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Acetonitrilebis(nitrato-κ^2O,O')(1,10-phenanthroline)cobalt(II)

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In the title compound, $[Co(NO_3)_2(C_2H_3N)(C_{12}H_8N_2)]$, the cobalt(II) centre adopts a seven-coordinate distorted pentagonal–bipyramidal geometry, being coordinated by a bidentate 1,10-phenanthroline, two bidentate nitrate anions and an acetonitrile ligand. The two axial sites are occupied by the acetonitrile ligand and one N-atom donor from the phenanthroline. The major distortions from ideal geometry occur within the equatorial plane, and are due to the narrow bite angle of the bidentate nitrate anions.

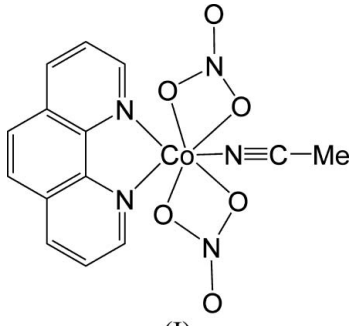
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.069
Data-to-parameter ratio = 15.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The field of coordination frameworks and their potential applications have been increasingly growing over the last few decades (Braga *et al.*, 2005; Champness *et al.*, 2006). Our studies have led us to investigate a variety of transition metal(II) nitrate salts in combination with soft N-donor ligands (Barnett *et al.*, 2001; Barnett *et al.*, 2003*a*,*b*; Blake *et al.*, 2000; Khlobystov *et al.*, 2003). During our investigations, we have encountered the title compound, (I), as a by-product from an attempt to prepare a coordination polymer with the ligand 4,4′-(1,4-phenylene)bis(3,6-dipyridin-2-ylpyridazine). Thus, a new crystal structure containing the widely studied 1,10-phenanthroline ligand has been obtained and characterized.



(I)

The cobalt(II) centre adopts a seven-coordinate distorted pentagonal–bipyramidal geometry, the donor atoms being two N atoms supplied by a bidentate 1,10-phenanthroline, four O atoms from two bidentate nitrate anions and an N atom from an acetonitrile ligand. The two axial sites are occupied by the acetonitrile ligand and one N-atom donor from the phenanthroline; as the other phenanthroline N-atom donor occupies an equatorial site, this ligand bridges axial and equatorial sites. The major distortions from ideal geometry occur within the equatorial plane, and are due to the narrow bite angle (ca. 57°) of the nitrate anions.

A dihedral angle of 4.05 (14)° is observed between the least-squares planes through the two nitrate anions which occupy four of the five equatorial positions of the cobalt(II) coordination environment. Dihedral angles of 105.1 (12) and 108.7 (12)° are observed between the plane through the 1,10-phenanthroline group and those of the nitrates.

Experimental

The title compound was prepared by slow reaction of $Co(NO_3)_2{\cdot}6H_2O$ (10 mg, 0.034 mmol) and 1,10-phenanthroline (6 mg, 0.033 mmol) in acetonitrile (10 ml) in the presence of 4,4′-(1,4-phenylene)bis(3,6-dipyridin-2-ylpyridazine). Crystals were left to grow over a period of six months before being taken from the mother liquor for single-crystal X-ray diffraction studies.

Crystal data

$[Co(NO_3)_2(C_2H_3N)(C_{12}H_8N_2)]$
M_r = 404.2
Monoclinic, $P2_1/c$
a = 7.1414 (9) Å
b = 14.3837 (17) Å
c = 15.4670 (19) Å
β = 92.906 (2)°
V = 1586.7 (3) Å^3
Z = 4
D_x = 1.692 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 150 (2) K
Block, orange
0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SHELXTL*; Bruker, 2001)
T_{min} = 0.575, T_{max} = 0.614
(expected range = 0.840–0.896)
9772 measured reflections
3637 independent reflections
2323 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.069
S = 0.88
3637 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—N1	2.1087 (19)	Co—O3	2.2583 (18)
Co—N2	2.1180 (19)	Co—O4	2.3289 (19)
Co—N5	2.079 (2)	Co—O5	2.1224 (17)
Co—O1	2.2375 (17)		
N1—Co—N2	78.48 (7)	N5—Co—O1	87.02 (7)
N1—Co—N5	95.89 (7)	N5—Co—O3	93.68 (7)
N1—Co—O3	137.22 (7)	N5—Co—O4	85.53 (7)
N1—Co—O4	86.07 (7)	N5—Co—O5	94.82 (7)
N1—Co—O5	141.12 (7)	O1—Co—O3	56.74 (6)
N1—Co—O1	82.23 (7)	O1—Co—O4	165.41 (6)
N2—Co—N5	172.54 (8)	O1—Co—O5	135.63 (6)
N2—Co—O1	87.36 (7)	O3—Co—O4	136.29 (6)
N2—Co—O3	87.34 (7)	O3—Co—O5	78.93 (6)
N2—Co—O4	98.85 (7)	O4—Co—O5	57.68 (6)
N2—Co—O5	92.63 (7)		

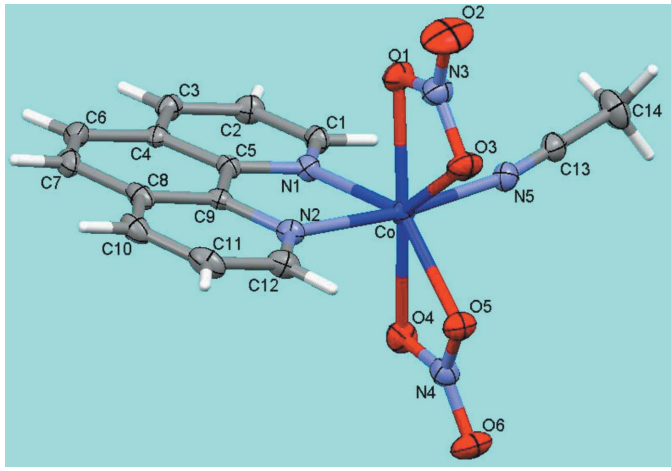


Figure 1
A view of the structure of the title compound, showing the atom-numbering scheme adopted. Displacement ellipsoids are drawn at the 50% probability level.

The methyl H atoms on the acetonitrile molecule were located in ΔF syntheses and refined as part of a rigid rotating group, with C—H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$. Aryl H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* and *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Macrae *et al.*, 2006); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2003) and publCIF (Westrip, 2006).

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Crystal data

$[Co(NO_3)_2(C_2H_3N)(C_{12}H_8N_2)]$
$M_r = 404.2$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.1414$ (9) Å
$b = 14.3837$ (17) Å
$c = 15.4670$ (19) Å
$\beta = 92.906$ (2)°
$V = 1586.7$ (3) Å^3
$Z = 4$
$F(000) = 820$
$D_x = 1.692$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2176 reflections
$\theta = 2.6$–26.3°
$\mu = 1.13$ mm^{-1}
$T = 150$ K
Block, orange
0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SHELXTL; Bruker, 2001)
$T_{min} = 0.575$, $T_{max} = 0.614$
9772 measured reflections
3637 independent reflections
2323 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -9 \rightarrow 8$
$k = -18 \rightarrow 9$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.069$
$S = 0.88$
3637 reflections
236 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
$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co	0.28718 (5)	0.22598 (2)	0.06541 (2)	0.02146 (10)
O1	0.5768 (2)	0.27548 (12)	0.10332 (10)	0.0303 (4)
O2	0.7271 (3)	0.23194 (16)	0.22143 (14)	0.0651 (7)

O3	0.4572 (3)	0.17059 (12)	0.18127 (11)	0.0357 (5)
O4	0.0056 (3)	0.18769 (12)	−0.00861 (11)	0.0324 (5)
O5	0.1019 (2)	0.12420 (11)	0.11177 (10)	0.0295 (4)
O6	−0.1564 (3)	0.07419 (13)	0.04586 (12)	0.0429 (5)
N1	0.2889 (3)	0.34430 (13)	−0.01504 (12)	0.0202 (5)
N2	0.1867 (3)	0.32986 (14)	0.14833 (12)	0.0220 (5)
N3	0.5916 (3)	0.22588 (16)	0.17027 (14)	0.0326 (5)
N4	−0.0217 (3)	0.12728 (15)	0.04871 (13)	0.0290 (5)
N5	0.4106 (3)	0.13693 (14)	−0.02096 (13)	0.0260 (5)
C1	0.3322 (3)	0.35013 (17)	−0.09734 (15)	0.0237 (6)
H1	0.3635	0.2946	−0.1267	0.028*
C2	0.3341 (3)	0.43379 (17)	−0.14275 (15)	0.0257 (6)
H2	0.3640	0.4347	−0.2019	0.031*
C3	0.2925 (3)	0.51460 (17)	−0.10130 (15)	0.0245 (6)
H3	0.2934	0.5721	−0.1315	0.029*
C4	0.2485 (3)	0.51208 (16)	−0.01379 (15)	0.0205 (5)
C5	0.2464 (3)	0.42474 (16)	0.02636 (14)	0.0189 (5)
C6	0.2058 (3)	0.59309 (17)	0.03556 (16)	0.0262 (6)
H6	0.2059	0.6525	0.0087	0.031*
C7	0.1654 (3)	0.58598 (17)	0.11965 (16)	0.0273 (6)
H7	0.1413	0.6408	0.1515	0.033*
C8	0.1583 (3)	0.49767 (18)	0.16172 (15)	0.0247 (6)
C9	0.1962 (3)	0.41704 (17)	0.11497 (14)	0.0194 (5)
C10	0.1106 (3)	0.48547 (19)	0.24808 (16)	0.0304 (7)
H10	0.0865	0.5379	0.2831	0.036*
C11	0.0991 (4)	0.3977 (2)	0.28134 (16)	0.0322 (7)
H11	0.0657	0.3888	0.3394	0.039*
C12	0.1368 (3)	0.32119 (18)	0.22956 (15)	0.0279 (6)
H12	0.1265	0.2606	0.2533	0.034*
C13	0.4936 (4)	0.10035 (17)	−0.07133 (16)	0.0268 (6)
C14	0.5977 (4)	0.05468 (19)	−0.13782 (16)	0.0413 (8)
H14A	0.7129	0.0276	−0.1115	0.062*
H14B	0.6298	0.1003	−0.1817	0.062*
H14C	0.5204	0.0054	−0.1650	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.02299 (19)	0.02063 (19)	0.02087 (18)	0.00052 (16)	0.00219 (13)	0.00219 (16)
O1	0.0333 (11)	0.0272 (10)	0.0301 (10)	−0.0034 (9)	−0.0005 (8)	0.0113 (9)
O2	0.0500 (15)	0.0784 (17)	0.0632 (15)	−0.0177 (13)	−0.0356 (12)	0.0239 (13)
O3	0.0335 (12)	0.0356 (12)	0.0380 (11)	−0.0096 (9)	0.0032 (9)	0.0136 (9)
O4	0.0351 (12)	0.0331 (11)	0.0294 (10)	0.0024 (9)	0.0050 (9)	0.0107 (8)
O5	0.0281 (11)	0.0337 (12)	0.0262 (10)	−0.0050 (8)	−0.0019 (8)	0.0061 (8)
O6	0.0332 (13)	0.0471 (14)	0.0480 (13)	−0.0188 (10)	−0.0035 (10)	0.0050 (10)
N1	0.0212 (12)	0.0221 (12)	0.0174 (11)	0.0014 (9)	0.0011 (9)	−0.0009 (9)
N2	0.0217 (12)	0.0256 (12)	0.0186 (11)	−0.0005 (9)	0.0016 (9)	0.0002 (9)
N3	0.0290 (14)	0.0320 (14)	0.0361 (13)	−0.0020 (12)	−0.0027 (11)	0.0060 (12)

N4	0.0280 (14)	0.0299 (14)	0.0292 (13)	0.0025 (11)	0.0039 (11)	−0.0020 (11)
N5	0.0272 (13)	0.0230 (13)	0.0279 (12)	0.0019 (10)	0.0010 (10)	0.0018 (10)
C1	0.0251 (15)	0.0237 (15)	0.0224 (14)	0.0019 (11)	0.0029 (11)	−0.0042 (11)
C2	0.0279 (16)	0.0305 (16)	0.0189 (13)	−0.0010 (12)	0.0025 (11)	0.0033 (12)
C3	0.0244 (15)	0.0226 (15)	0.0262 (14)	−0.0021 (11)	−0.0024 (12)	0.0055 (11)
C4	0.0172 (13)	0.0192 (14)	0.0247 (14)	−0.0016 (10)	−0.0036 (11)	−0.0001 (11)
C5	0.0171 (14)	0.0220 (14)	0.0173 (12)	0.0020 (10)	−0.0020 (10)	−0.0026 (11)
C6	0.0243 (15)	0.0188 (15)	0.0353 (16)	−0.0017 (11)	−0.0008 (12)	−0.0007 (11)
C7	0.0253 (16)	0.0226 (15)	0.0336 (16)	0.0023 (11)	−0.0020 (12)	−0.0096 (12)
C8	0.0182 (14)	0.0329 (16)	0.0227 (14)	0.0043 (11)	−0.0025 (11)	−0.0079 (12)
C9	0.0138 (13)	0.0238 (15)	0.0205 (13)	0.0001 (10)	−0.0007 (10)	0.0001 (11)
C10	0.0245 (16)	0.0394 (18)	0.0269 (15)	0.0072 (13)	−0.0014 (12)	−0.0098 (13)
C11	0.0268 (16)	0.051 (2)	0.0186 (14)	0.0054 (13)	0.0035 (12)	−0.0020 (13)
C12	0.0241 (16)	0.0372 (17)	0.0226 (14)	0.0011 (12)	0.0012 (12)	0.0043 (12)
C13	0.0263 (16)	0.0232 (15)	0.0304 (15)	0.0021 (12)	−0.0019 (13)	0.0038 (12)
C14	0.044 (2)	0.046 (2)	0.0344 (17)	0.0139 (15)	0.0064 (14)	−0.0080 (14)

Geometric parameters (Å, º)

Co—N1	2.1087 (19)	C2—H2	0.9500
Co—N2	2.1180 (19)	C3—C4	1.405 (3)
Co—N5	2.079 (2)	C3—H3	0.9500
Co—O1	2.2375 (17)	C4—C5	1.402 (3)
Co—O3	2.2583 (18)	C4—C6	1.434 (3)
Co—O4	2.3289 (19)	C5—C9	1.438 (3)
Co—O5	2.1224 (17)	C6—C7	1.350 (3)
O1—N3	1.258 (2)	C6—H6	0.9500
O2—N3	1.222 (3)	C7—C8	1.429 (3)
O3—N3	1.264 (3)	C7—H7	0.9500
O4—N4	1.264 (2)	C8—C9	1.400 (3)
O5—N4	1.283 (2)	C8—C10	1.406 (3)
O6—N4	1.227 (3)	C10—C11	1.368 (3)
N1—C1	1.328 (3)	C10—H10	0.9500
N1—C5	1.364 (3)	C11—C12	1.395 (3)
N2—C12	1.329 (3)	C11—H11	0.9500
N2—C9	1.359 (3)	C12—H12	0.9500
N5—C13	1.132 (3)	C13—C14	1.456 (3)
C1—C2	1.394 (3)	C14—H14A	0.9800
C1—H1	0.9500	C14—H14B	0.9800
C2—C3	1.367 (3)	C14—H14C	0.9800
N1—Co—N2	78.48 (7)	C3—C2—C1	119.3 (2)
N1—Co—N5	95.89 (7)	C3—C2—H2	120.3
N1—Co—O3	137.22 (7)	C1—C2—H2	120.3
N1—Co—O4	86.07 (7)	C2—C3—C4	119.6 (2)
N1—Co—O5	141.12 (7)	C2—C3—H3	120.2
N1—Co—O1	82.23 (7)	C4—C3—H3	120.2
N2—Co—N5	172.54 (8)	C5—C4—C3	117.2 (2)

N2—Co—O1	87.36 (7)	C5—C4—C6	119.0 (2)
N2—Co—O3	87.34 (7)	C3—C4—C6	123.8 (2)
N2—Co—O4	98.85 (7)	N1—C5—C4	123.0 (2)
N2—Co—O5	92.63 (7)	N1—C5—C9	117.0 (2)
N5—Co—O1	87.02 (7)	C4—C5—C9	120.0 (2)
N5—Co—O3	93.68 (7)	C7—C6—C4	120.8 (2)
N5—Co—O4	85.53 (7)	C7—C6—H6	119.6
N5—Co—O5	94.82 (7)	C4—C6—H6	119.6
O1—Co—O3	56.74 (6)	C6—C7—C8	121.3 (2)
O1—Co—O4	165.41 (6)	C6—C7—H7	119.3
O1—Co—O5	135.63 (6)	C8—C7—H7	119.3
O3—Co—O4	136.29 (6)	C9—C8—C10	116.7 (2)
O3—Co—O5	78.93 (6)	C9—C8—C7	119.3 (2)
O4—Co—O5	57.68 (6)	C10—C8—C7	124.0 (2)
N3—O1—Co	94.19 (14)	N2—C9—C8	123.6 (2)
N3—O3—Co	93.02 (14)	N2—C9—C5	116.9 (2)
N4—O4—Co	88.74 (14)	C8—C9—C5	119.5 (2)
N4—O5—Co	97.83 (13)	C11—C10—C8	119.6 (2)
C1—N1—C5	117.7 (2)	C11—C10—H10	120.2
C1—N1—Co	128.71 (16)	C8—C10—H10	120.2
C5—N1—Co	113.54 (15)	C10—C11—C12	119.7 (2)
C12—N2—C9	117.8 (2)	C10—C11—H11	120.2
C12—N2—Co	128.42 (17)	C12—C11—H11	120.2
C9—N2—Co	113.33 (15)	N2—C12—C11	122.5 (2)
O2—N3—O1	121.6 (2)	N2—C12—H12	118.7
O2—N3—O3	122.6 (2)	C11—C12—H12	118.7
O1—N3—O3	115.8 (2)	N5—C13—C14	178.5 (3)
O6—N4—O4	123.5 (2)	C13—C14—H14A	109.5
O6—N4—O5	120.9 (2)	C13—C14—H14B	109.5
O4—N4—O5	115.6 (2)	H14A—C14—H14B	109.5
C13—N5—Co	169.2 (2)	C13—C14—H14C	109.5
N1—C1—C2	123.1 (2)	H14A—C14—H14C	109.5
N1—C1—H1	118.4	H14B—C14—H14C	109.5
C2—C1—H1	118.4		