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[Bis(2-pyridyl)amine-*N*,*N*′](nitrato-*O*,*O*′)cobalt(II) nitrate. Corrigendum

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.076; data-to-parameter ratio = 12.8.

The chemical name and formula in the paper by Castillo, Luque, De la Pinta & Román [*Acta Cryst.* (2001), E**57**, m384–m386] is corrected.

In the paper by Castillo, Luque, De la Pinta & Román (2001), the ligand reported as nitrate should be carbonate and the oxidation state of the cobalt metal atom should be Co^{III} rather than Co^{II}, thus making the correct chemical composition $[Co(CO_3)(C_{10}H_9N_3)_2]NO_3$ and the correct chemical name '[Bis(2-pyridyl)amine-κ^2N,N'](carbonato-κ^2O,O')cobalt(III) nitrate'.

Experimental

Crystal data

$[Co(CO_3)(C_{10}H_9N_3)_2]NO_3$
M_r = 523.35
Monoclinic, $P2_1/n$
a = 17.191 (3) Å
b = 7.3080 (10) Å
c = 17.843 (5) Å
β = 104.94 (3)°
V = 2165.9 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 293 K
0.42 × 0.20 × 0.08 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: numerical (Stoe & Cie, 1998)
T_{min} = 0.815, T_{max} = 0.934
14084 measured reflections
4037 independent reflections
2598 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.076
S = 0.82
4037 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Data collection, cell refinement and data reduction: *IPDS Software* (Stoe & Cie, 1998); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT9068).

References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
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supporting information

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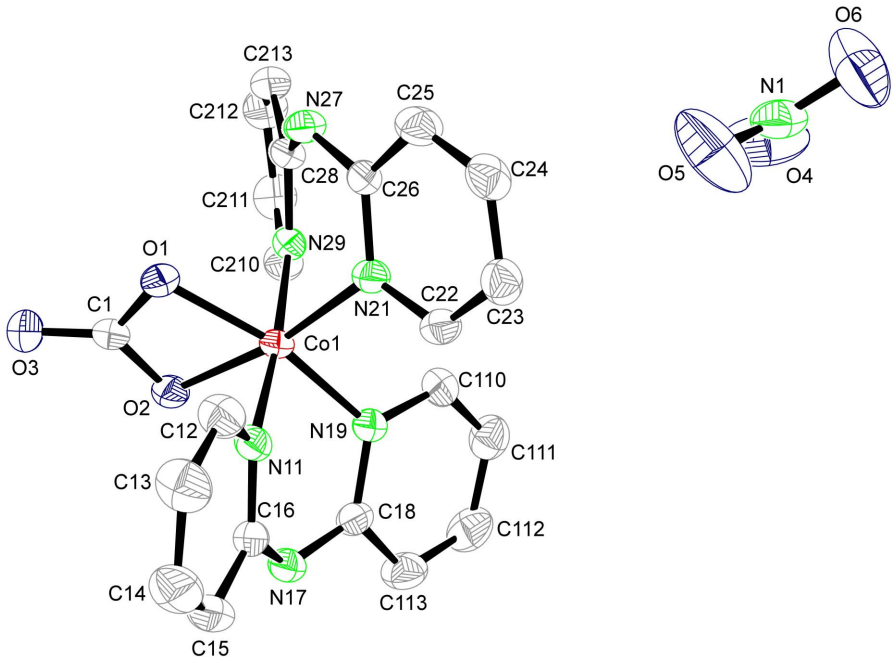

Figure 1

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[Bis(2-pyridyl)amine-κ^2N,N'](carbonato- κ^2O,O')cobalt(III) nitrate

Crystal data

$[Co(CO_3)(C_{10}H_9N_3)_2]NO_3$
$M_r = 523.35$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 17.191$ (3) Å
$b = 7.308$ (1) Å
$c = 17.843$ (5) Å
$\beta = 104.94$ (3)°
$V = 2165.9$ (8) Å^3
$Z = 4$
$F(000) = 1072$
$D_x = 1.605$ Mg m^{-3}
$D_m = 1.620$ (10) Mg m^{-3}
D_m measured by flotation in a mixture of carbon tetrachloride and bromoform
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14084 reflections
$\theta = 2.5$–25.8°
$\mu = 0.85$ mm^{-1}
$T = 293$ K
Irregular, red
0.42 × 0.20 × 0.08 mm

Data collection

Stoe IPDS diffractometer
Radiation source: x-ray tube
area detection scans
Absorption correction: numerical (Stoe & Cie, 1998)
T_{min} = 0.815, T_{max} = 0.934
14084 measured reflections
4037 independent reflections
2598 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.8°, θ_{min} = 2.5°
h = −21→20
k = −8→8
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.076
S = 0.82
4037 reflections
316 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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 on F^2 for ALL reflections except for 0 with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating _refine_ls_R_factor_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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.208061 (17)	0.99837 (6)	0.017580 (17)	0.02336 (10)
O1	0.23991 (9)	1.2048 (3)	0.08392 (10)	0.0312 (4)
O2	0.12415 (9)	1.1761 (3)	0.00121 (10)	0.0303 (4)
O3	0.14776 (12)	1.4292 (3)	0.07612 (14)	0.0527 (6)
C1	0.16896 (15)	1.2835 (4)	0.05558 (16)	0.0334 (6)
N11	0.16489 (11)	0.8897 (3)	0.09726 (11)	0.0272 (5)
N17	0.04511 (11)	0.8079 (3)	0.00592 (11)	0.0292 (5)
H17	−0.0038	0.7780	−0.0020	0.035*
N19	0.14971 (11)	0.8210 (3)	−0.05761 (11)	0.0264 (5)
N21	0.30490 (11)	0.8520 (3)	0.04848 (11)	0.0263 (5)
N27	0.38277 (11)	1.1071 (3)	0.03429 (12)	0.0296 (5)
H27	0.4362	1.1583	0.0483	0.050*
N29	0.25563 (11)	1.1244 (3)	−0.05511 (11)	0.0259 (5)
C12	0.20818 (16)	0.8977 (5)	0.17273 (14)	0.0368 (7)
H12	0.2618	0.9338	0.1836	0.044*
C13	0.17653 (18)	0.8552 (5)	0.23277 (16)	0.0475 (8)
H13	0.2080	0.8596	0.2836	0.057*
C14	0.09590 (18)	0.8048 (5)	0.21652 (17)	0.0476 (8)
H14	0.0723	0.7798	0.2568	0.057*

C15	0.05152 (16)	0.7923 (4)	0.14141 (16)	0.0388 (7)
H15	−0.0025	0.7588	0.1299	0.047*
C16	0.08865 (14)	0.8307 (4)	0.08200 (14)	0.0286 (6)
C18	0.07418 (14)	0.7711 (4)	−0.05744 (14)	0.0270 (6)
C22	0.30150 (15)	0.6729 (4)	0.06686 (15)	0.0310 (6)
H22	0.2517	0.6149	0.0551	0.037*
C23	0.36824 (16)	0.5742 (4)	0.10194 (15)	0.0360 (7)
H23	0.3643	0.4505	0.1126	0.043*
C24	0.44253 (16)	0.6626 (4)	0.12152 (16)	0.0371 (7)
H24	0.4885	0.6006	0.1486	0.045*
C25	0.44716 (15)	0.8400 (4)	0.10075 (15)	0.0368 (7)
H25	0.4966	0.8999	0.1128	0.044*
C26	0.37755 (14)	0.9325 (4)	0.06117 (14)	0.0257 (6)
C28	0.33230 (13)	1.1815 (4)	−0.03170 (14)	0.0262 (6)
C110	0.17778 (16)	0.7693 (4)	−0.11929 (15)	0.0337 (7)
H110	0.2309	0.7958	−0.1184	0.040*
C111	0.13110 (17)	0.6804 (4)	−0.18228 (15)	0.0403 (7)
H111	0.1518	0.6489	−0.2238	0.048*
C112	0.05219 (18)	0.6379 (5)	−0.18306 (16)	0.0459 (8)
H112	0.0189	0.5799	−0.2259	0.055*
C113	0.02388 (16)	0.6817 (4)	−0.12057 (16)	0.0402 (7)
H113	−0.0286	0.6522	−0.1201	0.048*
C210	0.21007 (15)	1.1863 (4)	−0.12503 (14)	0.0333 (7)
H210	0.1570	1.1467	−0.1422	0.040*
C211	0.23921 (17)	1.3034 (5)	−0.17036 (15)	0.0408 (7)
H211	0.2082	1.3357	−0.2194	0.049*
C212	0.31612 (17)	1.3739 (4)	−0.14214 (16)	0.0414 (7)
H212	0.3358	1.4613	−0.1705	0.050*
C213	0.36287 (15)	1.3141 (4)	−0.07247 (15)	0.0343 (6)
H213	0.4143	1.3612	−0.0526	0.041*
O4	0.53958 (14)	0.2616 (4)	0.07243 (14)	0.0776 (9)
O5	0.55625 (16)	0.2594 (5)	0.19487 (16)	0.0915 (10)
O6	0.63851 (15)	0.1193 (4)	0.14682 (14)	0.0788 (9)
N1	0.57871 (13)	0.2135 (4)	0.13843 (14)	0.0422 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01698 (14)	0.0260 (2)	0.02727 (16)	−0.00198 (16)	0.00593 (10)	−0.00171 (17)
O1	0.0240 (9)	0.0335 (13)	0.0360 (9)	−0.0073 (8)	0.0077 (7)	−0.0083 (8)
O2	0.0193 (8)	0.0297 (12)	0.0413 (10)	−0.0005 (8)	0.0064 (7)	−0.0016 (8)
O3	0.0444 (12)	0.0309 (15)	0.0910 (17)	−0.0032 (9)	0.0320 (12)	−0.0187 (11)
C1	0.0273 (13)	0.029 (2)	0.0489 (16)	−0.0061 (12)	0.0189 (12)	−0.0044 (13)
N11	0.0226 (10)	0.0309 (15)	0.0285 (11)	0.0006 (9)	0.0075 (8)	−0.0024 (9)
N17	0.0180 (10)	0.0356 (15)	0.0348 (12)	−0.0048 (9)	0.0081 (8)	−0.0040 (10)
N19	0.0238 (10)	0.0274 (14)	0.0286 (11)	−0.0016 (9)	0.0077 (8)	−0.0023 (9)
N21	0.0221 (10)	0.0276 (15)	0.0292 (11)	−0.0014 (9)	0.0067 (8)	−0.0001 (9)
N27	0.0196 (10)	0.0305 (16)	0.0362 (12)	−0.0046 (9)	0.0027 (9)	0.0032 (10)

N29	0.0212 (10)	0.0255 (15)	0.0309 (11)	0.0012 (9)	0.0066 (9)	−0.0011 (9)
C12	0.0308 (14)	0.047 (2)	0.0304 (14)	−0.0005 (13)	0.0048 (11)	−0.0027 (13)
C13	0.0497 (17)	0.065 (3)	0.0288 (15)	−0.0016 (16)	0.0109 (13)	0.0004 (14)
C14	0.0548 (18)	0.058 (2)	0.0374 (16)	−0.0080 (16)	0.0255 (14)	0.0009 (15)
C15	0.0331 (14)	0.044 (2)	0.0448 (17)	−0.0084 (13)	0.0192 (12)	−0.0034 (14)
C16	0.0264 (13)	0.0239 (17)	0.0367 (14)	0.0003 (11)	0.0105 (11)	−0.0014 (11)
C18	0.0238 (12)	0.0241 (17)	0.0318 (13)	−0.0012 (11)	0.0051 (10)	0.0020 (11)
C22	0.0272 (13)	0.0292 (19)	0.0374 (14)	−0.0049 (12)	0.0101 (11)	0.0010 (12)
C23	0.0407 (16)	0.0305 (18)	0.0394 (15)	0.0032 (12)	0.0151 (12)	0.0037 (12)
C24	0.0307 (14)	0.038 (2)	0.0410 (15)	0.0100 (12)	0.0066 (12)	0.0093 (13)
C25	0.0229 (13)	0.040 (2)	0.0444 (16)	0.0006 (12)	0.0032 (11)	0.0031 (13)
C26	0.0237 (12)	0.0258 (17)	0.0279 (13)	−0.0012 (10)	0.0073 (10)	−0.0027 (11)
C28	0.0211 (12)	0.0284 (18)	0.0303 (13)	−0.0006 (11)	0.0087 (10)	−0.0023 (11)
C110	0.0336 (14)	0.0332 (19)	0.0375 (15)	0.0004 (12)	0.0152 (11)	−0.0026 (12)
C111	0.0507 (17)	0.037 (2)	0.0344 (15)	−0.0013 (14)	0.0130 (13)	−0.0035 (13)
C112	0.0496 (18)	0.046 (2)	0.0364 (16)	−0.0112 (15)	0.0008 (13)	−0.0112 (14)
C113	0.0315 (14)	0.045 (2)	0.0413 (16)	−0.0094 (13)	0.0043 (12)	−0.0042 (14)
C210	0.0259 (13)	0.038 (2)	0.0326 (14)	0.0016 (12)	0.0014 (11)	−0.0021 (12)
C211	0.0472 (17)	0.043 (2)	0.0305 (14)	0.0032 (14)	0.0067 (12)	0.0060 (13)
C212	0.0491 (17)	0.038 (2)	0.0411 (16)	−0.0024 (14)	0.0188 (13)	0.0104 (14)
C213	0.0302 (14)	0.0324 (19)	0.0426 (15)	−0.0052 (12)	0.0138 (12)	−0.0004 (13)
O4	0.0512 (14)	0.106 (3)	0.0602 (15)	−0.0266 (14)	−0.0127 (12)	0.0321 (15)
O5	0.0806 (18)	0.131 (3)	0.0775 (18)	0.0419 (18)	0.0468 (16)	0.0180 (18)
O6	0.0589 (15)	0.101 (2)	0.0700 (16)	0.0344 (15)	0.0055 (13)	−0.0195 (15)
N1	0.0273 (12)	0.0479 (19)	0.0486 (15)	−0.0107 (12)	0.0046 (11)	0.0006 (13)

Geometric parameters (Å, º)

Co1—O2	1.9067 (18)	C15—C16	1.400 (4)
Co1—O1	1.9083 (18)	C15—H15	0.9300
Co1—N11	1.935 (2)	C18—C113	1.393 (4)
Co1—N21	1.935 (2)	C22—C23	1.363 (4)
Co1—N29	1.936 (2)	C22—H22	0.9300
Co1—N19	1.947 (2)	C23—C24	1.393 (4)
Co1—C1	2.343 (3)	C23—H23	0.9300
O1—C1	1.325 (3)	C24—C25	1.356 (4)
O2—C1	1.329 (3)	C24—H24	0.9300
O3—C1	1.212 (3)	C25—C26	1.397 (4)
N11—C16	1.340 (3)	C25—H25	0.9300
N11—C12	1.362 (3)	C28—C213	1.394 (4)
N17—C18	1.375 (3)	C110—C111	1.365 (4)
N17—C16	1.381 (3)	C110—H110	0.9300
N17—H17	0.8447	C111—C112	1.388 (4)
N19—C18	1.350 (3)	C111—H111	0.9300
N19—C110	1.364 (3)	C112—C113	1.365 (4)
N21—C26	1.346 (3)	C112—H112	0.9300
N21—C22	1.355 (4)	C113—H113	0.9300
N27—C26	1.374 (3)	C210—C211	1.359 (4)

N27—C28	1.381 (3)	C210—H210	0.9300
N27—H27	0.9632	C211—C212	1.387 (4)
N29—C28	1.342 (3)	C211—H211	0.9300
N29—C210	1.368 (3)	C212—C213	1.366 (4)
C12—C13	1.357 (4)	C212—H212	0.9300
C12—H12	0.9300	C213—H213	0.9300
C13—C14	1.390 (4)	O4—N1	1.247 (3)
C13—H13	0.9300	O5—N1	1.215 (3)
C14—C15	1.364 (4)	O6—N1	1.214 (3)
C14—H14	0.9300		

O2—Co1—O1	68.99 (8)	C13—C14—H14	120.1
O2—Co1—N11	88.49 (8)	C14—C15—C16	118.8 (2)
O1—Co1—N11	88.37 (8)	C14—C15—H15	120.6
O2—Co1—N21	168.88 (8)	C16—C15—H15	120.6
O1—Co1—N21	99.89 (8)	N11—C16—N17	119.5 (2)
N11—Co1—N21	91.64 (9)	N11—C16—C15	121.6 (2)
O2—Co1—N29	90.39 (8)	N17—C16—C15	118.9 (2)
O1—Co1—N29	86.35 (8)	N19—C18—N17	120.2 (2)
N11—Co1—N29	174.65 (9)	N19—C18—C113	121.5 (2)
N21—Co1—N29	88.44 (9)	N17—C18—C113	118.4 (2)
O2—Co1—N19	96.48 (8)	N21—C22—C23	122.6 (2)
O1—Co1—N19	165.44 (8)	N21—C22—H22	118.7
N11—Co1—N19	90.35 (9)	C23—C22—H22	118.7
N21—Co1—N19	94.64 (9)	C22—C23—C24	118.6 (3)
N29—Co1—N19	94.97 (9)	C22—C23—H23	120.7
O2—Co1—C1	34.55 (8)	C24—C23—H23	120.7
O1—Co1—C1	34.45 (8)	C25—C24—C23	119.3 (3)
N11—Co1—C1	87.67 (9)	C25—C24—H24	120.4
N21—Co1—C1	134.34 (9)	C23—C24—H24	120.4
N29—Co1—C1	88.45 (9)	C24—C25—C26	119.8 (3)
N19—Co1—C1	131.01 (9)	C24—C25—H25	120.1
C1—O1—Co1	91.03 (15)	C26—C25—H25	120.1
C1—O2—Co1	91.00 (15)	N21—C26—N27	119.2 (2)
O3—C1—O1	125.8 (3)	N21—C26—C25	120.7 (3)
O3—C1—O2	125.2 (3)	N27—C26—C25	120.1 (2)
O1—C1—O2	109.0 (2)	N29—C28—N27	119.6 (2)
O3—C1—Co1	178.6 (2)	N29—C28—C213	121.7 (2)
O1—C1—Co1	54.52 (13)	N27—C28—C213	118.7 (2)
O2—C1—Co1	54.46 (13)	C111—C110—N19	122.7 (2)
C16—N11—C12	118.1 (2)	C111—C110—H110	118.6
C16—N11—Co1	121.55 (17)	N19—C110—H110	118.6
C12—N11—Co1	119.59 (17)	C110—C111—C112	118.7 (3)
C18—N17—C16	127.72 (19)	C110—C111—H111	120.6
C18—N17—H17	111.6	C112—C111—H111	120.6
C16—N17—H17	117.4	C113—C112—C111	119.5 (3)
C18—N19—C110	117.9 (2)	C113—C112—H112	120.2
C18—N19—Co1	120.23 (17)	C111—C112—H112	120.2

C110—N19—Co1	120.91 (17)	C112—C113—C18	119.5 (2)
C26—N21—C22	118.5 (2)	C112—C113—H113	120.2
C26—N21—Co1	119.95 (18)	C18—C113—H113	120.2
C22—N21—Co1	121.02 (16)	C211—C210—N29	122.6 (2)
C26—N27—C28	125.4 (2)	C211—C210—H210	118.7
C26—N27—H27	114.4	N29—C210—H210	118.7
C28—N27—H27	114.6	C210—C211—C212	118.7 (3)
C28—N29—C210	117.8 (2)	C210—C211—H211	120.6
C28—N29—Co1	119.33 (16)	C212—C211—H211	120.6
C210—N29—Co1	121.81 (16)	C213—C212—C211	119.6 (3)
C13—C12—N11	122.9 (3)	C213—C212—H212	120.2
C13—C12—H12	118.6	C211—C212—H212	120.2
N11—C12—H12	118.6	C212—C213—C28	119.0 (2)
C12—C13—C14	118.5 (3)	C212—C213—H213	120.5
C12—C13—H13	120.8	C28—C213—H213	120.5
C14—C13—H13	120.8	O6—N1—O5	119.6 (3)
C15—C14—C13	119.9 (3)	O6—N1—O4	120.7 (3)
C15—C14—H14	120.1	O5—N1—O4	119.7 (3)