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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

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[*N*,*N*′-(*o*-Phenylene)dipicolinamide-κ^4N]-nickel(II)

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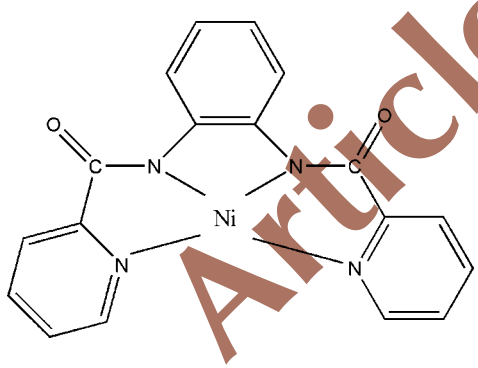
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.045; wR factor = 0.119; data-to-parameter ratio = 12.3.

The title compound, $[Ni(C_{18}H_{12}N_4O_2)]$, which was synthesized by reaction of *N*-[2-(picolinamido)phenyl]picolinamide with $Ni(NO_3)_2{\cdot}6H_2O$ in ethanol, is a mononuclear complex in which the nickel(II) ion is coordinated by four N atoms and displays a distorted square-planar coordination geometry.

Related literature

For related literature, see: Liu *et al.* (2007).



Experimental

Crystal data

$[Ni(C_{18}H_{12}N_4O_2)]$
M_r = 375.01
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 = 1.30 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*; Bruker, 1997)
T_{min} = 0.679, T_{max} = 0.750
9286 measured reflections
2784 independent reflections
2087 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.119
S = 1.00
2784 reflections
226 parameters
234 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); 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* (Siemens, 1996); 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: BV2070).

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Siemens (1996). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2007). E**63**, m2684 [**doi:10.1107/S1600536807048386**]

[*N*,*N*'-(*o*-Phenylene)dipicolinamide-κ^4N]nickel(II)

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

Comment

As shown in Fig. 1, the title compound is a mononuclear complex in which each nickel(II) ion is coordinated by four N atoms from the same *N*-(2-(picolinamido)phenyl)picolinamide molecule and displays a distorted planar quadrilateral coordination geometry. The coordination bonds of Ni1—N are between 1.920 (4) Å and 2.016 (4) Å, atoms N1, N2, N3, and N4 are approximately coplanar with the central nickel(II) ion with a maximum deviation from the least squares plane of 0.0876 (2) Å for atom N1. Along the *a* axis, the benzene rings and pyridine rings of adjacent *N*-(2-(picolinamido)phenyl)picolinamide molecules are nearly parallel to each other impling there may exist π-π interactions between them. In the complex no classical hydrogen bonds are found and the three-dimensional network of the crystal is mainly consolidated by π-π interactions and weak interactions involving O atoms and the H atoms of adjacent pyridine rings.

Experimental

A mixture of *N*-(2-(picolinamido)phenyl)picolinamide(0.314 g, 0.001 mol) and $Ni(NO_3)_2{\cdot}6H_2O$(0.288 g, 0.001 mol) was added to 20 ml e thanol, The mixture was closed in a steel tomb and heated at 418 K for 4 days, Single crystals suitable for X-ray diffraction analysis formed after it cooled down untouched in the air.

Refinement

All H atoms were located at calculated positions and refined as riding on their parent C atoms with the C—H bond length fixed at 0.93Å with U_{iso}(H) = 1.2 times U_{eq}(C). In the final refinement cycles the anistropic parameters of atoms bonding to each other were constrained to be approximately equal.

Figures

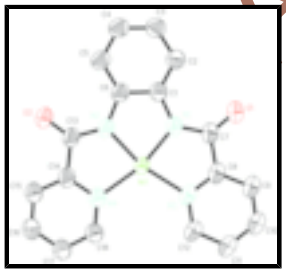

Fig. 1. The molecular unit of (I), showing 50% probability displacement ellipsoids.

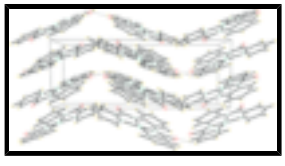

Fig. 2. The packing diagram of (I), viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

[*N*,*N*'-(*o*-Phenylene)dipicolinamide-κ^4*N*]nickel(II)

Crystal data

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

M_r = 375.01

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

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

F_{000} = 768.0

D_x = 1.644 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å

Cell parameters from 6201 reflections

θ = 2.8–27.9°

μ = 1.30 mm^{-1}

T = 293 (2) K

Block, blue

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; Bruker, 1997)

T_{min} = 0.679, T_{max} = 0.750

9286 measured reflections

2784 independent reflections

2087 reflections with $I > 2\sigma(I)$

R_{int} = 0.035

θ_{max} = 25.5°

θ_{min} = 2.1°

h = −8→8

k = −22→22

l = −14→14

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.045

$wR(F^2)$ = 0.119

S = 1.00

2784 reflections

226 parameters

234 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

$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 1.4239P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.003

$\Delta\rho_{max}$ = 0.48 e Å^{-3}

$\Delta\rho_{min}$ = −0.56 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}
Ni1	0.27023 (8)	0.49353 (2)	0.04659 (5)	0.0392 (2)
N4	0.3749 (5)	0.54985 (19)	0.1888 (3)	0.0491 (5)
C18	0.3852 (7)	0.5336 (3)	0.2993 (4)	0.0525 (6)
H18	0.3490	0.4871	0.3189	0.063*
C17	0.4466 (7)	0.5821 (2)	0.3866 (4)	0.0557 (6)
H17	0.4515	0.5686	0.4627	0.067*
C16	0.5004 (7)	0.6508 (3)	0.3581 (4)	0.0562 (6)
H16	0.5412	0.6848	0.4148	0.067*
C15	0.4931 (7)	0.6685 (3)	0.2443 (4)	0.0537 (6)
H15	0.5306	0.7144	0.2234	0.064*
C14	0.4297 (7)	0.6176 (2)	0.1617 (4)	0.0496 (5)
C13	0.4132 (7)	0.6356 (2)	0.0369 (4)	0.0492 (5)
C6	0.2871 (7)	0.5805 (2)	−0.1482 (4)	0.0479 (5)
C5	0.3207 (7)	0.6352 (2)	−0.2235 (4)	0.0513 (6)
H5	0.3875	0.6768	−0.1959	0.062*
C4	0.2551 (7)	0.6281 (3)	−0.3395 (4)	0.0545 (6)
H4	0.2796	0.6647	−0.3896	0.065*
C3	0.1537 (7)	0.5672 (3)	−0.3814 (4)	0.0556 (6)
H3	0.1078	0.5636	−0.4592	0.067*
C2	0.1194 (7)	0.5110 (2)	−0.3080 (4)	0.0530 (6)
H2	0.0524	0.4697	−0.3367	0.064*
C1	0.1860 (7)	0.5172 (2)	−0.1916 (4)	0.0487 (5)
C7	0.0884 (7)	0.3988 (2)	−0.1232 (4)	0.0508 (5)
C8	0.0954 (7)	0.3593 (2)	−0.0110 (4)	0.0509 (5)
C9	0.0197 (7)	0.2900 (3)	−0.0066 (4)	0.0548 (6)
H9	−0.0386	0.2672	−0.0731	0.066*
C10	0.0318 (7)	0.2553 (2)	0.0974 (4)	0.0570 (6)
H10	−0.0191	0.2089	0.1017	0.068*
C11	0.1188 (7)	0.2894 (2)	0.1942 (4)	0.0554 (6)
H11	0.1289	0.2664	0.2649	0.067*
C12	0.1923 (7)	0.3591 (2)	0.1851 (4)	0.0524 (6)
H12	0.2520	0.3823	0.2509	0.063*
N3	0.1797 (5)	0.39376 (18)	0.0844 (3)	0.0492 (5)

N1	0.1611 (5)	0.46607 (19)	−0.1063 (3)	0.0477 (5)
N2	0.3430 (5)	0.57963 (18)	−0.0291 (3)	0.0467 (5)
O1	0.0220 (5)	0.36873 (16)	−0.2133 (3)	0.0565 (6)
O2	0.4605 (4)	0.69673 (16)	0.0071 (3)	0.0542 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0475 (4)	0.0257 (3)	0.0445 (3)	0.0000 (2)	0.0071 (2)	−0.0003 (2)
N4	0.0594 (12)	0.0381 (9)	0.0502 (8)	−0.0017 (9)	0.0098 (10)	−0.0048 (7)
C18	0.0640 (13)	0.0437 (11)	0.0501 (8)	−0.0017 (11)	0.0093 (12)	−0.0053 (8)
C17	0.0667 (14)	0.0470 (12)	0.0532 (10)	−0.0011 (11)	0.0087 (12)	−0.0080 (9)
C16	0.0660 (14)	0.0458 (11)	0.0566 (10)	−0.0014 (11)	0.0085 (12)	−0.0101 (10)
C15	0.0625 (13)	0.0408 (10)	0.0578 (10)	−0.0023 (10)	0.0088 (12)	−0.0086 (9)
C14	0.0584 (11)	0.0359 (9)	0.0549 (8)	−0.0023 (8)	0.0095 (10)	−0.0059 (7)
C13	0.0583 (11)	0.0329 (8)	0.0569 (9)	−0.0038 (8)	0.0101 (9)	−0.0018 (7)
C6	0.0558 (11)	0.0379 (9)	0.0507 (8)	0.0020 (8)	0.0108 (9)	0.0026 (7)
C5	0.0587 (13)	0.0433 (10)	0.0528 (10)	0.0032 (10)	0.0117 (11)	0.0052 (9)
C4	0.0617 (13)	0.0495 (11)	0.0530 (10)	0.0045 (10)	0.0113 (11)	0.0056 (10)
C3	0.0625 (13)	0.0521 (12)	0.0525 (10)	0.0041 (11)	0.0095 (11)	0.0028 (9)
C2	0.0598 (13)	0.0480 (11)	0.0514 (9)	0.0028 (10)	0.0089 (11)	−0.0007 (9)
C1	0.0559 (11)	0.0408 (9)	0.0499 (7)	0.0020 (8)	0.0095 (9)	−0.0012 (7)
C7	0.0559 (11)	0.0366 (9)	0.0601 (9)	−0.0029 (8)	0.0097 (9)	−0.0076 (7)
C8	0.0544 (11)	0.0338 (8)	0.0656 (10)	−0.0025 (8)	0.0129 (10)	−0.0034 (7)
C9	0.0577 (13)	0.0363 (10)	0.0717 (12)	−0.0031 (9)	0.0139 (11)	−0.0023 (9)
C10	0.0599 (13)	0.0378 (11)	0.0748 (13)	−0.0027 (10)	0.0155 (12)	0.0026 (9)
C11	0.0595 (13)	0.0372 (11)	0.0714 (12)	−0.0016 (10)	0.0158 (12)	0.0065 (9)
C12	0.0573 (13)	0.0353 (10)	0.0664 (11)	−0.0011 (10)	0.0151 (12)	0.0063 (8)
N3	0.0540 (12)	0.0323 (9)	0.0629 (10)	−0.0015 (9)	0.0136 (11)	0.0020 (7)
N1	0.0549 (11)	0.0367 (9)	0.0518 (8)	−0.0018 (8)	0.0090 (9)	−0.0044 (7)
N2	0.0562 (11)	0.0325 (8)	0.0519 (8)	−0.0019 (8)	0.0098 (9)	0.0012 (7)
O1	0.0618 (13)	0.0426 (11)	0.0642 (11)	−0.0040 (10)	0.0072 (11)	−0.0110 (9)
O2	0.0641 (13)	0.0352 (10)	0.0633 (12)	−0.0068 (10)	0.0101 (12)	−0.0001 (9)

Geometric parameters (Å, °)

Ni1—N1	1.920 (4)	C5—H5	0.9300
Ni1—N2	1.926 (3)	C4—C3	1.378 (7)
Ni1—N4	2.016 (4)	C4—H4	0.9300
Ni1—N3	2.015 (3)	C3—C2	1.395 (6)
N4—C18	1.332 (6)	C3—H3	0.9300
N4—C14	1.357 (5)	C2—C1	1.389 (7)
C18—C17	1.382 (6)	C2—H2	0.9300
C18—H18	0.9300	C1—N1	1.409 (6)
C17—C16	1.374 (7)	C7—O1	1.228 (5)
C17—H17	0.9300	C7—N1	1.342 (5)
C16—C15	1.378 (7)	C7—C8	1.506 (7)
C16—H16	0.9300	C8—N3	1.350 (6)
C15—C14	1.375 (6)	C8—C9	1.385 (6)

C15—H15	0.9300	C9—C10	1.377 (6)
C14—C13	1.500 (6)	C9—H9	0.9300
C13—O2	1.238 (5)	C10—C11	1.365 (7)
C13—N2	1.339 (5)	C10—H10	0.9300
C6—C5	1.388 (6)	C11—C12	1.392 (6)
C6—N2	1.403 (6)	C11—H11	0.9300
C6—C1	1.419 (6)	C12—N3	1.341 (6)
C5—C4	1.386 (6)	C12—H12	0.9300
N1—Ni1—N2	82.83 (15)	C4—C3—C2	120.6 (5)
N1—Ni1—N4	164.32 (15)	C4—C3—H3	119.7
N2—Ni1—N4	82.89 (15)	C2—C3—H3	119.7
N1—Ni1—N3	82.82 (16)	C1—C2—C3	119.4 (5)
N2—Ni1—N3	165.30 (16)	C1—C2—H2	120.3
N4—Ni1—N3	111.72 (15)	C3—C2—H2	120.3
C18—N4—C14	117.6 (4)	C2—C1—N1	126.5 (4)
C18—N4—Ni1	131.4 (3)	C2—C1—C6	120.0 (4)
C14—N4—Ni1	110.8 (3)	N1—C1—C6	113.4 (4)
N4—C18—C17	123.4 (5)	O1—C7—N1	129.1 (5)
N4—C18—H18	118.3	O1—C7—C8	120.3 (4)
C17—C18—H18	118.3	N1—C7—C8	110.7 (4)
C18—C17—C16	118.5 (5)	N3—C8—C9	121.5 (4)
C18—C17—H17	120.8	N3—C8—C7	117.5 (4)
C16—C17—H17	120.8	C9—C8—C7	121.1 (4)
C17—C16—C15	119.1 (4)	C10—C9—C8	119.3 (5)
C17—C16—H16	120.5	C10—C9—H9	120.4
C15—C16—H16	120.5	C8—C9—H9	120.4
C14—C15—C16	119.4 (4)	C11—C10—C9	119.6 (4)
C14—C15—H15	120.3	C11—C10—H10	120.2
C16—C15—H15	120.3	C9—C10—H10	120.2
N4—C14—C15	122.0 (4)	C10—C11—C12	118.9 (5)
N4—C14—C13	116.9 (4)	C10—C11—H11	120.6
C15—C14—C13	121.1 (4)	C12—C11—H11	120.6
O2—C13—N2	128.5 (4)	N3—C12—C11	122.1 (5)
O2—C13—C14	119.7 (4)	N3—C12—H12	119.0
N2—C13—C14	111.7 (4)	C11—C12—H12	119.0
C5—C6—N2	127.0 (4)	C12—N3—C8	118.7 (4)
C5—C6—C1	119.2 (4)	C12—N3—Ni1	130.5 (3)
N2—C6—C1	113.7 (4)	C8—N3—Ni1	110.8 (3)
C6—C5—C4	120.2 (5)	C7—N1—C1	126.5 (4)
C6—C5—H5	119.9	C7—N1—Ni1	118.1 (3)
C4—C5—H5	119.9	C1—N1—Ni1	115.0 (3)
C3—C4—C5	120.5 (5)	C13—N2—C6	126.7 (4)
C3—C4—H4	119.7	C13—N2—Ni1	117.5 (3)
C5—C4—H4	119.7	C6—N2—Ni1	114.9 (3)

Fig. 1

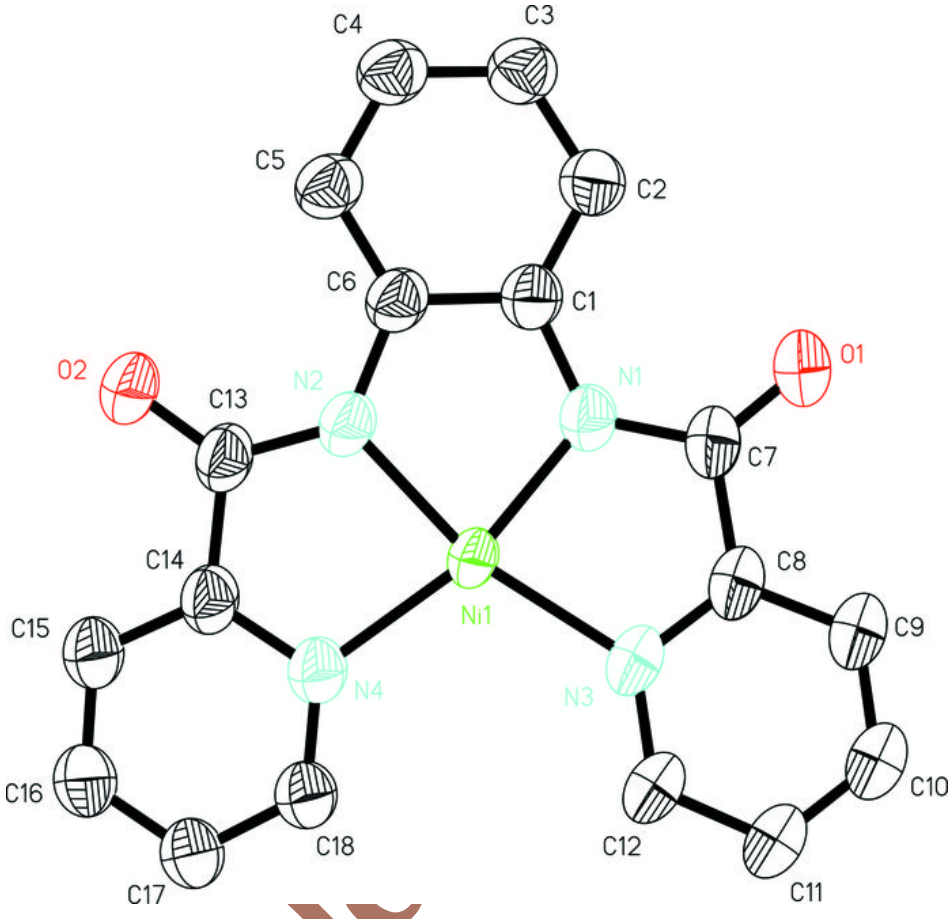

Fig. 2