)	0.0445 (9)
H19A	0.7852	0.2833	-0.2026	0.080*
C20	0.7206 (3)	0.4910 (3)	-0.1634 (2)	0.0497 (9)
H20A	0.6939	0.4688	-0.2174	0.080*
C21	0.6942 (3)	0.5958 (3)	-0.1325 (2)	0.0557 (10)
H21A	0.6491	0.6481	-0.1645	0.080*
C22	0.7337 (3)	0.6249 (3)	-0.0535 (2)	0.0604 (11)
H22A	0.7150	0.6982	-0.0312	0.080*
C23	0.7984 (3)	0.5520 (3)	-0.0082 (2)	0.0554 (11)
H23A	0.8260	0.5757	0.0453	0.080*
C24	0.8269 (3)	0.4429 (3)	-0.0374 (2)	0.0398 (8)
C25	0.7865 (3)	0.4134 (3)	-0.1165 (2)	0.0390 (8)
C26	1.3363 (3)	0.0714 (3)	0.1094 (2)	0.0684 (12)
H26A	1.3701	0.0566	0.0566	0.080*
H26B	1.3529	0.0097	0.1465	0.080*
H26C	1.3666	0.1407	0.1318	0.080*
C27	1.2099 (3)	0.0826 (3)	0.0986 (2)	0.0417 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0557 (3)	0.0357 (3)	0.0299 (3)	0.0030 (2)	0.0046 (2)	-0.0040 (2)
Co2	0.0490 (4)	0.0338 (3)	0.0270 (4)	0.0048 (3)	0.0043 (3)	-0.0027 (3)
O1	0.0589 (16)	0.0341 (12)	0.0299 (14)	0.0000 (11)	0.0084 (11)	-0.0010 (11)
O2	0.0565 (16)	0.0313 (11)	0.0313 (14)	0.0058 (11)	0.0013 (11)	-0.0032 (10)
O3	0.0463 (16)	0.0503 (14)	0.0387 (15)	0.0043 (11)	0.0018 (12)	-0.0072 (12)
O4	0.0517 (16)	0.0486 (14)	0.0362 (15)	0.0058 (11)	-0.0015 (12)	-0.0063 (11)
N1	0.0506 (19)	0.0381 (16)	0.0324 (18)	0.0000 (13)	0.0027 (14)	-0.0056 (13)
N2	0.0478 (19)	0.0343 (14)	0.0343 (17)	0.0022 (13)	-0.0016 (14)	-0.0033 (14)
C1	0.042 (2)	0.0394 (19)	0.029 (2)	0.0004 (15)	0.0037 (16)	-0.0009 (16)
C2	0.039 (2)	0.0370 (19)	0.030 (2)	0.0047 (15)	0.0035 (16)	-0.0010 (16)
C3	0.052 (2)	0.0390 (19)	0.034 (2)	-0.0020 (16)	0.0086 (17)	-0.0056 (16)
C4	0.053 (3)	0.041 (2)	0.043 (3)	-0.0027 (17)	0.0077 (18)	-0.0085 (18)
C5	0.054 (3)	0.044 (2)	0.049 (3)	-0.0059 (17)	0.0082 (19)	0.0035 (18)
C6	0.057 (3)	0.057 (2)	0.049 (3)	-0.0078 (19)	0.012 (2)	0.014 (2)
C7	0.065 (3)	0.070 (3)	0.036 (2)	-0.004 (2)	0.005 (2)	0.008 (2)
C8	0.057 (3)	0.055 (2)	0.035 (2)	-0.0049 (19)	0.0078 (18)	0.0027 (19)
C9	0.041 (2)	0.0382 (19)	0.038 (2)	0.0007 (15)	0.0070 (17)	-0.0005 (17)
C10	0.039 (2)	0.045 (2)	0.033 (2)	0.0039 (16)	0.0063 (16)	0.0028 (17)
C11	0.051 (2)	0.050 (2)	0.025 (2)	-0.0043 (17)	0.0029 (16)	0.0012 (17)
C12	0.071 (3)	0.046 (2)	0.032 (2)	-0.0096 (18)	0.0030 (19)	-0.0083 (17)
C13	0.062 (3)	0.043 (2)	0.042 (2)	-0.0078 (18)	0.0055 (19)	-0.0175 (18)
C14	0.059 (3)	0.044 (2)	0.038 (2)	-0.0038 (17)	-0.0046 (19)	-0.0080 (17)
C15	0.052 (2)	0.0312 (18)	0.040 (2)	0.0012 (16)	0.0055 (18)	-0.0044 (17)
C16	0.046 (2)	0.0338 (18)	0.030 (2)	0.0008 (15)	0.0029 (16)	-0.0014 (15)

C17	0.041 (2)	0.0379 (18)	0.031 (2)	-0.0001 (16)	0.0045 (16)	0.0031 (16)
C18	0.055 (2)	0.0402 (19)	0.029 (2)	0.0029 (16)	0.0049 (18)	-0.0025 (16)
C19	0.052 (2)	0.046 (2)	0.036 (2)	-0.0022 (17)	-0.0017 (18)	-0.0021 (17)
C20	0.053 (2)	0.049 (2)	0.047 (2)	-0.0042 (18)	-0.0040 (18)	0.0018 (19)
C21	0.060 (3)	0.048 (2)	0.059 (3)	0.0060 (19)	-0.003 (2)	0.012 (2)
C22	0.084 (3)	0.042 (2)	0.056 (3)	0.015 (2)	0.000 (2)	-0.001 (2)
C23	0.081 (3)	0.040 (2)	0.044 (2)	0.013 (2)	-0.006 (2)	-0.0053 (18)
C24	0.048 (2)	0.0349 (18)	0.036 (2)	-0.0028 (16)	0.0049 (17)	0.0029 (16)
C25	0.047 (2)	0.0387 (19)	0.032 (2)	-0.0002 (16)	-0.0004 (17)	0.0019 (16)
C26	0.057 (3)	0.079 (3)	0.069 (3)	0.016 (2)	-0.011 (2)	-0.012 (2)
C27	0.048 (3)	0.0341 (19)	0.043 (3)	0.0043 (17)	0.0031 (19)	0.0078 (18)

Geometric parameters (Å, °)

Co1—O1	1.998 (2)	C8—H8A	0.9597
Co1—O4	2.018 (2)	C9—C10	1.415 (4)
Co1—N2	2.019 (3)	C11—H11	0.9300
Co1—O2	2.036 (2)	C12—C13	1.506 (4)
Co1—N1	2.052 (3)	C12—H12A	0.9597
Co2—O3	2.065 (2)	C12—H12B	0.9603
Co2—O3 ⁱ	2.065 (2)	C13—C14	1.510 (4)
Co2—O2 ⁱ	2.095 (2)	C13—H13A	0.9599
Co2—O2	2.095 (2)	C13—H13B	0.9597
Co2—O1 ⁱ	2.137 (2)	C14—H14A	0.9598
Co2—O1	2.137 (2)	C14—H14B	0.9597
O1—C2	1.318 (3)	C15—C16	1.442 (4)
O2—C17	1.317 (3)	C15—H15	0.9300
O3—C27	1.257 (4)	C16—C17	1.406 (4)
O4—C27	1.263 (4)	C16—C24	1.446 (4)
N1—C11	1.294 (4)	C17—C18	1.428 (4)
N1—C12	1.479 (4)	C18—C19	1.356 (4)
N2—C15	1.279 (3)	C18—H18A	0.9599
N2—C14	1.467 (4)	C19—C25	1.421 (4)
C1—C2	1.412 (4)	C19—H19A	0.9600
C1—C11	1.429 (4)	C20—C21	1.366 (4)
C1—C10	1.453 (4)	C20—C25	1.413 (4)
C2—C3	1.421 (4)	C20—H20A	0.9600
C3—C4	1.344 (4)	C21—C22	1.396 (5)
C3—H3A	0.9602	C21—H21A	0.9599
C4—C9	1.418 (4)	C22—C23	1.355 (4)
C4—H4A	0.9599	C22—H22A	0.9599
C5—C6	1.356 (4)	C23—C24	1.409 (4)
C5—C9	1.408 (4)	C23—H23A	0.9600
C5—H5A	0.9598	C24—C25	1.402 (4)
C6—C7	1.396 (5)	C26—C27	1.502 (5)
C6—H6A	0.9600	C26—H26A	0.9600
C7—C8	1.367 (4)	C26—H26B	0.9600
C7—H7A	0.9602	C26—H26C	0.9600

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C8—C10	1.413 (4)		
O1—Co1—O4	98.24 (9)	C8—C10—C9	116.5 (3)
O1—Co1—N2	158.02 (10)	C8—C10—C1	124.4 (3)
O4—Co1—N2	102.36 (10)	C9—C10—C1	119.1 (3)
O1—Co1—O2	81.12 (8)	N1—C11—C1	129.6 (3)
O4—Co1—O2	100.13 (9)	N1—C11—H11	115.2
N2—Co1—O2	87.76 (9)	C1—C11—H11	115.2
O1—Co1—N1	89.09 (9)	N1—C12—C13	114.2 (3)
O4—Co1—N1	95.61 (10)	N1—C12—H12A	107.2
N2—Co1—N1	96.38 (10)	C13—C12—H12A	106.7
O2—Co1—N1	162.48 (10)	N1—C12—H12B	109.6
O3—Co2—O3 ⁱ	180.00 (17)	C13—C12—H12B	111.0
O3—Co2—O2 ⁱ	91.69 (8)	H12A—C12—H12B	107.9
O3 ⁱ —Co2—O2 ⁱ	88.31 (8)	C12—C13—C14	115.4 (3)
O3—Co2—O2	88.31 (8)	C12—C13—H13A	109.2
O3 ⁱ —Co2—O2	91.69 (8)	C14—C13—H13A	109.7
O2 ⁱ —Co2—O2	180.00 (15)	C12—C13—H13B	107.0
O3—Co2—O1 ⁱ	88.83 (9)	C14—C13—H13B	107.4
O3 ⁱ —Co2—O1 ⁱ	91.17 (9)	H13A—C13—H13B	107.9
O2 ⁱ —Co2—O1 ⁱ	76.60 (7)	N2—C14—C13	112.0 (3)
O2—Co2—O1 ⁱ	103.40 (7)	N2—C14—H14A	109.6
O3—Co2—O1	91.17 (9)	C13—C14—H14A	110.6
O3 ⁱ —Co2—O1	88.83 (9)	N2—C14—H14B	108.7
O2 ⁱ —Co2—O1	103.40 (7)	C13—C14—H14B	107.7
O2—Co2—O1	76.60 (7)	H14A—C14—H14B	108.2
O1 ⁱ —Co2—O1	180.00 (15)	N2—C15—C16	128.5 (3)
C2—O1—Co1	130.82 (19)	N2—C15—H15	115.8
C2—O1—Co2	133.59 (18)	C16—C15—H15	115.8
Co1—O1—Co2	94.87 (8)	C17—C16—C15	122.1 (3)
C17—O2—Co1	128.05 (19)	C17—C16—C24	119.9 (3)
C17—O2—Co2	134.18 (19)	C15—C16—C24	118.0 (3)
Co1—O2—Co2	95.05 (8)	O2—C17—C16	122.7 (3)
C27—O3—Co2	134.7 (2)	O2—C17—C18	118.8 (3)
C27—O4—Co1	122.2 (2)	C16—C17—C18	118.5 (3)
C11—N1—C12	115.8 (3)	C19—C18—C17	121.3 (3)
C11—N1—Co1	124.3 (2)	C19—C18—H18A	120.0
C12—N1—Co1	119.57 (19)	C17—C18—H18A	118.7
C15—N2—C14	117.4 (3)	C18—C19—C25	121.7 (3)
C15—N2—Co1	125.8 (2)	C18—C19—H19A	119.2
C14—N2—Co1	116.8 (2)	C25—C19—H19A	119.2
C2—C1—C11	122.5 (3)	C21—C20—C25	120.9 (3)
C2—C1—C10	119.4 (3)	C21—C20—H20A	120.3
C11—C1—C10	118.1 (3)	C25—C20—H20A	118.8
O1—C2—C1	123.1 (3)	C20—C21—C22	118.7 (3)
O1—C2—C3	117.9 (3)	C20—C21—H21A	120.6
C1—C2—C3	119.0 (3)	C22—C21—H21A	120.7

C4—C3—C2	121.1 (3)	C23—C22—C21	121.1 (3)
C4—C3—H3A	120.1	C23—C22—H22A	119.8
C2—C3—H3A	118.8	C21—C22—H22A	119.1
C3—C4—C9	122.4 (3)	C22—C23—C24	122.1 (3)
C3—C4—H4A	118.9	C22—C23—H23A	118.9
C9—C4—H4A	118.6	C24—C23—H23A	119.0
C6—C5—C9	121.6 (3)	C25—C24—C23	116.7 (3)
C6—C5—H5A	119.6	C25—C24—C16	119.7 (3)
C9—C5—H5A	118.8	C23—C24—C16	123.5 (3)
C5—C6—C7	118.4 (3)	C24—C25—C20	120.4 (3)
C5—C6—H6A	120.4	C24—C25—C19	118.8 (3)
C7—C6—H6A	121.1	C20—C25—C19	120.7 (3)
C8—C7—C6	121.6 (3)	C27—C26—H26A	109.5
C8—C7—H7A	119.5	C27—C26—H26B	109.5
C6—C7—H7A	118.9	H26A—C26—H26B	109.5
C7—C8—C10	121.4 (3)	C27—C26—H26C	109.5
C7—C8—H8A	119.5	H26A—C26—H26C	109.5
C10—C8—H8A	119.1	H26B—C26—H26C	109.5
C5—C9—C10	120.4 (3)	O3—C27—O4	125.4 (3)
C5—C9—C4	121.0 (3)	O3—C27—C26	117.2 (3)
C10—C9—C4	118.6 (3)	O4—C27—C26	117.4 (3)

Symmetry codes: (i) $-x+2, -y, -z$.

Fig. 1

