

Crystal structure of bis(2,2':6',2''-terpyridine- κ^3N,N',N'')nickel(II) dicyanidoaurate(I)

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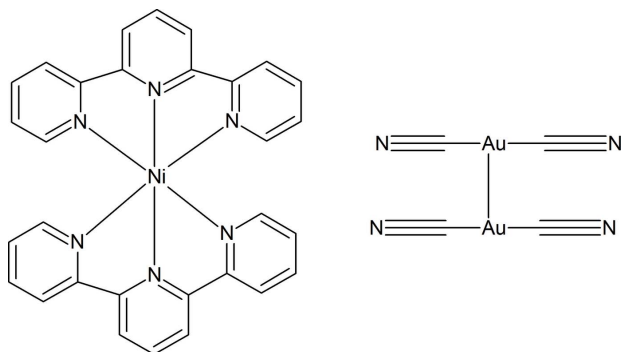
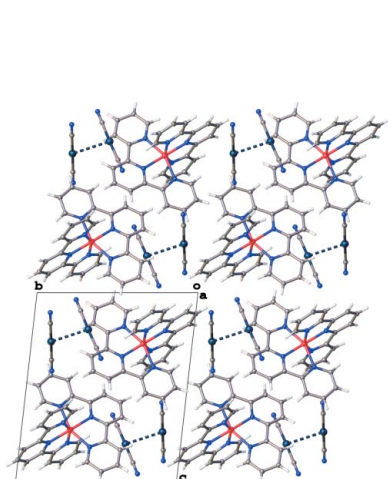
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Keywords: crystal structure; terpyridine; aurophilic interaction; dicyanidoaurate**CCDC reference:** 1033527**Supporting information:** this article has supporting information at journals.iucr.org/e

The title compound, $[\text{Ni}(\text{C}_{15}\text{H}_{11}\text{N}_3)_2][\text{Au}(\text{CN})_2]_2$, is an ionic compound composed of bis(2,2':6',2''-terpyridine)nickel(II) dication and dicyanidoaurate(I) anions in a 1:2 ratio. The two tridentate terpyridine ligands define the coordination of the Ni^{2+} cation, resulting in a nearly octahedral coordination sphere, although there is not any imposed crystallographic symmetry about the Ni^{2+} site. The two nearly linear dicyanidoaurate(I) anions [$\text{C}-\text{Au}-\text{C} = 179.0(2)$ and $178.2(2)^\circ$] contain a short aurophilic interaction of $3.1017(3)$ Å. The structure does not demonstrate any $\pi-\pi$ stacking. Non-classical $\text{C}-\text{H}\cdots\text{N}$ interactions between the cations and anions build up a three-dimensional network.

1. Chemical context

Derivatives of the compound $[\text{M}(\text{terpy})_2](\text{X})$ (M = transition metal; terpy = 2,2':6',2''-terpyridine; X = anion) have been known since the 1970's (Harris & Lockyer, 1970). Transition metal-terpyridine complexes have been known to exhibit interesting properties such as their photophysical and spin-state properties (Pal *et al.*, 2014). These allow transition metal-terpyridine complexes to have useful applications in molecular electronics and as building blocks for copolymers (Katz *et al.*, 2008; Pal *et al.*, 2014; Schubert *et al.*, 2001). However, it was not until recently that the incorporation of gold cyanidometallates has been introduced into these systems (Ovens *et al.*, 2010). We report here the synthesis and crystal structure of another metal-terpyridine cyanidoaurate, $[\text{Ni}(\text{C}_{15}\text{H}_{11}\text{N}_3)_2][\text{Au}(\text{CN})_2]_2$, (I).



2. Structural commentary

The structure of compound (I) contains an Ni^{2+} ion coordinated by two tridentate 2,2':6',2''-terpyridine ligands. The coordination of the terpyridine ligands around the metal cation gives an approximate octahedral coordination sphere. Included in the structure are two dicyanidoaurate(I) anions that are non-coordinating to the Ni^{2+} cation, as shown in Fig. 1.

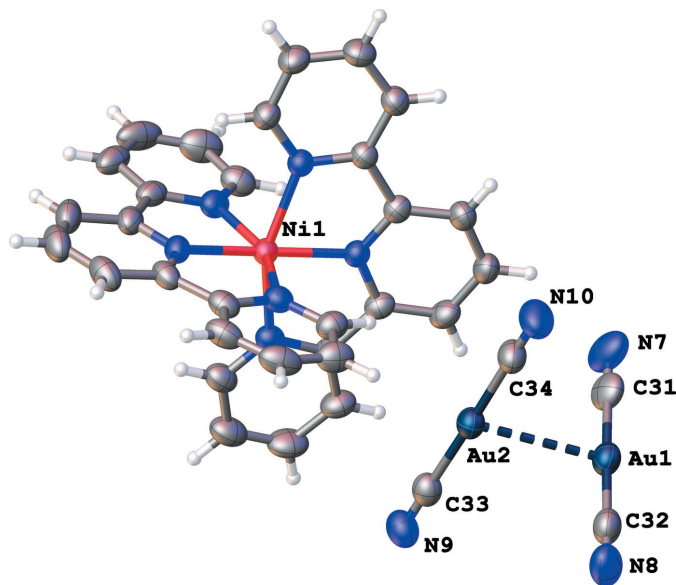


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids for non-hydrogen atoms are drawn at the 50% probability level.

Recently, the compound $[\text{Ni}(\text{terpy})][\text{Au}(\text{Br})_2(\text{CN})_2]_2$ was synthesized and analysed (Ovens *et al.*, 2010). Its crystal structure contains a gold(III) cyanidometallate anion and a complex $[\text{Ni}(\text{terpy})]^{2+}$ cation. The title compound has some similarity, given that it too contains a $[\text{Ni}(\text{terpy})]^{2+}$ cation with dicyanidoaurate(I) anions. However, the important difference between the two compounds is that there are no metal–metal interactions in the $[\text{Ni}(\text{terpy})][\text{Au}(\text{Br})_2(\text{CN})_2]_2$ structure containing the d^8 Au(III) ion, whereas the $[\text{Ni}(\text{terpy})_2]$ -

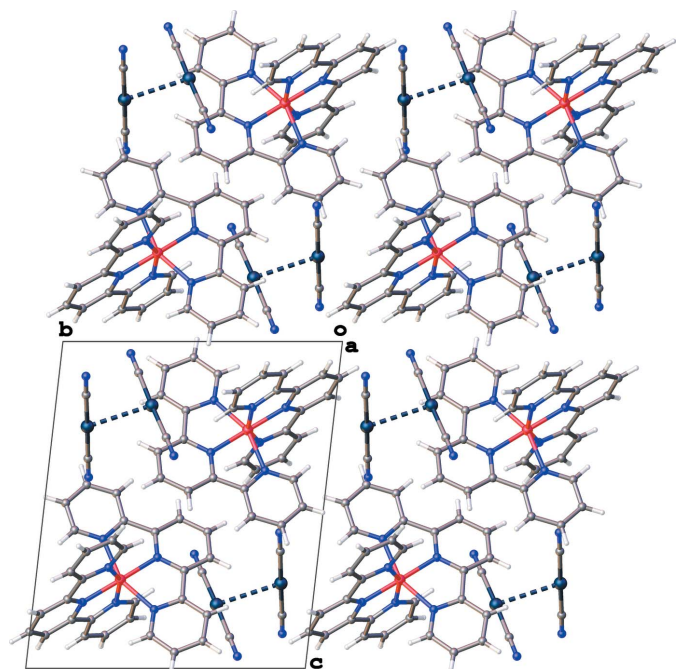


Figure 2
An illustration of the packing of the molecular entities of (I).

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C1-H1\cdots N10^i$	0.93	2.57	3.235 (7)	129
$C7-H7\cdots N8^{ii}$	0.93	2.51	3.356 (9)	151
$C8-H8\cdots N9^{iii}$	0.93	2.54	3.421 (7)	157
$C22-H22\cdots N10^{iv}$	0.93	2.43	3.364 (8)	179
$C23-H23\cdots N7$	0.93	2.51	3.274 (7)	139
$C30-H30\cdots N9^v$	0.93	2.41	3.280 (7)	156

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

$[\text{Au}(\text{CN})_2]_2$ structure contains a d^{10} gold(I) dicyanidoaurate(I) anion that has a strong propensity to form aurophilic interactions. This makes the title compound of interest because it contains short aurophilic interactions, contained within dimeric $[\text{Au}(\text{CN})_2]_2$ moieties, with $\text{Au}\cdots\text{Au}$ distances of 3.1017 (3) \AA (Fig. 1).

3. Supramolecular features

A packing diagram of the title compound is illustrated in Fig. 2. There are not any classical hydrogen bonds within the structure of the title compound. However, the cation and anion are stabilized by relatively weak non-classical hydrogen-bonding interactions from H atoms on the terpyridine rings to terminal N atoms on the cyanidometallates. There are six such interactions ranging from 3.235 (7) to 3.421 (7) \AA , if using a $D\cdots A$ distance of 3.5 \AA as the upper defined limit. Details of the interactions can be found in Table 1. The other type of non-

Table 2
Experimental details.

Crystal data	
Chemical formula	$[\text{Ni}(\text{C}_{15}\text{H}_{11}\text{N}_3)_2][\text{Au}(\text{CN})_2]_2$
M_r	1023.26
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	180
a, b, c (\AA)	8.8374 (3), 12.6707 (4), 14.7497 (4)
α, β, γ ($^\circ$)	83.401 (2), 88.788 (3), 81.078 (3)
V (\AA^3)	1620.82 (9)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	9.65
Crystal size (mm)	0.09 \times 0.06 \times 0.05
Data collection	
Diffractometer	Agilent Xcalibur Eos
Absorption correction	Multi-scan (<i>CrystAlis PRO</i> ; Agilent, 2014)
$T_{\text{min}}, T_{\text{max}}$	0.299, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41260, 5928, 5305
R_{int}	0.045
$(\sin \theta/\lambda)_{\text{max}}$ (\AA^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.070, 1.06
No. of reflections	5928
No. of parameters	424
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ($e \text{\AA}^{-3}$)	1.18, -0.51

Computer programs: *CrystAlis PRO* (Agilent, 2014), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

classical intermolecular interactions that exists in the structure is the one aurophilic interaction discussed in the *Structural commentary* above. There are no π - π stacking interactions in the structure.

4. Synthesis and crystallization

Ethanol solutions of 0.1 M Ni(NO₃)₂ (1 ml) and 0.1 M 2,2':6'.2"-terpyridine (1 ml) were mixed together. Following the mixture of these two compounds, 2 ml of 0.05 M KAu(CN)₂ (50:50 ethanol/water *v/v*) was added dropwise. A precipitate formed and the suspension was mixed thoroughly and centrifuged. The brownish-red solution was decanted from the solid precipitate and placed in a test tube to allow for slow evaporation. After approximately one week, the formation of brownish-red crystals had begun. The grown single crystals were then gathered and isolated.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in calculated positions and allowed to ride on their parent atoms during

subsequent refinement, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and C-H distances of 0.93 Å.

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supporting information

Acta Cryst. (2014). E70, 519-521 [doi:10.1107/S1600536814024672]

Crystal structure of bis(2,2':6',2''-terpyridine- κ^3N,N',N'')nickel(II) dicyanidoaurate(I)

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Bis(2,2':6',2''-terpyridine- κ^3N,N',N'')nickel(II) dicyanidoaurate(I)

Crystal data

[Ni(C₁₅H₁₁N₃)₂][Au(CN)₂]₂

M_r = 1023.26

Triclinic, *P*1

a = 8.8374 (3) Å

b = 12.6707 (4) Å

c = 14.7497 (4) Å

α = 83.401 (2)°

β = 88.788 (3)°

γ = 81.078 (3)°

V = 1620.82 (9) Å³

Z = 2

F(000) = 964

D_x = 2.097 Mg m⁻³

Mo *K* α radiation, λ = 0.7107 Å

Cell parameters from 15517 reflections

θ = 2.6–28.0°

μ = 9.65 mm⁻¹

T = 180 K

Irregular, red

0.09 × 0.06 × 0.05 mm

Data collection

Agilent Xcalibur Eos
diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 16.0514 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*CrysAlis PRO*; Agilent, 2014)

T_{min} = 0.299, *T_{max}* = 1.000

41260 measured reflections

5928 independent reflections

5305 reflections with *I* > 2 σ (*I*)

R_{int} = 0.045

θ_{\max} = 25.4°, θ_{\min} = 2.6°

h = -10→10

k = -15→15

l = -17→17

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2 σ (*F*²)] = 0.027

wR(*F*²) = 0.070

S = 1.06

5928 reflections

424 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

$$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 1.8409P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.18 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.39267 (2)	0.878031 (15)	0.259898 (14)	0.05010 (8)
Au2	0.37167 (2)	0.656248 (15)	0.195383 (13)	0.04589 (7)
Ni1	0.03978 (6)	0.30283 (4)	0.27059 (4)	0.03278 (13)
N4	0.1366 (4)	0.2245 (3)	0.3954 (2)	0.0343 (8)
N5	0.0613 (4)	0.4262 (3)	0.3394 (2)	0.0341 (8)
N6	-0.0595 (4)	0.4355 (3)	0.1801 (2)	0.0367 (8)
N3	0.2540 (4)	0.2959 (3)	0.2017 (2)	0.0386 (8)
N2	0.0398 (4)	0.1761 (3)	0.2020 (2)	0.0371 (8)
N1	-0.1736 (4)	0.2555 (3)	0.3086 (3)	0.0407 (9)
C21	0.1440 (5)	0.4070 (4)	0.4172 (3)	0.0355 (9)
C20	0.1790 (5)	0.2913 (3)	0.4515 (3)	0.0343 (9)
C26	-0.0609 (5)	0.5321 (4)	0.2110 (3)	0.0385 (10)
C16	0.1583 (5)	0.1185 (4)	0.4230 (3)	0.0412 (10)
H16	0.1277	0.0722	0.3847	0.049*
C19	0.2464 (5)	0.2534 (4)	0.5352 (3)	0.0428 (11)
H19	0.2749	0.3008	0.5731	0.051*
C22	0.1874 (6)	0.4908 (4)	0.4572 (3)	0.0430 (11)
H22	0.2452	0.4773	0.5104	0.052*
C30	-0.1275 (5)	0.4324 (4)	0.1000 (3)	0.0458 (11)
H30	-0.1253	0.3665	0.0777	0.055*
C5	-0.1995 (5)	0.1651 (4)	0.2730 (3)	0.0436 (11)
C11	0.2842 (5)	0.2140 (4)	0.1487 (3)	0.0405 (10)
C24	0.0583 (6)	0.6150 (4)	0.3379 (3)	0.0446 (11)
H24	0.0272	0.6849	0.3110	0.054*
C23	0.1440 (6)	0.5948 (4)	0.4175 (3)	0.0452 (11)
H23	0.1723	0.6517	0.4442	0.054*
C15	0.3549 (5)	0.3636 (4)	0.2029 (3)	0.0437 (11)
H15	0.3334	0.4202	0.2384	0.052*
C25	0.0205 (5)	0.5273 (3)	0.2995 (3)	0.0367 (10)
C1	-0.2761 (6)	0.3004 (4)	0.3657 (3)	0.0491 (12)
H1	-0.2587	0.3625	0.3892	0.059*
C10	0.1623 (6)	0.1451 (4)	0.1495 (3)	0.0407 (11)

C18	0.2705 (6)	0.1439 (4)	0.5616 (3)	0.0503 (12)
H18	0.3180	0.1167	0.6169	0.060*
C6	-0.0791 (6)	0.1213 (4)	0.2111 (3)	0.0434 (11)
C17	0.2241 (6)	0.0754 (4)	0.5057 (3)	0.0480 (12)
H17	0.2368	0.0017	0.5233	0.058*
C27	-0.1337 (6)	0.6270 (4)	0.1636 (4)	0.0503 (12)
H27	-0.1335	0.6924	0.1863	0.060*
C9	0.1660 (7)	0.0561 (4)	0.1017 (4)	0.0540 (14)
H9	0.2483	0.0354	0.0640	0.065*
C14	0.4912 (6)	0.3535 (5)	0.1532 (4)	0.0527 (13)
H14	0.5592	0.4023	0.1550	0.063*
C4	-0.3309 (6)	0.1213 (4)	0.2956 (4)	0.0551 (14)
H4	-0.3497	0.0606	0.2704	0.066*
C12	0.4186 (6)	0.1984 (5)	0.0993 (3)	0.0509 (13)
H12	0.4394	0.1407	0.0649	0.061*
C13	0.5218 (6)	0.2694 (5)	0.1016 (4)	0.0576 (15)
H13	0.6123	0.2602	0.0680	0.069*
C7	-0.0793 (7)	0.0300 (4)	0.1661 (4)	0.0546 (14)
H7	-0.1607	-0.0088	0.1728	0.066*
C3	-0.4349 (6)	0.1692 (6)	0.3568 (4)	0.0683 (18)
H3	-0.5229	0.1397	0.3734	0.082*
C32	0.5489 (7)	0.8954 (4)	0.1631 (4)	0.0557 (14)
C8	0.0441 (8)	-0.0008 (4)	0.1118 (4)	0.0609 (16)
H8	0.0457	-0.0611	0.0812	0.073*
C2	-0.4084 (6)	0.2576 (6)	0.3916 (4)	0.0638 (16)
H2	-0.4773	0.2899	0.4324	0.077*
C31	0.2372 (8)	0.8628 (4)	0.3579 (4)	0.0621 (15)
N8	0.6378 (7)	0.9036 (5)	0.1061 (4)	0.0765 (16)
C29	-0.2014 (6)	0.5252 (5)	0.0493 (4)	0.0579 (14)
H29	-0.2469	0.5213	-0.0062	0.070*
C28	-0.2056 (7)	0.6228 (5)	0.0831 (4)	0.0615 (15)
H28	-0.2570	0.6853	0.0514	0.074*
N7	0.1488 (8)	0.8529 (4)	0.4154 (4)	0.0830 (18)
N9	0.1436 (6)	0.7521 (4)	0.0368 (3)	0.0576 (11)
C33	0.2250 (6)	0.7165 (4)	0.0954 (4)	0.0477 (12)
N10	0.6060 (7)	0.5566 (4)	0.3494 (4)	0.0765 (16)
C34	0.5206 (7)	0.5917 (4)	0.2936 (4)	0.0536 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.05730 (14)	0.03953 (12)	0.05524 (14)	-0.00962 (9)	-0.00594 (10)	-0.00889 (9)
Au2	0.05153 (13)	0.04074 (12)	0.04712 (12)	-0.00948 (9)	-0.00261 (9)	-0.00856 (8)
Ni1	0.0342 (3)	0.0307 (3)	0.0338 (3)	-0.0050 (2)	-0.0024 (2)	-0.0048 (2)
N4	0.0348 (19)	0.0319 (19)	0.0361 (19)	-0.0043 (15)	-0.0009 (15)	-0.0048 (15)
N5	0.0363 (19)	0.0318 (19)	0.0347 (19)	-0.0057 (15)	0.0012 (15)	-0.0052 (15)
N6	0.0339 (19)	0.040 (2)	0.0350 (19)	-0.0041 (16)	-0.0002 (15)	-0.0017 (16)
N3	0.039 (2)	0.040 (2)	0.035 (2)	-0.0022 (17)	-0.0027 (16)	-0.0018 (16)

N2	0.042 (2)	0.0314 (19)	0.038 (2)	-0.0051 (16)	-0.0059 (17)	-0.0048 (16)
N1	0.037 (2)	0.043 (2)	0.041 (2)	-0.0082 (17)	-0.0077 (17)	0.0007 (17)
C21	0.033 (2)	0.034 (2)	0.039 (2)	-0.0037 (18)	0.0030 (18)	-0.0053 (18)
C20	0.033 (2)	0.035 (2)	0.034 (2)	-0.0026 (18)	0.0008 (18)	-0.0054 (18)
C26	0.038 (2)	0.034 (2)	0.042 (2)	-0.0034 (19)	0.0026 (19)	-0.0027 (19)
C16	0.046 (3)	0.034 (2)	0.044 (3)	-0.007 (2)	-0.003 (2)	-0.0037 (19)
C19	0.046 (3)	0.043 (3)	0.040 (3)	-0.007 (2)	-0.006 (2)	-0.005 (2)
C22	0.051 (3)	0.043 (3)	0.037 (2)	-0.010 (2)	0.000 (2)	-0.009 (2)
C30	0.042 (3)	0.057 (3)	0.038 (3)	-0.008 (2)	-0.005 (2)	-0.001 (2)
C5	0.043 (3)	0.044 (3)	0.043 (3)	-0.012 (2)	-0.011 (2)	0.010 (2)
C11	0.041 (2)	0.044 (3)	0.033 (2)	0.005 (2)	-0.0050 (19)	-0.0035 (19)
C24	0.055 (3)	0.030 (2)	0.047 (3)	-0.003 (2)	0.005 (2)	-0.003 (2)
C23	0.058 (3)	0.037 (3)	0.044 (3)	-0.013 (2)	0.001 (2)	-0.010 (2)
C15	0.042 (3)	0.041 (3)	0.047 (3)	-0.005 (2)	-0.002 (2)	0.001 (2)
C25	0.035 (2)	0.031 (2)	0.042 (2)	0.0004 (18)	0.0039 (19)	-0.0009 (18)
C1	0.044 (3)	0.057 (3)	0.043 (3)	0.000 (2)	-0.003 (2)	-0.002 (2)
C10	0.049 (3)	0.038 (2)	0.033 (2)	0.005 (2)	-0.010 (2)	-0.0073 (19)
C18	0.057 (3)	0.049 (3)	0.042 (3)	-0.006 (2)	-0.009 (2)	0.004 (2)
C6	0.051 (3)	0.037 (2)	0.043 (3)	-0.011 (2)	-0.016 (2)	0.000 (2)
C17	0.054 (3)	0.036 (2)	0.051 (3)	-0.005 (2)	-0.007 (2)	0.004 (2)
C27	0.053 (3)	0.039 (3)	0.054 (3)	-0.002 (2)	-0.003 (2)	0.008 (2)
C9	0.066 (3)	0.050 (3)	0.044 (3)	0.010 (3)	-0.012 (2)	-0.016 (2)
C14	0.038 (3)	0.061 (3)	0.056 (3)	-0.006 (2)	0.002 (2)	0.005 (3)
C4	0.053 (3)	0.050 (3)	0.062 (3)	-0.020 (3)	-0.020 (3)	0.017 (3)
C12	0.049 (3)	0.063 (3)	0.035 (3)	0.007 (3)	0.001 (2)	-0.004 (2)
C13	0.038 (3)	0.082 (4)	0.045 (3)	0.001 (3)	0.004 (2)	0.009 (3)
C7	0.067 (4)	0.041 (3)	0.059 (3)	-0.015 (3)	-0.023 (3)	-0.006 (2)
C3	0.040 (3)	0.089 (5)	0.070 (4)	-0.022 (3)	-0.009 (3)	0.032 (4)
C32	0.062 (4)	0.049 (3)	0.061 (4)	-0.016 (3)	-0.008 (3)	-0.013 (3)
C8	0.083 (4)	0.041 (3)	0.059 (3)	-0.002 (3)	-0.025 (3)	-0.015 (3)
C2	0.039 (3)	0.086 (5)	0.060 (4)	-0.004 (3)	0.002 (3)	0.008 (3)
C31	0.083 (4)	0.032 (3)	0.072 (4)	-0.003 (3)	0.005 (3)	-0.016 (3)
N8	0.079 (4)	0.088 (4)	0.074 (4)	-0.040 (3)	0.007 (3)	-0.024 (3)
C29	0.053 (3)	0.074 (4)	0.044 (3)	-0.009 (3)	-0.011 (2)	0.007 (3)
C28	0.058 (3)	0.061 (4)	0.057 (3)	0.001 (3)	-0.012 (3)	0.017 (3)
N7	0.111 (5)	0.046 (3)	0.095 (4)	-0.017 (3)	0.032 (4)	-0.019 (3)
N9	0.059 (3)	0.058 (3)	0.056 (3)	0.000 (2)	-0.007 (2)	-0.017 (2)
C33	0.048 (3)	0.048 (3)	0.049 (3)	-0.009 (2)	0.003 (2)	-0.013 (2)
N10	0.095 (4)	0.061 (3)	0.073 (4)	-0.008 (3)	-0.031 (3)	-0.006 (3)
C34	0.063 (3)	0.043 (3)	0.056 (3)	-0.010 (3)	-0.013 (3)	-0.008 (2)

Geometric parameters (Å, °)

Au1—Au2	3.1017 (3)	C11—C12	1.381 (7)
Au1—C32	1.983 (7)	C24—H24	0.9300
Au1—C31	1.987 (7)	C24—C23	1.388 (7)
Au2—C33	1.989 (5)	C24—C25	1.391 (7)
Au2—C34	1.994 (5)	C23—H23	0.9300

Ni1—N4	2.119 (4)	C15—H15	0.9300
Ni1—N5	1.994 (4)	C15—C14	1.393 (7)
Ni1—N6	2.110 (4)	C1—H1	0.9300
Ni1—N3	2.124 (4)	C1—C2	1.392 (8)
Ni1—N2	1.993 (4)	C10—C9	1.393 (7)
Ni1—N1	2.112 (4)	C18—H18	0.9300
N4—C20	1.346 (5)	C18—C17	1.375 (7)
N4—C16	1.344 (6)	C6—C7	1.399 (7)
N5—C21	1.351 (6)	C17—H17	0.9300
N5—C25	1.346 (5)	C27—H27	0.9300
N6—C26	1.353 (6)	C27—C28	1.368 (8)
N6—C30	1.344 (6)	C9—H9	0.9300
N3—C11	1.361 (6)	C9—C8	1.382 (8)
N3—C15	1.331 (6)	C14—H14	0.9300
N2—C10	1.352 (6)	C14—C13	1.370 (8)
N2—C6	1.343 (6)	C4—H4	0.9300
N1—C5	1.365 (6)	C4—C3	1.395 (9)
N1—C1	1.331 (6)	C12—H12	0.9300
C21—C20	1.481 (6)	C12—C13	1.381 (8)
C21—C22	1.379 (6)	C13—H13	0.9300
C20—C19	1.385 (6)	C7—H7	0.9300
C26—C25	1.493 (6)	C7—C8	1.373 (9)
C26—C27	1.391 (6)	C3—H3	0.9300
C16—H16	0.9300	C3—C2	1.338 (9)
C16—C17	1.380 (7)	C32—N8	1.146 (8)
C19—H19	0.9300	C8—H8	0.9300
C19—C18	1.381 (7)	C2—H2	0.9300
C22—H22	0.9300	C31—N7	1.150 (8)
C22—C23	1.380 (7)	C29—H29	0.9300
C30—H30	0.9300	C29—C28	1.381 (8)
C30—C29	1.396 (7)	C28—H28	0.9300
C5—C6	1.472 (7)	N9—C33	1.141 (7)
C5—C4	1.382 (7)	N10—C34	1.132 (7)
C11—C10	1.487 (7)		
C32—Au1—Au2	87.27 (15)	C23—C24—C25	117.8 (4)
C32—Au1—C31	179.0 (2)	C25—C24—H24	121.1
C31—Au1—Au2	93.69 (15)	C22—C23—C24	120.5 (4)
C33—Au2—Au1	94.33 (14)	C22—C23—H23	119.8
C33—Au2—C34	178.2 (2)	C24—C23—H23	119.8
C34—Au2—Au1	87.35 (15)	N3—C15—H15	118.5
N4—Ni1—N3	93.99 (14)	N3—C15—C14	122.9 (5)
N5—Ni1—N4	77.69 (14)	C14—C15—H15	118.5
N5—Ni1—N6	78.00 (14)	N5—C25—C26	112.9 (4)
N5—Ni1—N3	96.88 (15)	N5—C25—C24	121.3 (4)
N5—Ni1—N1	106.69 (15)	C24—C25—C26	125.7 (4)
N6—Ni1—N4	155.47 (14)	N1—C1—H1	118.9
N6—Ni1—N3	92.12 (14)	N1—C1—C2	122.2 (6)

N6—Ni1—N1	93.45 (14)	C2—C1—H1	118.9
N2—Ni1—N4	99.88 (14)	N2—C10—C11	114.0 (4)
N2—Ni1—N5	174.57 (15)	N2—C10—C9	120.2 (5)
N2—Ni1—N6	104.62 (14)	C9—C10—C11	125.8 (5)
N2—Ni1—N3	78.36 (15)	C19—C18—H18	120.1
N2—Ni1—N1	78.06 (16)	C17—C18—C19	119.7 (4)
N1—Ni1—N4	90.39 (14)	C17—C18—H18	120.1
N1—Ni1—N3	156.42 (15)	N2—C6—C5	113.6 (4)
C20—N4—Ni1	114.3 (3)	N2—C6—C7	120.6 (5)
C16—N4—Ni1	127.2 (3)	C7—C6—C5	125.8 (5)
C16—N4—C20	118.5 (4)	C16—C17—H17	120.8
C21—N5—Ni1	118.6 (3)	C18—C17—C16	118.5 (4)
C25—N5—Ni1	119.4 (3)	C18—C17—H17	120.8
C25—N5—C21	120.6 (4)	C26—C27—H27	120.4
C26—N6—Ni1	114.5 (3)	C28—C27—C26	119.2 (5)
C30—N6—Ni1	126.9 (3)	C28—C27—H27	120.4
C30—N6—C26	118.5 (4)	C10—C9—H9	120.9
C11—N3—Ni1	113.9 (3)	C8—C9—C10	118.3 (5)
C15—N3—Ni1	127.4 (3)	C8—C9—H9	120.9
C15—N3—C11	118.6 (4)	C15—C14—H14	121.0
C10—N2—Ni1	119.1 (3)	C13—C14—C15	118.0 (5)
C6—N2—Ni1	119.5 (3)	C13—C14—H14	121.0
C6—N2—C10	121.4 (4)	C5—C4—H4	120.4
C5—N1—Ni1	113.7 (3)	C5—C4—C3	119.1 (6)
C1—N1—Ni1	127.0 (4)	C3—C4—H4	120.4
C1—N1—C5	119.2 (4)	C11—C12—H12	120.4
N5—C21—C20	113.3 (4)	C11—C12—C13	119.2 (5)
N5—C21—C22	120.5 (4)	C13—C12—H12	120.4
C22—C21—C20	126.2 (4)	C14—C13—C12	120.1 (5)
N4—C20—C21	114.7 (4)	C14—C13—H13	120.0
N4—C20—C19	121.8 (4)	C12—C13—H13	120.0
C19—C20—C21	123.5 (4)	C6—C7—H7	120.9
N6—C26—C25	114.4 (4)	C8—C7—C6	118.2 (5)
N6—C26—C27	121.9 (4)	C8—C7—H7	120.9
C27—C26—C25	123.7 (4)	C4—C3—H3	119.9
N4—C16—H16	118.7	C2—C3—C4	120.1 (5)
N4—C16—C17	122.6 (4)	C2—C3—H3	119.9
C17—C16—H16	118.7	N8—C32—Au1	178.4 (5)
C20—C19—H19	120.6	C9—C8—H8	119.3
C18—C19—C20	118.8 (4)	C7—C8—C9	121.4 (5)
C18—C19—H19	120.6	C7—C8—H8	119.3
C21—C22—H22	120.4	C1—C2—H2	120.5
C21—C22—C23	119.3 (4)	C3—C2—C1	119.0 (6)
C23—C22—H22	120.4	C3—C2—H2	120.5
N6—C30—H30	119.0	N7—C31—Au1	179.0 (6)
N6—C30—C29	122.0 (5)	C30—C29—H29	120.6
C29—C30—H30	119.0	C28—C29—C30	118.8 (5)
N1—C5—C6	115.0 (4)	C28—C29—H29	120.6

N1—C5—C4	120.3 (5)	C27—C28—C29	119.6 (5)
C4—C5—C6	124.7 (5)	C27—C28—H28	120.2
N3—C11—C10	114.6 (4)	C29—C28—H28	120.2
N3—C11—C12	121.2 (5)	N9—C33—Au2	178.4 (5)
C12—C11—C10	124.2 (5)	N10—C34—Au2	178.9 (5)
C23—C24—H24	121.1		

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C1—H1...N10 ⁱ	0.93	2.57	3.235 (7)	129
C7—H7...N8 ⁱⁱ	0.93	2.51	3.356 (9)	151
C8—H8...N9 ⁱⁱⁱ	0.93	2.54	3.421 (7)	157
C22—H22...N10 ^{iv}	0.93	2.43	3.364 (8)	179
C23—H23...N7	0.93	2.51	3.274 (7)	139
C30—H30...N9 ^v	0.93	2.41	3.280 (7)	156

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