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Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^2N^2:$N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

 doi:10.1107/S1600536809054300

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O′-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

References

Chen, Q. (2006). *Acta Cryst.* E**62**, m56–m57.
Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2091–m2092.
Chen, J.-R., Sui, Y., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* E**64**, m562–m563.
Han, Z.-Q. (2008). *Acta Cryst.* E**64**, m592.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* E**64**, m8–m9.
Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* E**63**, m2039–m2040.
Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* E**63**, m2356–m2357.
Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* E**65**, m1161–m1162.
Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* E**62**, m1038–m1039.
Li, N.-G., Tao, R.-M. & Fu, B.-F (2007). *Acta Cryst.* E**63**, o4228.
Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* E**64**, m215.
Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* E**62**, m2507–m2508.
Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* E**62**, m2165–m2166.
Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* E**63**, m3094.
Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* E**63**, m2928.
Liu, Y.-Q. & Zeng, X.-R. (2007*a*). *Acta Cryst.* E**63**, m2547.
Liu, Y.-Q. & Zeng, X.-R. (2007*b*). *Acta Cryst.* E**63**, m2684.
Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* E**63**, m2462.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m2396.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m2854.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*a*). *Acta Cryst.* E**63**, o2892.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*b*). *Acta Cryst.* E**63**, o2932.
Qiu, X.-Y. (2006). *Acta Cryst.* E**62**, m1190–m1191.
Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* E**63**, m2135–m2136.
Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* E**63**, m2275–m2276.
Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* E**63**, m2093–m2094.
Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* E**63**, m2277–m2278.
Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m3205–m3207.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2256–m2257.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* E**63**, m2089–m2090.
Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* E**61**, m354–m355.
Wang, Q. & Fang, Z.-N. (2006). *Acta Cryst.* E**62**, m1492–m1493.
Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* E**65**, o2198.
Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* E**64**, m806–m807.
Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* E**64**, m804–m805.
Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* E**61**, m863–m864.
Yang, X.-M. (2007). *Acta Cryst.* E**63**, o4453.
Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* E**63**, m1613.
Zhang, P. (2004). *Acta Cryst.* E**60**, m1808–m1810.

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[*N*,*N*′-(*o*-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)

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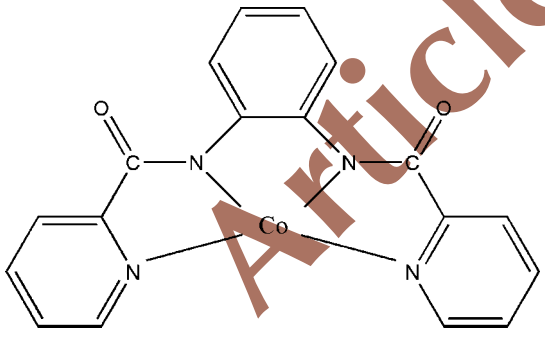
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.114; data-to-parameter ratio = 16.0.

In the title complex, $[Co(C_{18}H_{12}N_4O_2)]$, the Co^{II} ion is coordinated by four N atoms from one *o*-phenylenebis(picolinamide) ligand in a square-planar coordination geometry. Weak C—H···O hydrogen bonding exists in the crystal structure.

Related literature

For the structure of a related complex, $[Zn(C_{20}H_{14}N_2O_2)]$, see: Liu *et al.* (2007).



Experimental

Crystal data

$[Co(C_{18}H_{12}N_4O_2)]$
M_r = 375.25
Monoclinic, $P2_1/c$
a = 7.052 (2) Å
b = 18.383 (5) Å
c = 11.826 (3) Å
β = 98.827 (4)°
V = 1514.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 293 (2) K
0.31 × 0.27 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.708, T_{max} = 0.776
11141 measured reflections
3607 independent reflections
2420 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.114
S = 0.98
3607 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	1.916 (3)	Co1—N3	2.015 (3)
Co1—N2	1.926 (3)	Co1—N4	2.016 (3)
N1—Co1—N2	82.85 (12)	N1—Co1—N4	164.37 (12)
N1—Co1—N3	82.80 (12)	N2—Co1—N4	82.93 (12)
N2—Co1—N3	165.31 (13)	N3—Co1—N4	111.67 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1	0.93	2.39	2.963 (5)	120
C5—H5···O2	0.93	2.40	2.974 (5)	120
C10—H10···O1^{i}	0.93	2.59	3.200 (5)	124
C16—H16···O2^{ii}	0.93	2.54	3.344 (4)	145

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); 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: XU2308).

References

Bruker (1997). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007). *Acta Cryst.* E**63**, m2396.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m2547 [**doi:10.1107/S1600536807044571**]

[*N*,*N*'-(*o*-Phenylene)bis(picolinamido)-κ^4*N*,*N*',*N*'',*N*''']cobalt(II)

Y.-Q. Liu and X.-R. Zeng

Comment

Transition metal complexes with organic ligands, possessing diverse structures and special optical and electromagnetic properties, have aroused great interest among researchers. In the title complex, each cobalt(II) ion is four-coordinated in a square-planar geometry by four N atoms from one *N*-(2-(picolinamido)phenyl)picolinamide molecule (Fig. 1). The Co—N bond lengths are listed in Table 1. Atom N1, N2, N3 and N4 are approximately coplanar with the central Co1 ion, the maximum deviation from the least-squares plane through all five atoms being 0.0816 (1) Å for atom N1.

π-π stacking is observed between benzene ring and N3^{i}-pyridine [symmetry code: (i) −*x*, 1 − *y*, −*z*], verified by the centroid–centroid distance of 3.818 (2) Å and dihedral angle of 3.08° No strong hydrogen bonds exist in the crystal, but weak C—H···O hydrogen bonding occurs in the crystal structure (Table 2).

Experimental

A mixture of *N*-(2-(picolinamido)phenyl)picolinamide (0.316 g, 1 mmol) and $Co(NO_3)_2{\cdot}6H_2O$ (0.291 g, 1 mmol) was dissolved in ethanol (20 ml). The mixture was closed in a steel tomb and heated at 418 K for 4 d. Single crystals suitable for X-ray diffraction analysis were obtained after cooling to room temperature.

Refinement

All H atoms were located at calculated positions with C—h = 0.93 Å and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C).

Figures

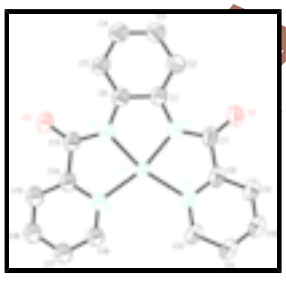

Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids.

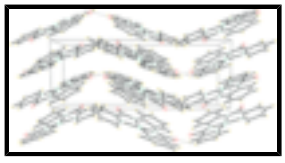

Fig. 2. The packing diagram of (I), viewed along *c* axis, Hydrogen bonds shown as dash lines.

[*N*,*N*'-(*o*-Phenylene)bis(picolinamido)- κ^4*N*,*N*',*N*'',*N*''']cobalt(II)

Crystal data

$[Co(C_{18}H_{12}N_4O_2)]$

$M_r = 375.25$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.052$ (2) Å

$b = 18.383$ (5) Å

$c = 11.826$ (3) Å

$\beta = 98.827$ (4)°

$V = 1514.8$ (7) Å^3

$Z = 4$

$F_{000} = 764.0$

$D_x = 1.645$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 6407 reflections

$\theta = 2.8$–27.9°

$\mu = 1.15$ mm^{-1}

$T = 293$ (2) K

Block, brown

0.31 × 0.27 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2002)

$T_{min} = 0.708$, $T_{max} = 0.776$

11141 measured reflections

3607 independent reflections

2420 reflections with $I > 2\sigma(I)$

$R_{int} = 0.036$

$\theta_{max} = 28.3$°

$\theta_{min} = 2.1$°

$h = -8\rightarrow9$

$k = -24\rightarrow24$

$l = -15\rightarrow15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.114$

$S = 0.98$

3607 reflections

226 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 2.409P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.58$ e Å^{-3}

$\Delta\rho_{min} = -0.67$ e Å^{-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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1858 (5)	0.51706 (18)	−0.1917 (3)	0.0499 (8)
C2	0.1192 (6)	0.5110 (2)	−0.3077 (3)	0.0545 (9)
H2	0.0519	0.4698	−0.3364	0.065*
C3	0.1539 (6)	0.5673 (2)	−0.3815 (3)	0.0573 (10)
H3	0.1084	0.5636	−0.4593	0.069*
C4	0.2551 (6)	0.6282 (2)	−0.3395 (3)	0.0560 (9)
H4	0.2795	0.6649	−0.3895	0.067*
C5	0.3209 (5)	0.63537 (19)	−0.2233 (3)	0.0526 (9)
H5	0.3876	0.6770	−0.1957	0.063*
C6	0.2872 (5)	0.58037 (18)	−0.1481 (3)	0.0489 (9)
C7	0.0889 (5)	0.39877 (18)	−0.1229 (3)	0.0519 (9)
C8	0.0961 (5)	0.35929 (18)	−0.0110 (3)	0.0520 (9)
C9	0.0198 (5)	0.29003 (19)	−0.0069 (4)	0.0563 (10)
H9	−0.0388	0.2673	−0.0734	0.068*
C10	0.0321 (6)	0.25519 (19)	0.0976 (4)	0.0586 (10)
H10	−0.0186	0.2087	0.1019	0.070*
C11	0.1191 (5)	0.28933 (19)	0.1943 (4)	0.0569 (10)
H11	0.1295	0.2664	0.2651	0.068*
C12	0.1920 (5)	0.35912 (18)	0.1852 (4)	0.0537 (9)
H12	0.2512	0.3825	0.2510	0.064*
C13	0.4128 (5)	0.63559 (17)	0.0370 (3)	0.0506 (9)
C14	0.4296 (5)	0.61761 (18)	0.1615 (3)	0.0510 (9)
C15	0.4930 (6)	0.6686 (2)	0.2440 (3)	0.0555 (9)
H15	0.5304	0.7146	0.2230	0.067*
C16	0.5007 (6)	0.6509 (2)	0.3582 (3)	0.0581 (10)
H16	0.5417	0.6849	0.4149	0.070*
C17	0.4466 (6)	0.5820 (2)	0.3865 (3)	0.0573 (10)
H17	0.4516	0.5685	0.4627	0.069*
C18	0.3848 (6)	0.5335 (2)	0.2996 (3)	0.0538 (9)
H18	0.3484	0.4871	0.3191	0.065*
Co1	0.27021 (6)	0.49353 (2)	0.04659 (4)	0.03724 (14)
N1	0.1613 (4)	0.46612 (15)	−0.1059 (3)	0.0487 (7)
N2	0.3428 (4)	0.57967 (14)	−0.0291 (3)	0.0477 (7)

N3	0.1795 (4)	0.39377 (14)	0.0844 (3)	0.0503 (7)
N4	0.3747 (4)	0.54978 (15)	0.1889 (3)	0.0502 (7)
O1	0.0223 (4)	0.36877 (13)	−0.2134 (2)	0.0581 (7)
O2	0.4601 (4)	0.69679 (12)	0.0071 (2)	0.0561 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.058 (2)	0.0421 (18)	0.050 (2)	0.0018 (15)	0.0098 (17)	−0.0009 (15)
C2	0.062 (2)	0.050 (2)	0.052 (2)	0.0025 (17)	0.0091 (18)	−0.0002 (17)
C3	0.065 (3)	0.054 (2)	0.053 (2)	0.0039 (18)	0.010 (2)	0.0036 (18)
C4	0.064 (2)	0.051 (2)	0.054 (2)	0.0044 (18)	0.0116 (19)	0.0064 (17)
C5	0.061 (2)	0.0445 (19)	0.054 (2)	0.0032 (16)	0.0121 (19)	0.0060 (16)
C6	0.058 (2)	0.0388 (17)	0.051 (2)	0.0018 (15)	0.0113 (18)	0.0032 (15)
C7	0.058 (2)	0.0372 (17)	0.061 (2)	−0.0034 (15)	0.0095 (19)	−0.0082 (16)
C8	0.056 (2)	0.0337 (17)	0.067 (2)	−0.0029 (15)	0.0128 (19)	−0.0036 (16)
C9	0.060 (2)	0.0366 (18)	0.074 (3)	−0.0034 (16)	0.014 (2)	−0.0023 (18)
C10	0.062 (3)	0.0384 (18)	0.077 (3)	−0.0029 (16)	0.015 (2)	0.0028 (19)
C11	0.062 (2)	0.0375 (18)	0.073 (3)	−0.0021 (16)	0.016 (2)	0.0071 (18)
C12	0.059 (2)	0.0354 (17)	0.068 (2)	−0.0016 (15)	0.0153 (19)	0.0072 (16)
C13	0.060 (2)	0.0334 (17)	0.058 (2)	−0.0046 (15)	0.0104 (19)	−0.0018 (15)
C14	0.061 (2)	0.0363 (17)	0.056 (2)	−0.0030 (15)	0.0095 (18)	−0.0065 (15)
C15	0.065 (2)	0.0416 (19)	0.059 (2)	−0.0029 (17)	0.0088 (19)	−0.0092 (17)
C16	0.069 (3)	0.047 (2)	0.058 (2)	−0.0019 (17)	0.008 (2)	−0.0107 (17)
C17	0.070 (3)	0.048 (2)	0.054 (2)	−0.0012 (18)	0.009 (2)	−0.0086 (17)
C18	0.067 (3)	0.0446 (19)	0.050 (2)	−0.0017 (17)	0.0091 (19)	−0.0060 (16)
Co1	0.0450 (3)	0.0240 (2)	0.0429 (2)	0.00014 (17)	0.00702 (18)	−0.00024 (18)
N1	0.0566 (18)	0.0376 (14)	0.0520 (17)	−0.0022 (13)	0.0090 (15)	−0.0046 (13)
N2	0.0580 (19)	0.0330 (14)	0.0527 (17)	−0.0026 (12)	0.0103 (14)	0.0017 (12)
N3	0.0558 (19)	0.0321 (14)	0.0643 (19)	−0.0019 (12)	0.0137 (16)	0.0025 (13)
N4	0.0617 (19)	0.0385 (15)	0.0507 (18)	−0.0019 (13)	0.0097 (15)	−0.0054 (13)
O1	0.0637 (17)	0.0441 (13)	0.0657 (17)	−0.0042 (12)	0.0071 (14)	−0.0120 (12)
O2	0.0665 (18)	0.0362 (13)	0.0658 (17)	−0.0076 (11)	0.0105 (14)	0.0002 (11)

Geometric parameters (Å, °)

C1—C2	1.385 (5)	C11—C12	1.392 (5)
C1—N1	1.411 (5)	C11—H11	0.9300
C1—C6	1.420 (5)	C12—N3	1.342 (5)
C2—C3	1.399 (5)	C12—H12	0.9300
C2—H2	0.9300	C13—O2	1.240 (4)
C3—C4	1.379 (5)	C13—N2	1.339 (4)
C3—H3	0.9300	C13—C14	1.496 (5)
C4—C5	1.387 (5)	C14—N4	1.359 (4)
C4—H4	0.9300	C14—C15	1.377 (5)
C5—C6	1.390 (5)	C15—C16	1.382 (5)
C5—H5	0.9300	C15—H15	0.9300
C6—N2	1.402 (4)	C16—C17	1.379 (5)
C7—O1	1.231 (4)	C16—H16	0.9300

C7—N1	1.343 (4)	C17—C18	1.380 (5)
C7—C8	1.503 (5)	C17—H17	0.9300
C8—N3	1.349 (5)	C18—N4	1.334 (5)
C8—C9	1.386 (5)	C18—H18	0.9300
C9—C10	1.382 (5)	Co1—N1	1.916 (3)
C9—H9	0.9300	Co1—N2	1.926 (3)
C10—C11	1.365 (5)	Co1—N3	2.015 (3)
C10—H10	0.9300	Co1—N4	2.016 (3)
C2—C1—N1	126.8 (3)	O2—C13—N2	128.4 (3)
C2—C1—C6	120.0 (3)	O2—C13—C14	119.8 (3)
N1—C1—C6	113.2 (3)	N2—C13—C14	111.8 (3)
C1—C2—C3	119.5 (4)	N4—C14—C15	122.0 (4)
C1—C2—H2	120.3	N4—C14—C13	117.0 (3)
C3—C2—H2	120.3	C15—C14—C13	121.0 (3)
C4—C3—C2	120.5 (4)	C14—C15—C16	119.4 (4)
C4—C3—H3	119.8	C14—C15—H15	120.3
C2—C3—H3	119.8	C16—C15—H15	120.3
C3—C4—C5	120.6 (4)	C17—C16—C15	118.9 (4)
C3—C4—H4	119.7	C17—C16—H16	120.5
C5—C4—H4	119.7	C15—C16—H16	120.5
C4—C5—C6	120.0 (4)	C16—C17—C18	118.7 (4)
C4—C5—H5	120.0	C16—C17—H17	120.7
C6—C5—H5	120.0	C18—C17—H17	120.7
C5—C6—N2	126.8 (3)	N4—C18—C17	123.3 (4)
C5—C6—C1	119.3 (3)	N4—C18—H18	118.4
N2—C6—C1	113.8 (3)	C17—C18—H18	118.4
O1—C7—N1	129.0 (4)	N1—Co1—N2	82.85 (12)
O1—C7—C8	120.4 (3)	N1—Co1—N3	82.80 (12)
N1—C7—C8	110.7 (3)	N2—Co1—N3	165.31 (13)
N3—C8—C9	121.6 (4)	N1—Co1—N4	164.37 (12)
N3—C8—C7	117.5 (3)	N2—Co1—N4	82.93 (12)
C9—C8—C7	120.9 (3)	N3—Co1—N4	111.67 (12)
C10—C9—C8	119.1 (4)	C7—N1—C1	126.2 (3)
C10—C9—H9	120.5	C7—N1—Co1	118.2 (3)
C8—C9—H9	120.5	C1—N1—Co1	115.3 (2)
C11—C10—C9	119.6 (3)	C13—N2—C6	126.9 (3)
C11—C10—H10	120.2	C13—N2—Co1	117.4 (2)
C9—C10—H10	120.2	C6—N2—Co1	114.9 (2)
C10—C11—C12	118.9 (4)	C12—N3—C8	118.8 (3)
C10—C11—H11	120.6	C12—N3—Co1	130.5 (2)
C12—C11—H11	120.6	C8—N3—Co1	110.7 (2)
N3—C12—C11	122.1 (4)	C18—N4—C14	117.7 (3)
N3—C12—H12	119.0	C18—N4—Co1	131.4 (2)
C11—C12—H12	119.0	C14—N4—Co1	110.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.93	2.39	2.963 (5)	120

C5—H5···O2	0.93	2.40	2.974 (5)	120
C10—H10···O1^{i}	0.93	2.59	3.200 (5)	124
C16—H16···O2^{ii}	0.93	2.54	3.344 (4)	145

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

Fig. 1

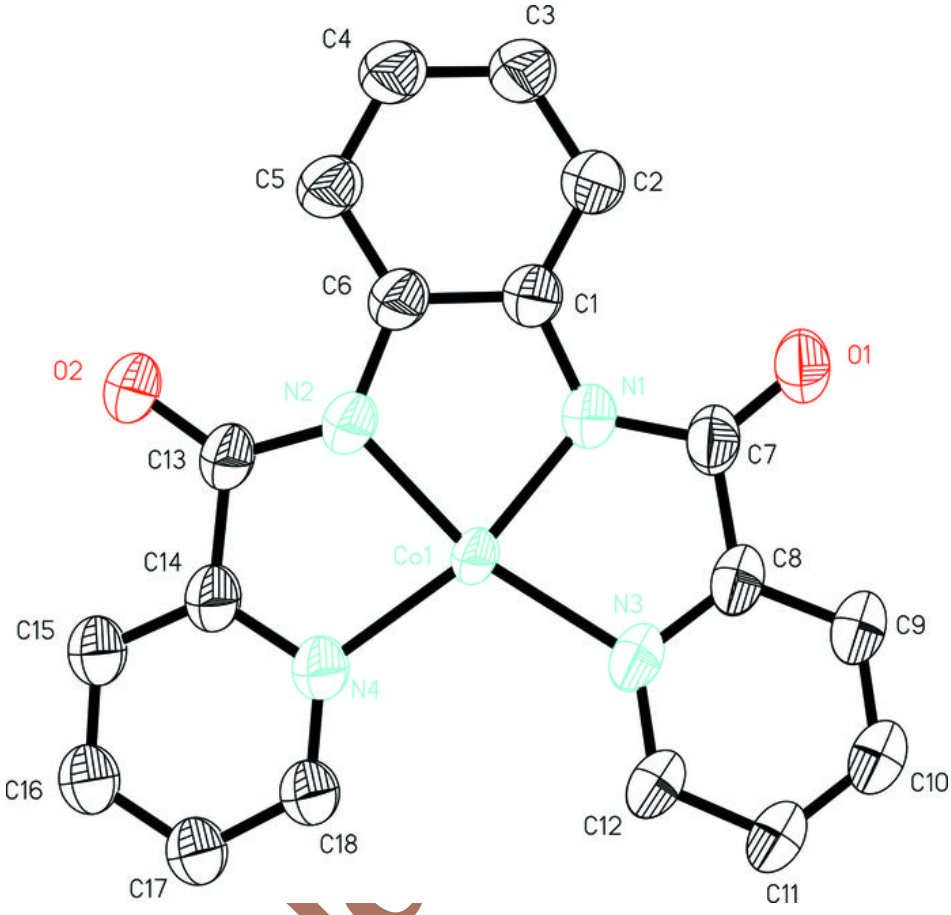

Fig. 2