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Tetraaquabis[2-(2-nitrophenyl)acetato-κO]cobalt(II)

Muhammad Danish,[a] Muhammad Nawaz Tahir,[b]* Sana Iftikhar,[a] Muhammad Asam Raza[a] and Muhammad Ashfaq[a]

[a]Department of Chemistry, Institute of Chemical and Biological Sciences, University of Gujrat, Gujrat 50700, Pakistan, and [b]Department of Physics, University of Sargodha, Sargodha, Punjab, Pakistan. *Correspondence e-mail: dmntahir_uos@yahoo.com

The molecule of the title compound, $[Co(C_8H_6NO_4)_2(H_2O)_4]$, is centrosymmetric. It is a cobalt(II) complex, bearing two (2-nitrophenyl)acetate and four aqua ligands. The coordination around the Co^{II} atom is distorted octahedral, defined by four O atoms of water molecules in the equatorial plane and by two carboxylate O atoms at axial positions. The dihedral angles between the benzene ring and the acetate and nitro groups are 61.90 (10) and 19.21 (11)°, respectively. The water molecules form O—H···O hydrogen bonds with the nitro and carboxylate groups, leading to a layered structural arrangement parallel to (001).

1. Related literature

The title compound is structurally related to tetraaquabis-(acetato-κO)cobalt(II) (Sobolev *et al.*, 2003), tetraaquabis(2-nitrophenoxyethanoato-κO)cobalt(II) dihydrate (Kennard *et al.*, 1985), tetraaquabis((2,4-dichlorophenoxy)acetato-κO)-cobalt(II) dihydrate (Tan *et al.*, 2011), tetraaquabis[2-(6-amino-9H-purin-9-yl)acetato-κO]cobalt(II) (Mishra *et al.*, 2011) and tetraaquabis(3,5-dinitrobenzoato-κO)cobalt(II) tetrahydrate (Tahir *et al.*, 1996).
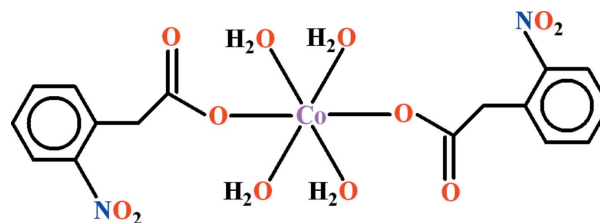
2. Experimental

2.1. Crystal data

$[Co(C_8H_6NO_4)_2(H_2O)_4]$	$V = 998.96 (10)$ Å^3
$M_r = 491.27$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 5.4431 (3)$ Å	$\mu = 0.93$ mm^{-1}
$b = 6.4313 (4)$ Å	$T = 296$ K
$c = 28.5697 (15)$ Å	$0.32 \times 0.24 \times 0.20$ mm
$\beta = 92.762 (2)°$	

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer	8913 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)	2156 independent reflections
$T_{min} = 0.758$, $T_{max} = 0.835$	1937 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.026$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.070$	
$S = 1.04$	
2156 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O1^i	0.82 (2)	2.00 (2)	2.7984 (16)	166 (2)
O5—H5B···O2^{ii}	0.82 (2)	1.89 (2)	2.6797 (17)	161 (2)
O6—H6A···O2^{iii}	0.78 (2)	1.93 (2)	2.6979 (17)	169 (2)
O6—H6B···O3	0.81 (2)	2.22 (2)	2.988 (2)	159 (2)

Symmetry codes: (i) $-x + 1, -y, -z$; (ii) $-x + 2, -y, -z$; (iii) $x, y - 1, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

data reports

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supporting information

Tetraaquabis[2-(2-nitrophenyl)acetato-*κO*]cobalt(II)

Muhammad Danish, Muhammad Nawaz Tahir, Sana Iftikhar, Muhammad Asam Raza and Muhammad Ashfaq

S1. Experimental

The sodium salt of (2-nitrophenyl)acetic acid was prepared by mixing aqueous solutions of (2-nitrophenyl)acetic acid and Na(HCO$_3$) in the molar ratio 1:1. To this solution a 0.5 molar equivalent of cobalt(II) acetate was added and the mixture refluxed for 4 h. The resulting solution was evaporated for crystal growth. Light-orange prisms suitable for X-ray data collection were obtained after one week.

S2. Refinement

The coordinates of water H-atoms were refined freely, with $U_{iso}(H) = 1.2U_{eq}(O)$. The other H-atoms were positioned geometrically (C—H = 0.93—0.97 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.
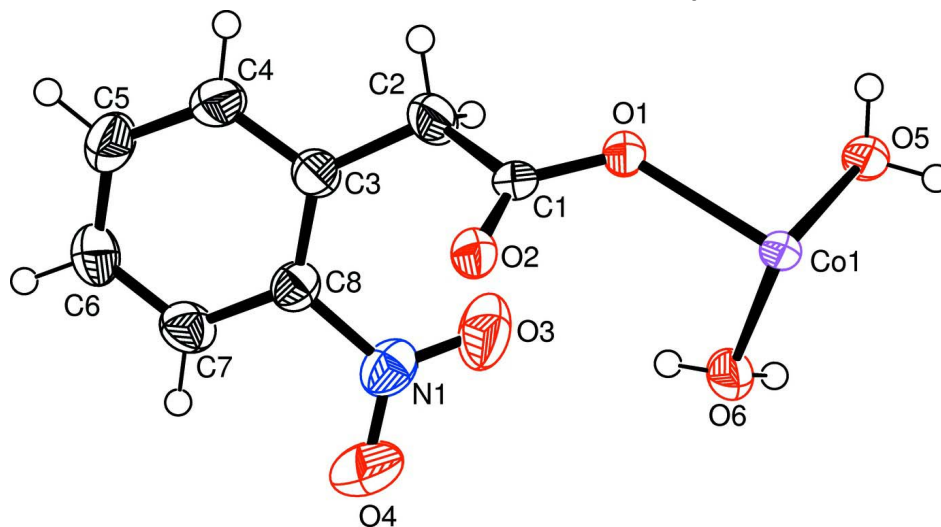

Figure 1

View of the asymmetric unit of title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H-atoms are shown as small circles of arbitrary radius.
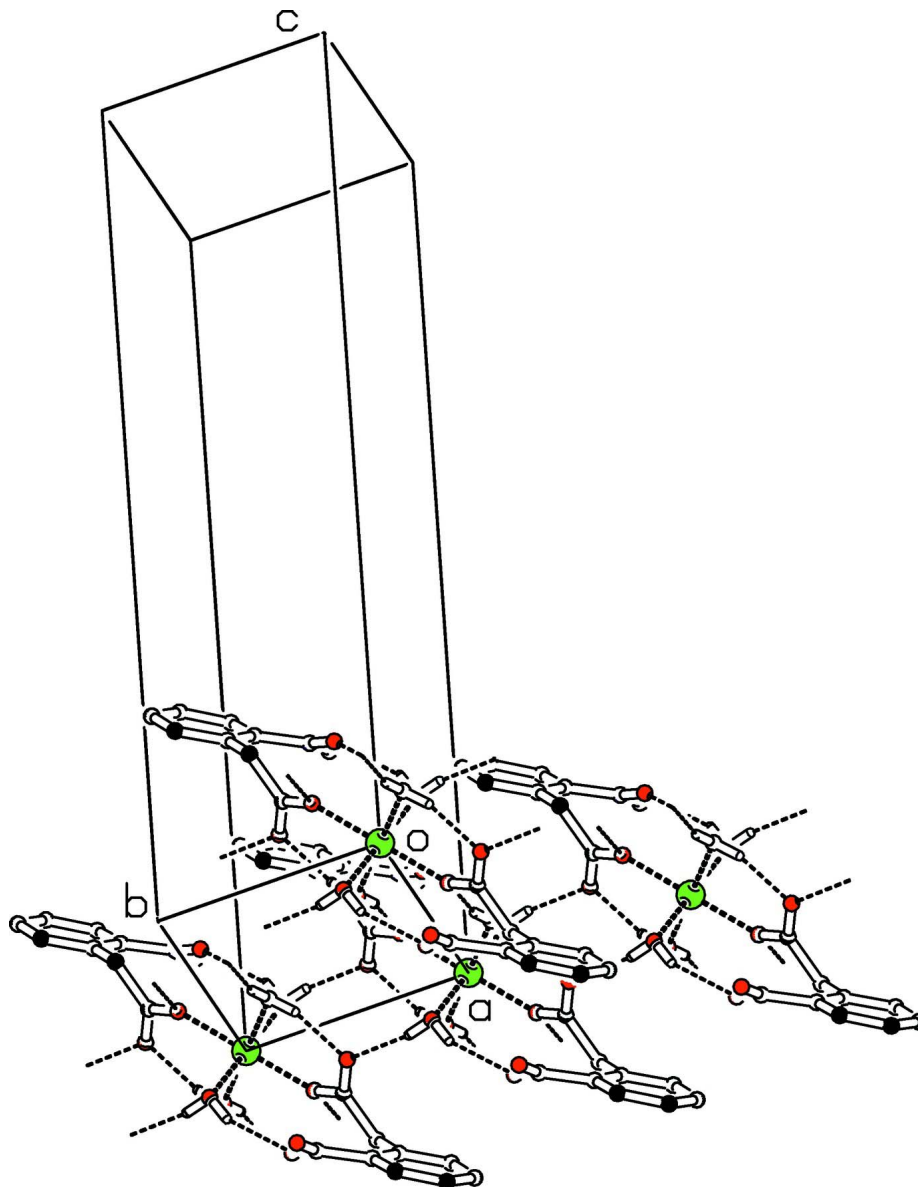
Figure 2

A partial packing diagram of the title compound showing the layered organisation of molecules held together by O—H···O interactions (dashed lines). H atoms not involved in hydrogen bonding are omitted for clarity.

Tetraaquabis[2-(2-nitrophenyl)acetato-*κO*]cobalt(II)

Crystal data

$[Co(C_8H_6NO_4)_2(H_2O)_4]$	$F(000) = 506$
$M_r = 491.27$	$D_x = 1.633$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 5.4431$ (3) Å	Cell parameters from 2154 reflections
$b = 6.4313$ (4) Å	$\theta = 2.9$–27.0°
$c = 28.5697$ (15) Å	$\mu = 0.93$ mm^{-1}
$\beta = 92.762$ (2)°	$T = 296$ K
$V = 998.96$ (10) Å^3	Prism, light-orange
$Z = 2$	$0.32 \times 0.24 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	8913 measured reflections
Radiation source: fine-focus sealed tube	2156 independent reflections
Graphite monochromator	1937 reflections with $I > 2\sigma(I)$
Detector resolution: 7.80 pixels mm^{-1}	$R_{int} = 0.026$
ω scans	$\theta_{max} = 27.0°$, $\theta_{min} = 2.9°$
Absorption correction: multi-scan ($SADABS$; Bruker, 2007)	$h = -6\rightarrow5$
	$k = -8\rightarrow8$
$T_{min} = 0.758$, $T_{max} = 0.835$	$l = -36\rightarrow36$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.028$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.070$	
$S = 1.04$	H atoms treated by a mixture of independent and constrained refinement
2156 reflections	
154 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.3677P]$ where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.27$ e Å^{-3}
	$\Delta\rho_{min} = -0.28$ e Å^{-3}

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}
Co1	1.0000	0.0000	0.0000	0.02745 (10)
O1	0.78213 (19)	0.21130 (18)	0.03439 (4)	0.0354 (3)
O2	1.0428 (2)	0.45515 (17)	0.06128 (4)	0.0349 (3)
O3	0.9861 (3)	0.1663 (2)	0.13936 (6)	0.0656 (4)
O4	1.2715 (3)	0.2897 (3)	0.18485 (7)	0.0860 (6)
O5	0.7121 (2)	−0.21593 (19)	−0.00252 (5)	0.0367 (3)
H5A	0.572 (4)	−0.193 (3)	−0.0126 (7)	0.044*
H5B	0.761 (4)	−0.309 (3)	−0.0197 (7)	0.044*
O6	1.1243 (2)	−0.1312 (2)	0.06473 (5)	0.0396 (3)
H6A	1.089 (4)	−0.249 (4)	0.0668 (7)	0.047*
H6B	1.076 (4)	−0.079 (4)	0.0883 (8)	0.047*
N1	1.0723 (3)	0.3042 (2)	0.16413 (5)	0.0449 (4)
C1	0.8429 (3)	0.3604 (2)	0.06134 (5)	0.0302 (3)
C2	0.6512 (3)	0.4255 (4)	0.09495 (7)	0.0465 (5)
H2A	0.5280	0.5076	0.0776	0.056*

H2B	0.5702	0.3010	0.1056	0.056*
C3	0.7378 (3)	0.5481 (3)	0.13750 (6)	0.0360 (4)
C4	0.6146 (4)	0.7320 (3)	0.14716 (7)	0.0477 (5)
H4	0.4881	0.7762	0.1265	0.057*
C5	0.6733 (4)	0.8505 (3)	0.18614 (7)	0.0501 (5)
H5	0.5823	0.9693	0.1920	0.060*
C6	0.8658 (4)	0.7945 (3)	0.21649 (7)	0.0478 (5)
H6	0.9062	0.8753	0.2427	0.057*
C7	0.9977 (3)	0.6180 (3)	0.20765 (6)	0.0419 (4)
H7	1.1312	0.5804	0.2274	0.050*
C8	0.9304 (3)	0.4964 (2)	0.16911 (6)	0.0340 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01995 (16)	0.02718 (16)	0.03467 (18)	0.00213 (11)	−0.00444 (11)	−0.00896 (12)
O1	0.0242 (5)	0.0371 (6)	0.0445 (7)	0.0033 (5)	−0.0030 (5)	−0.0170 (5)
O2	0.0296 (6)	0.0312 (6)	0.0437 (7)	0.0001 (5)	−0.0005 (5)	−0.0103 (5)
O3	0.0995 (13)	0.0358 (8)	0.0613 (9)	0.0115 (8)	0.0019 (9)	−0.0049 (7)
O4	0.0700 (11)	0.0865 (13)	0.0987 (14)	0.0409 (10)	−0.0245 (10)	−0.0129 (11)
O5	0.0227 (6)	0.0368 (6)	0.0501 (7)	0.0005 (5)	−0.0034 (5)	−0.0142 (6)
O6	0.0452 (7)	0.0307 (6)	0.0417 (7)	0.0038 (5)	−0.0094 (6)	−0.0072 (5)
N1	0.0545 (10)	0.0427 (9)	0.0380 (8)	0.0124 (7)	0.0064 (7)	0.0062 (7)
C1	0.0244 (8)	0.0328 (8)	0.0328 (8)	0.0075 (6)	−0.0058 (6)	−0.0059 (6)
C2	0.0287 (9)	0.0635 (12)	0.0468 (11)	0.0016 (8)	−0.0009 (8)	−0.0240 (9)
C3	0.0286 (9)	0.0451 (9)	0.0345 (9)	0.0011 (7)	0.0027 (7)	−0.0089 (7)
C4	0.0394 (10)	0.0592 (12)	0.0439 (10)	0.0161 (9)	−0.0047 (8)	−0.0120 (9)
C5	0.0569 (12)	0.0461 (11)	0.0473 (11)	0.0134 (9)	0.0030 (9)	−0.0123 (9)
C6	0.0560 (12)	0.0498 (11)	0.0374 (10)	0.0006 (9)	0.0010 (8)	−0.0146 (8)
C7	0.0417 (10)	0.0530 (11)	0.0305 (8)	0.0021 (8)	−0.0034 (7)	−0.0011 (8)
C8	0.0351 (9)	0.0353 (9)	0.0319 (8)	0.0026 (7)	0.0054 (7)	0.0003 (7)

Geometric parameters (Å, º)

Co1—O1^i	2.0810 (11)	C1—C2	1.511 (2)
Co1—O1	2.0810 (11)	C2—C3	1.505 (2)
Co1—O5	2.0925 (12)	C2—H2A	0.9700
Co1—O5^i	2.0925 (12)	C2—H2B	0.9700
Co1—O6	2.1141 (13)	C3—C8	1.391 (2)
Co1—O6^i	2.1141 (13)	C3—C4	1.394 (3)
O1—C1	1.2637 (18)	C4—C5	1.374 (3)
O2—C1	1.2473 (19)	C4—H4	0.9300
O3—N1	1.214 (2)	C5—C6	1.376 (3)
O4—N1	1.213 (2)	C5—H5	0.9300
O5—H5A	0.82 (2)	C6—C7	1.373 (3)
O5—H5B	0.82 (2)	C6—H6	0.9300
O6—H6A	0.78 (2)	C7—C8	1.385 (2)
O6—H6B	0.81 (2)	C7—H7	0.9300

N1—C8	1.468 (2)		
O1ⁱ—Co1—O1	180.0	O2—C1—C2	119.65 (14)
O1ⁱ—Co1—O5	89.61 (5)	O1—C1—C2	115.40 (14)
O1—Co1—O5	90.39 (5)	C3—C2—C1	117.33 (14)
O1ⁱ—Co1—O5ⁱ	90.39 (5)	C3—C2—H2A	108.0
O1—Co1—O5ⁱ	89.61 (5)	C1—C2—H2A	108.0
O5—Co1—O5ⁱ	180.0	C3—C2—H2B	108.0
O1ⁱ—Co1—O6	89.23 (5)	C1—C2—H2B	108.0
O1—Co1—O6	90.77 (5)	H2A—C2—H2B	107.2
O5—Co1—O6	88.44 (5)	C8—C3—C4	115.41 (16)
O5ⁱ—Co1—O6	91.56 (5)	C8—C3—C2	126.60 (16)
O1ⁱ—Co1—O6ⁱ	90.77 (5)	C4—C3—C2	117.98 (16)
O1—Co1—O6ⁱ	89.23 (5)	C5—C4—C3	122.40 (18)
O5—Co1—O6ⁱ	91.56 (5)	C5—C4—H4	118.8
O5ⁱ—Co1—O6ⁱ	88.44 (5)	C3—C4—H4	118.8
O6—Co1—O6ⁱ	180.00 (6)	C4—C5—C6	120.38 (18)
C1—O1—Co1	130.14 (10)	C4—C5—H5	119.8
Co1—O5—H5A	125.5 (15)	C6—C5—H5	119.8
Co1—O5—H5B	103.7 (14)	C7—C6—C5	119.33 (17)
H5A—O5—H5B	104 (2)	C7—C6—H6	120.3
Co1—O6—H6A	112.4 (16)	C5—C6—H6	120.3
Co1—O6—H6B	117.5 (16)	C6—C7—C8	119.51 (17)
H6A—O6—H6B	104 (2)	C6—C7—H7	120.2
O4—N1—O3	122.64 (18)	C8—C7—H7	120.2
O4—N1—C8	118.61 (17)	C7—C8—C3	122.90 (16)
O3—N1—C8	118.75 (16)	C7—C8—N1	115.63 (16)
O2—C1—O1	124.94 (15)	C3—C8—N1	121.46 (15)
Co1—O1—C1—O2	25.0 (2)	C6—C7—C8—C3	2.2 (3)
Co1—O1—C1—C2	−156.08 (13)	C6—C7—C8—N1	−176.35 (17)
O2—C1—C2—C3	−20.9 (3)	C4—C3—C8—C7	−0.1 (3)
O1—C1—C2—C3	160.19 (17)	C2—C3—C8—C7	−179.68 (18)
C1—C2—C3—C8	−50.9 (3)	C4—C3—C8—N1	178.29 (16)
C1—C2—C3—C4	129.5 (2)	C2—C3—C8—N1	−1.3 (3)
C8—C3—C4—C5	−2.3 (3)	O4—N1—C8—C7	−19.3 (3)
C2—C3—C4—C5	177.3 (2)	O3—N1—C8—C7	160.92 (17)
C3—C4—C5—C6	2.6 (3)	O4—N1—C8—C3	162.21 (19)
C4—C5—C6—C7	−0.5 (3)	O3—N1—C8—C3	−17.6 (3)
C5—C6—C7—C8	−1.8 (3)		

Symmetry code: (i) −x+2, −y, −z.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O1ⁱⁱ	0.82 (2)	2.00 (2)	2.7984 (16)	166 (2)
O5—H5B···O2ⁱ	0.82 (2)	1.89 (2)	2.6797 (17)	161 (2)

O6—H6A···O2^{iii}	0.78 (2)	1.93 (2)	2.6979 (17)	169 (2)
O6—H6B···O3	0.81 (2)	2.22 (2)	2.988 (2)	159 (2)

Symmetry codes: (i) −x+2, −y, −z; (ii) −x+1, −y, −z; (iii) x, y−1, z.