Synthesis and molecular structure of biologically significant bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold(I) complexes with chloride and dichloridoaurate counter-ions

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Diffraction-quality single crystals of two gold(I) complexes, namely bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold(I) chloride benzene monosolvate, $[\text{Au}(\text{C}_{29}\text{H}_{26}\text{N}_2\text{O}_2)_2]\text{Cl}\cdot\text{C}_6\text{H}_6$ or $[(\text{NQMe})_2\text{Au}]\text{Cl}\cdot\text{C}_6\text{H}_6$, **2**, and bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold(I) dichloridoaurate(I) dichloromethane disolvate, $[\text{Au}(\text{C}_{29}\text{H}_{26}\text{N}_2\text{O}_2)_2][\text{AuCl}_2]\cdot 2\text{CH}_2\text{Cl}_2$ or $[(\text{NQMe})_2\text{Au}][\text{AuCl}_2]\cdot 2\text{CH}_2\text{Cl}_2$, **4**, were isolated and studied with the aid of single-crystal X-ray diffraction analysis. Compound **2** crystallizes in a monoclinic space group $C2/c$ with eight molecules in the unit cell, while compound **4** crystallizes in the triclinic space group $P\bar{1}$ with two molecules in the unit cell. The crystal lattice of compound **2** reveals $\text{C}-\text{H}\cdots\text{Cl}^-$ interactions that are present throughout the entire structure representing head-to-tail contacts between the aromatic ($\text{C}-\text{H}$) hydrogens of naphthoquinone and Cl^- counter-ions. Compound **4** stacks with the aid of short interactions between a naphthoquinone O atom of one molecule and the mesityl methyl group of another molecule along the a axis, leading to a one-dimensional strand that is held together by strong $\pi-\eta^2$ interactions between the imidazolium backbone and the $[\text{AuCl}_2]^-$ counter-ion. The bond angles defined by the Au^{I} atom and two carbene C atoms $[\text{C}(\text{carbene})-\text{Au}-\text{C}(\text{carbene})]$ in compounds **2** and **4** are nearly rectilinear, with an average value of $\sim 174.1^\circ$. Though **2** and **4** share the same cation, they differ in their counter-anion, which alters the crystal lattice of the two compounds. The knowledge gleaned from these studies is expected to be useful in understanding the molecular interactions of **2** and **4** under physiological conditions.

1. Introduction

The development of organometallic compounds for therapeutic applications burgeoned after the discovery of cisplatin for cancer treatment (Rosenberg *et al.*, 1965; Dasari & Tchounwou, 2014; Kelland, 2007). An ideal organometallic drug design for therapeutic applications hinges directly on the judicious selection of the metal and the ligand; one such ligand system is N-heterocyclic carbene (NHC). More often, NHCs are used as ligands on transition metals to facilitate homogeneous catalysis (Hopkinson *et al.*, 2014; Cazin, 2011; Nolan & Cazin, 2018; Vougioukalakis & Grubbs, 2010; Ramón & Nolan, 2018). Such developments are attributed to the strong σ -donating properties of NHCs and the stability of the $M-\text{C}(\text{carbene})$ bond (Jacobsen *et al.*, 2009; Meng *et al.*, 2019; Tonner *et al.*, 2007), an important trait that could be exploited to withstand physiological conditions for organometallic therapeutic drugs. Recently, several NHC-based transition-metal (Pd, Pt, and Ag) complexes containing structurally different N-atom substitutions have been prepared and

Table 1
Experimental details.

	2	4
Crystal data		
Chemical formula	$[\text{Au}(\text{C}_{29}\text{H}_{26}\text{N}_2\text{O}_2)_2]\text{Cl}\cdot\text{C}_6\text{H}_6$	$[\text{Au}(\text{C}_{29}\text{H}_{26}\text{N}_2\text{O}_2)_2][\text{AuCl}_2]\cdot 2\text{CH}_2\text{Cl}_2$
M_r	1179.56	1503.72
Crystal system, space group	Monoclinic, $C2/c$	Triclinic, $P\bar{1}$
Temperature (K)	183	183
a, b, c (Å)	24.368 (3), 14.7921 (18), 33.349 (4)	11.9236 (11), 15.1244 (14), 18.4014 (16)
α, β, γ (°)	90, 103.630 (5), 90	100.460 (3), 105.164 (3), 103.994 (3)
V (Å ³)	11682 (3)	2999.8 (5)
Z	8	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	2.61	5.20
Crystal size (mm)	$0.56 \times 0.50 \times 0.20$	$0.74 \times 0.50 \times 0.25$
Data collection		
Diffractometer	Bruker SMART X2S benchtop	Bruker SMART X2S benchtop
Absorption correction	Multi-scan (SADABS; Bruker, 2014)	Multi-scan (SADABS; Bruker, 2014)
$T_{\min}, T_{\max}$	0.444, 1.000	0.413, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	64959, 10295, 7749	53862, 10522, 7802
R_{int}	0.127	0.105
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.595	0.596
Refinement		
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.050, 0.119, 1.00	0.052, 0.138, 0.99
No. of reflections	10295	10522
No. of parameters	675	697
No. of restraints	64	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.73, -0.76	2.29, -2.27

Computer programs: APEX2 (Bruker, 2014), SAINT (Bruker, 2014), SHELXT (Sheldrick, 2015a), SHELXL2017 (Sheldrick, 2015b), OLEX2 (Dolomanov *et al.*, 2009), PLATON (Spek, 2009) and Mercury (Macrae *et al.*, 2008).

studied as potential therapeutic agents (Youngs *et al.*, 2012; Liu & Gust, 2016; Karaca, Meier-Menches *et al.*, 2017; Oehninger *et al.*, 2013; Teyssot *et al.*, 2009). The prime advantage over conventional metal–phosphine-based complexes is the reduced deterioration of the M –C(carbene) bond under physiological conditions (Zou *et al.*, 2018) and the synthetic ease of accommodating various functionalities within it.

After the initial report of Berners–Price in 2004, NHC-ligated gold(I) complexes became of significant interest as

potential anticancer agents (Barnard *et al.*, 2004). Following this report, several bis(NHC)gold(I) complexes, *i.e.* $[(\text{NHC})_2\text{gold(I)}]^+$, were prepared and studied as potential cancer therapeutic agents (Tan *et al.*, 2018; Karaca, Scalcon *et al.*, 2017; Boscutti *et al.*, 2018; Hickey *et al.*, 2008; Muenzner *et al.*, 2016). Recently, our group disclosed the *in vitro* and *in vivo* testing of several dual-targeting redox-active bis(NHC)gold(I) complexes, *i.e.* $[(\text{rNHC})_2\text{gold(I)}]^+$, fused with either ferrocene (Arambula *et al.*, 2016) or naphthoquinone (McCall *et al.*, 2017) in human cancer cell lines. These redox-active

Figure 1
The synthetic scheme for the preparation of $[(\text{NQMes})_2\text{Au}]\text{Cl}$, **2**, and $[(\text{NQMes})_2\text{Au}][\text{AuCl}_2]$, **4**.

$[(rNHC)_2gold(I)]^+$ complexes were very effective in inhibiting cell proliferation of A549 cancer cells relative to other $[(NHC)_2gold(I)]^+$ complexes that lack redox-active moieties (Arambula *et al.*, 2016; McCall *et al.*, 2017). Moreover, $[(rNHC)_2gold(I)]^+$ complexes displayed excellent activity compared to auranofin, an approved antirheumatic agent and a potential anticancer drug (Furst, Li *et al.*, 2015; Park *et al.*, 2014).

The anticancer properties of ferrocene- and naphthoquinone-fused gold(I) complexes of $[(rNHC)_2gold(I)]^+$ are attributed to their bimodal network targeting capability (McCall *et al.*, 2017). These drugs are capable of simultaneously increasing reactive oxygen species (ROS) while inhibiting antioxidant enzymes such as thioredoxin reductase (TrxR). Such bimodal targeting capabilities are absent for simple $[(NHC)_2gold(I)]^+$ complexes and auranofin. Continuing with the development of naphthoquinone-based anticancer gold(I) complexes, we report herein an improved synthesis and the solid-state structural characterization of $[(NQMes)_2Au]Cl$, **2**, and $[(NQMes)_2Au][AuCl_2]$, **4** (NQMes is 1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene). In addition, solid-state structural variations with respect to the counter-ions are discussed in detail.

2. Experimental

2.1. Synthesis and crystallization

2.1.1. Preparation of bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold chloride, 2. Bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold dichloridoargentate (**1**; 100 mg, 0.8 mmol) was stirred in methanol (10 ml) for 3 d. During the course of the stirring, the formation of a precipitate of silver chloride was observed. The resulting hetero-

geneous mixture was filtered through a plug of Celite and washed with 2×2 ml of methanol. The volatiles were removed under reduced pressure. The resulting residue was dissolved in a minimal amount of dichloromethane, triturated with diethyl ether (15 ml), and subsequently washed with diethyl ether (15 ml) to yield a fine yellow precipitate of **2** (80 mg, 91% yield). 1H NMR (300 MHz, $CDCl_3$): δ 8.08–8.02 (*m*, 4H), 7.84–7.80 (*m*, 4H), 7.02 (*s*, 8H), 2.51 (*s*, 12H), 1.72 (*s*, 24H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 192.14, 173.83, 140.52, 135.36, 133.71, 132.14, 131.94, 131.74, 129.58, 127.50, 21.44, 17.35. Analysis calculated (%) for $C_{58}H_{52}AuClN_4O_4 \cdot 0.4CH_2Cl_2$: C 61.78, H 4.69, N 4.93; found: C 61.86, H 4.97, N 4.93.

2.1.2. Preparation of bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold dichloridoaurate, 4. 1,3-Dimesitylnaphthoquinoimidazolium chloride (95.4 mg, 0.2 mmol) was added to sodium bis(trimethylsilyl)amide (NaHMDS; 39 mg, 0.21 mmol) in a 20 ml scintillation vial and stirred at 25 °C for 16 h in toluene (4 ml). The resulting mixture was filtered through a plug of Celite into a preweighed 20 ml scintillation vial containing $(C_4H_8S)AuCl$ (64 mg, 0.2 mmol) and tetrahydrofuran (THF, 2 ml), and stirred at 25 °C for 24 h. Volatiles were removed under reduced pressure. The dark-green residue was washed with THF (3×5 ml) to yield a greenish yellow solid, which was dissolved in a minimal amount of dichloromethane, triturated with diethyl ether (15 ml), and subsequently washed with diethyl ether (15 ml) to yield a fine yellow precipitate of **4** (72 mg, 54% yield). 1H NMR (300 MHz, $CDCl_3$): δ 8.06–8.03 (*m*, 4H), 7.81–7.78 (*m*, 4H), 7.02 (*s*, 8H), 2.50 (*s*, 12H), 1.73 (*s*, 24H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 192.14, 173.93, 140.46, 135.25, 133.81, 132.21, 132.02, 131.88, 129.59, 127.49, 21.49, 17.45; Analysis calculated (%) for $C_{58}H_{52}Au_2Cl_2N_4O_4$: C 52.23, H 3.93, N 4.20; found: C 51.93, H 3.92, N 4.05.

Figure 2

The molecular structure of **2**, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. Selected bond angles and lengths are presented in Table 2.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Aromatic H atoms were added in calculated positions and allowed to ride on the C atoms to which they are attached, with C—H = 0.95 Å. Idealized methyl H atoms were refined as a rotating group and constrained to ride on their C atom; the methyl H atoms were fixed at a C—H distance of 0.98 Å. The disordered benzene molecule in **2** was treated using rigid-body restraints with idealized geometry. The distances and planarity were restrained with rigid-body restraints on atoms C1A, C1B, C1C, C1D, C1E and C1F, with a σ for 1–2 distances of 0.004 Å and a σ for 1–3 distances of 0.004 Å. Electron density at partially occupied sites for severely disordered benzene was removed using the SQUEEZE option (Spek, 2015) in PLATON (Spek, 2009). The disordered benzene molecules accounted for 99.4 electrons with a volume of 329.6 Å³.

3. Results and discussion

The synthetic scheme for the preparation of [(NQMes)₂Au]Cl, **2**, and [(NQMes)₂Au][AuCl₂], **4**, is presented in Fig. 1. The necessary starting materials, *i.e.* bis(1,3-dimesityl-4,5-naphtho-

quinoimidazol-2-ylidene)gold dichloridoargentate, **1**, and 1,3-dimesitylnaphthoquinimidazolium chloride, **3**, were prepared following the reported synthetic procedures of McCall *et al.* (2017) and Sanderson *et al.* (2006). Though our group has reported the synthesis of compound **2** previously, a detailed solid-state structural characterization of **2** was lacking (McCall *et al.*, 2017). Using an improved procedure, compound **2** was prepared by stirring **1** for 3 d in methanol. This led to the dissociation of [AgCl₂][−] into Cl[−] and AgCl (Baquero *et al.*, 2013), leaving [(NQMes)₂Au]Cl, **2**, in the methanol solution. The precipitate (AgCl) was removed by filtering the reaction mixture through a plug of Celite, followed by evaporation of the volatiles under reduced pressure. The obtained crude mixture was dissolved in a minimum amount of dichloromethane and triturated with diethyl ether (15 ml) to yield complex salt **2** in 91% yield. While compound **4** was prepared using the free carbene route, treatment of **3** with sodium bis(trimethylsilyl)amide (NaHMDS) in toluene led to the *in situ* formation of 1,3-dimesityl-4,5-naphthoquinimidazol-2-ylidene. The resulting ylidene was passed through a plug of Celite into a vial containing (C₄H₈S)AuCl and subsequently stirred for 24 h to yield **4** in 54% yield.

Single crystals of **2** were obtained by diffusion of benzene into a saturated solution of **2** in 1,2-dichloroethane. The

Figure 3

(a) Partial packing diagram for complex **2**. Dashed lines indicate C—H...Cl[−] hydrogen-bonding and C—H...O interactions. (b) Displacement ellipsoid plot showing two C—H... π interactions (marked as **1**, **1'** and **4**, **4'**), two C—H...O interactions (**2**, **2'** and **3**, **3'**) and six C—H...Cl[−] interactions (**5** to **10**). The distances (Å) are: **1/1'** 2.861 (6), **2/2'** 2.517 (5), **3/3'** 2.482 (5), **4/4'** 2.767 (6), **5** 2.862 (19), **6** 2.617 (19), **7** 2.911 (2), **8** 2.774 (2), **9** 2.670 (3) and **10** 2.823 (19). (c) Packing diagram showing the stacking into a two-dimensional sheet as a result of C—H...O interactions.

molecular structure is presented in Fig. 2. Compound **2** crystallized in the monoclinic space group $C2/c$ with eight molecules per unit cell. The average Au—C(carbene) bond length is 2.019 [6] Å, which closely matches other reported $[(NHC)_2Au]^+$ complexes (1.998–2.029 Å; de Frémont *et al.*, 2005; Gaillard *et al.*, 2010; Lazreg *et al.*, 2015; Collado *et al.*, 2016; Lozada-Rodríguez *et al.*, 2017). The bond angle defined by the Au^I atom and two carbene C atoms, *i.e.* C(carbene)—Au—C(carbene) is nearly rectilinear, with a value of 174.2 (2)°. The dihedral angle defined by the planes representing the two naphthoquinone-fused imidazolyliene (NHC) rings is 72.5 (2)°, indicative that they are near perpendicular to one another, with the N-mesityl groups projecting towards the top and bottom of the plane. This special arrangement of mesityl groups prevents the aurophilic ($Au^+ \cdots Au^+ = 3.372$ Å) interaction that is usually observed in the solid-state structures of less sterically hindered gold(I)–NHC complexes, such as $[\text{bis}(4,5\text{-dimethylimidazol-2-ylidene})\text{gold(I)}]^+$ (Britten *et al.*, 1992). The crystal packing diagram of compound **2** is presented in Fig. 3. The most striking feature observed is a nonclassical C—H $\cdots$ Cl[−] hydrogen-bonding network that is present throughout the solid-state structure (Fig. 3*a*). The network occurs in a head-to-tail fashion between aromatic C—H hydrogens of naphthoquinone and Cl[−] anions, forming a linear chain along the *a* axis (Fig. 3*a*). In addition, intermolecular interactions between naphthoquinone O atoms and naphthoquinone aromatic C—H hydrogens is also observed (Fig. 3*b*). A two-dimensional array of molecules, when viewed along the *b* axis, displays short interactions between the mesityl methyl H atoms and the naphthoquinone O atoms (Fig. 3*b*). Each chloride ion is held by six hydrogen-bonding interactions (C—H $\cdots$ Cl[−]). In general, the aromatic H atoms are not acidic and hence do not interact with the anions. However, the presence of two carbonyl groups on the

Table 2

Selected bond lengths (Å) and angles (°) for $[(NQMes)_2Au]Cl$, **2**, and $[(NQMes)_2Au][AuCl_2]$, **4**.

Compound	$[(NQMes)_2Au]Cl$, 2	$[(NQMes)_2Au][AuCl_2]$, 4
Au—C _{carbene} ^a	2.019 [6]	2.009 [6]
C1 _{carbene} —N ^a	1.362 [5]	1.357 [8]
C30 _{carbene} —N ^a	1.354 [5]	1.359 [8]
N1—C11/N2—C2	1.384 (7)/1.385 (8)	1.373 (9)/1.396 (10)
C2—C11	1.348 (8)	1.364 (10)
C2—C3	1.471 (9)	1.454 (10)
C—O ^a	1.214 [4]	1.205 [9]
Cl1—Au2	—	2.261 (3)
Au2—Cl2	—	2.254 (3)
Carbene—Au—Carbene	174.2 (2)	173.9 (3)
N1—C1—N2	106.2 (5)	105.9 (6)
C1—N2—C2	109.6 (5)	109.4 (6)
C1—N1—C11	109.2 (5)	111.1 (6)
Imi _{plane} —Au—Imi _{plane} ^c	72.5 (2)	61.8 (3)

Notes: (a) average interatomic distances are displayed when two identical bond types or angles are present; (b) average standard uncertainties were computed according to the reference (McRee, 1999); (c) Imi_{plane} denotes the plane defined by five atoms that constitutes the imidazolyliene ring.

naphthoquinone ligand coupled with the inductive effect displayed by the N atoms renders the whole NHC unit as an electron-deficient system (Shi *et al.*, 2016). Subsequently, complex **2** is more prone to nonclassical interactions, hence the aromatic C—H $\cdots$ Cl[−] interactions.

Crystals of **4** were obtained by diffusion of hexanes into a saturated solution of **4** in dichloromethane. The complex crystallizes in the triclinic space group $P\bar{1}$ with two molecules in the unit cell ($Z = 2$). The molecular structure is presented in Fig. 4. The Au—C(carbene) bond length [average 2.009 [6] Å] is consistent with earlier reported $[(NHC)_2Au]^+$ complexes (1.998–2.029 Å; de Frémont *et al.*, 2005; Gaillard *et al.*, 2010; Lazreg *et al.*, 2015; Collado *et al.*, 2016; Lozada-Rodríguez *et al.*, 2017). The Au center between the two carbene C atoms is

The molecular structure of complex **4**, with displacement ellipsoids drawn at the 50% probability level. H atoms and solvent molecules have been omitted for clarity. Selected bond lengths and angles are presented in Table 2.

Figure 5

(a) Partial packing diagram for complex **4**, viewed perpendicular to the *a* axis, with dashed lines indicating short interactions. (b) π - η^2 ...[Cl—Au—Cl][−] interaction between the [AuCl₂][−] anion and the imidazolylidene double bond [3.196 (5) Å], and C—H...Cl[−] hydrogen-bonding interactions [2.719 (3) Å] present in complex **4**. (c) Intercalation of the two-dimensional sheets via C...O, C—H...O and CH...CH short interactions. Solvent molecules have been omitted for clarity.

nearly rectilinear, with a C(carbene)—Au—C(carbene) bond angle of ~ 173.9 [3] $^\circ$, deviating slightly from 180 $^\circ$. The dihedral angle defined by the plane representing the two imidazolium rings of the two NHC ligands is 61.7 (2) $^\circ$ (Fig. 4), which is 10.8 (1) $^\circ$ less than the same angle of complex **2**. The crystal packing diagram of compound **4** is presented in Fig. 5. The complex crystallizes with [AuCl₂][−] anions and dichloromethane solvent molecules in the crystal lattice. [(NQMes)₂-Au][AuCl₂] stacks with the aid of short interactions (C—H...O) between a naphthoquinone O atom of one molecule and the mesityl methyl H atoms of another molecule along the *a* axis, leading to a one-dimensional strand. These strands were held together by secondary π - η^2 -type interactions between atoms C31 and C40 of the imidazolylidene ring and a Cl atom of [AuCl₂][−] (Fig. 5b). The π - η^2 and C—H...O interactions extend along the *b* axis, leading to a two-dimensional sheet. These sheets were stacked to give a three-dimensional structure that is held together by π - η^2 and C—H...O interactions throughout the crystal lattice (Fig. 5c).

In summary, the molecular structures for two redox-active bis(NHC)gold(I) complexes have been probed in detail. Their crystal lattices with respect to the counter-ions were investigated with the aid of single-crystal X-ray crystallography. The knowledge gleaned from these structural studies will be useful for simulating the interactions of these types of molecules under physiological conditions.

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Synthesis and molecular structure of biologically significant bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold(I) complexes with chloride and dichloridoaurate counter-ions

Jayaraman Selvakumar, Meredith H. Miles, David A. Grossie and Kuppuswamy Arumugam

Computing details

For both structures, data collection: *APEX2* (Bruker, 2014a); cell refinement: *APEX2* (Bruker, 2014a); data reduction: *SAINT* (Bruker, 2014b); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

Bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold(I) chloride benzene monosolvate (shelx_c2_c)

Crystal data

[Au(C₂₉H₂₆N₂O₂)₂]Cl·C₆H₆

M_r = 1179.56

Monoclinic, C2/c

a = 24.368 (3) Å

b = 14.7921 (18) Å

c = 33.349 (4) Å

β = 103.630 (5)°

V = 11682 (3) Å³

Z = 8

F(000) = 4784

D_x = 1.341 Mg m^{−3}

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 7468 reflections

θ = 19.9–2.3°

μ = 2.61 mm^{−1}

T = 183 K

Plate, yellow

0.56 × 0.50 × 0.20 mm

Data collection

Bruker SMART X2S benchtop

diffractometer

Radiation source: XOS X-beam microfocus
source

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2014)

T_{min} = 0.444, *T_{max}* = 1.000

64959 measured reflections

10295 independent reflections

7749 reflections with *I* > 2σ(*I*)

R_{int} = 0.127

θ_{max} = 25.0°, θ_{min} = 2.2°

h = −28→28

k = −17→16

l = −39→38

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.050

wR (*F*²) = 0.119

S = 1.00

10295 reflections

675 parameters

64 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 50.4155P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$

$$\Delta\rho_{\max} = 1.73 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.76 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Au1	0.79403 (2)	0.23012 (2)	0.88886 (2)	0.03146 (9)	
O1	0.78470 (19)	−0.1446 (3)	0.82538 (14)	0.0481 (12)	
O2	0.9877 (2)	−0.0364 (4)	0.91839 (18)	0.0720 (17)	
O3	0.7604 (2)	0.6044 (3)	0.82370 (15)	0.0510 (12)	
O4	0.6186 (2)	0.4954 (4)	0.91738 (19)	0.0759 (18)	
N1	0.8036 (2)	0.0380 (3)	0.86335 (15)	0.0324 (12)	
N2	0.8844 (2)	0.0807 (3)	0.90214 (15)	0.0339 (12)	
N3	0.7673 (2)	0.4220 (3)	0.86277 (15)	0.0315 (12)	
N4	0.7117 (2)	0.3786 (3)	0.90099 (15)	0.0320 (12)	
C1	0.8304 (2)	0.1086 (4)	0.88595 (19)	0.0342 (15)	
C2	0.8910 (3)	−0.0072 (4)	0.88981 (19)	0.0353 (15)	
C3	0.9422 (3)	−0.0635 (5)	0.8982 (2)	0.0507 (19)	
C4	0.9334 (3)	−0.1549 (5)	0.8801 (2)	0.0458 (17)	
C5	0.9787 (3)	−0.2149 (5)	0.8869 (3)	0.059 (2)	
H5	1.014697	−0.196192	0.902631	0.070*	
C6	0.9716 (4)	−0.3020 (6)	0.8708 (3)	0.068 (2)	
H6	1.002311	−0.343241	0.876229	0.082*	
C7	0.9202 (4)	−0.3283 (5)	0.8472 (3)	0.059 (2)	
H7	0.916005	−0.387860	0.836195	0.071*	
C8	0.8743 (3)	−0.2707 (5)	0.8389 (2)	0.0475 (17)	
H8	0.839010	−0.289935	0.822251	0.057*	
C9	0.8808 (3)	−0.1832 (4)	0.8555 (2)	0.0415 (16)	
C10	0.8304 (3)	−0.1226 (4)	0.8466 (2)	0.0407 (16)	
C11	0.8411 (2)	−0.0331 (4)	0.86554 (19)	0.0341 (15)	
C12	0.7462 (2)	0.0462 (4)	0.83762 (19)	0.0330 (14)	
C13	0.7401 (3)	0.0809 (4)	0.7986 (2)	0.0417 (16)	
C14	0.6848 (3)	0.0918 (5)	0.7753 (2)	0.0497 (18)	
H14	0.678948	0.114791	0.748055	0.060*	
C15	0.6386 (3)	0.0704 (4)	0.7906 (2)	0.0474 (18)	
C16	0.6469 (3)	0.0341 (4)	0.8293 (2)	0.0444 (17)	
H16	0.615097	0.017576	0.839637	0.053*	
C17	0.7017 (3)	0.0209 (4)	0.8543 (2)	0.0396 (16)	
C18	0.7898 (3)	0.1069 (6)	0.7819 (2)	0.062 (2)	
H18A	0.811591	0.154071	0.799298	0.093*	
H18B	0.776570	0.129810	0.753662	0.093*	
H18C	0.813866	0.053857	0.781681	0.093*	

C19	0.5788 (3)	0.0890 (5)	0.7657 (3)	0.071 (3)
H19A	0.573269	0.154347	0.762005	0.106*
H19B	0.551679	0.064841	0.780460	0.106*
H19C	0.573058	0.059762	0.738674	0.106*
C20	0.7100 (3)	−0.0172 (5)	0.8969 (2)	0.055 (2)
H20A	0.731628	−0.073558	0.898820	0.082*
H20B	0.673115	−0.029557	0.902724	0.082*
H20C	0.730618	0.026421	0.916969	0.082*
C21	0.9264 (2)	0.1398 (4)	0.9276 (2)	0.0388 (16)
C22	0.9396 (3)	0.1274 (5)	0.9705 (2)	0.0457 (17)
C23	0.9767 (3)	0.1913 (6)	0.9941 (3)	0.062 (2)
H23	0.986390	0.185905	1.023329	0.074*
C24	0.9995 (3)	0.2618 (6)	0.9756 (4)	0.073 (3)
C25	0.9859 (3)	0.2678 (5)	0.9326 (3)	0.065 (2)
H25	1.001880	0.315108	0.919847	0.079*
C26	0.9496 (3)	0.2066 (4)	0.9079 (2)	0.0459 (18)
C27	0.9156 (3)	0.0514 (5)	0.9904 (2)	0.058 (2)
H27A	0.874837	0.047328	0.978525	0.086*
H27B	0.922413	0.062489	1.020127	0.086*
H27C	0.933690	−0.005381	0.985566	0.086*
C28	1.0366 (3)	0.3318 (7)	1.0028 (3)	0.109 (4)
H28A	1.012689	0.373940	1.013781	0.163*
H28B	1.058288	0.365260	0.986425	0.163*
H28C	1.062516	0.301250	1.025724	0.163*
C29	0.9382 (3)	0.2110 (5)	0.8619 (3)	0.064 (2)
H29A	0.939546	0.149942	0.850820	0.096*
H29B	0.966835	0.248851	0.853917	0.096*
H29C	0.900705	0.237137	0.850933	0.096*
C30	0.7552 (2)	0.3516 (4)	0.88543 (18)	0.0320 (14)
C31	0.6962 (3)	0.4651 (4)	0.88839 (19)	0.0349 (15)
C32	0.6496 (3)	0.5212 (5)	0.8963 (2)	0.0497 (19)
C33	0.6457 (3)	0.6127 (4)	0.8771 (2)	0.0452 (17)
C34	0.6042 (3)	0.6715 (5)	0.8832 (3)	0.065 (2)
H34	0.578042	0.651936	0.898431	0.077*
C35	0.6004 (4)	0.7582 (5)	0.8674 (3)	0.074 (3)
H35	0.573409	0.799298	0.873366	0.089*
C36	0.6357 (3)	0.7845 (5)	0.8432 (3)	0.060 (2)
H36	0.631145	0.842581	0.830697	0.073*
C37	0.6776 (3)	0.7283 (5)	0.8367 (2)	0.055 (2)
H37	0.702944	0.748885	0.821003	0.066*
C38	0.6831 (3)	0.6416 (4)	0.8530 (2)	0.0404 (16)
C39	0.7283 (3)	0.5821 (4)	0.8446 (2)	0.0381 (15)
C40	0.7309 (3)	0.4927 (4)	0.86418 (19)	0.0352 (15)
C41	0.8092 (3)	0.4149 (4)	0.8379 (2)	0.0366 (16)
C42	0.8651 (3)	0.4388 (4)	0.8557 (2)	0.0383 (16)
C43	0.9049 (3)	0.4260 (5)	0.8326 (2)	0.0495 (19)
H43	0.943140	0.442199	0.843918	0.059*
C44	0.8893 (3)	0.3896 (5)	0.7930 (2)	0.052 (2)

C45	0.8335 (4)	0.3686 (5)	0.7768 (2)	0.057 (2)	
H45	0.823059	0.344699	0.749584	0.069*	
C46	0.7917 (3)	0.3808 (4)	0.7984 (2)	0.0434 (17)	
C47	0.8828 (3)	0.4757 (5)	0.8989 (2)	0.058 (2)	
H47A	0.864586	0.534311	0.900220	0.087*	
H47B	0.923901	0.483244	0.906482	0.087*	
H47C	0.871415	0.433473	0.918092	0.087*	
C48	0.9345 (4)	0.3673 (6)	0.7699 (3)	0.076 (3)	
H48A	0.925751	0.398010	0.743145	0.114*	
H48B	0.935485	0.301841	0.765689	0.114*	
H48C	0.971320	0.387735	0.786134	0.114*	
C49	0.7316 (3)	0.3555 (6)	0.7803 (2)	0.064 (2)	
H49A	0.720629	0.305946	0.796270	0.096*	
H49B	0.727492	0.336073	0.751620	0.096*	
H49C	0.707210	0.407879	0.781006	0.096*	
C50	0.6833 (3)	0.3172 (4)	0.9243 (2)	0.0360 (15)	
C51	0.6478 (3)	0.2523 (4)	0.9016 (2)	0.0409 (17)	
C52	0.6248 (3)	0.1888 (5)	0.9236 (2)	0.0487 (18)	
H52	0.601431	0.142215	0.909163	0.058*	
C53	0.6355 (3)	0.1921 (5)	0.9664 (3)	0.055 (2)	
C54	0.6687 (3)	0.2611 (5)	0.9873 (2)	0.052 (2)	
H54	0.674491	0.264444	1.016409	0.063*	
C55	0.6943 (3)	0.3262 (5)	0.9669 (2)	0.0430 (17)	
C56	0.6334 (3)	0.2510 (5)	0.8554 (2)	0.0521 (19)	
H56A	0.623919	0.312340	0.844894	0.078*	
H56B	0.601063	0.211007	0.845336	0.078*	
H56C	0.665943	0.228875	0.845676	0.078*	
C57	0.6116 (4)	0.1191 (6)	0.9901 (3)	0.083 (3)	
H57A	0.578043	0.092062	0.971974	0.124*	
H57B	0.601229	0.146416	1.014051	0.124*	
H57C	0.640163	0.072252	0.999394	0.124*	
C58	0.7293 (3)	0.4018 (5)	0.9896 (2)	0.058 (2)	
H58A	0.764540	0.406565	0.980514	0.086*	
H58B	0.737856	0.389470	1.019351	0.086*	
H58C	0.708270	0.458672	0.983938	0.086*	
C11	1.04519 (8)	0.47611 (13)	0.88765 (8)	0.0792 (8)	
C1A	0.8172 (10)	−0.2898 (16)	1.0212 (5)	0.096 (5)*	0.35
H1A	0.822300	−0.285239	1.050252	0.115*	0.35
C1B	0.7982 (9)	−0.3710 (13)	1.0007 (6)	0.098 (5)*	0.35
H1B	0.790513	−0.421274	1.016288	0.117*	0.35
C1C	0.7906 (9)	−0.3792 (12)	0.9591 (6)	0.074 (5)*	0.35
H1C	0.777685	−0.434473	0.945589	0.088*	0.35
C1D	0.8024 (10)	−0.3033 (15)	0.9363 (5)	0.089 (5)*	0.35
H1D	0.797473	−0.307832	0.907216	0.106*	0.35
C1E	0.8216 (10)	−0.2209 (13)	0.9567 (7)	0.091 (4)*	0.35
H1E	0.829354	−0.170067	0.941534	0.109*	0.35
C1F	0.8285 (10)	−0.2157 (12)	0.9984 (6)	0.095 (4)*	0.35
H1F	0.841353	−0.160753	1.012282	0.114*	0.35

C2A	0.8376 (5)	−0.2732 (9)	1.0218 (4)	0.095 (4)*	0.65
H2A	0.849029	−0.279806	1.050957	0.115*	0.65
C2B	0.8138 (5)	−0.3486 (9)	0.9980 (4)	0.090 (3)*	0.65
H2B	0.809607	−0.404226	1.011172	0.108*	0.65
C2C	0.7970 (5)	−0.3422 (8)	0.9565 (4)	0.082 (3)*	0.65
H2C	0.780802	−0.391592	0.939577	0.099*	0.65
C2D	0.8054 (6)	−0.2549 (9)	0.9398 (4)	0.084 (3)*	0.65
H2D	0.794028	−0.248385	0.910639	0.101*	0.65
C2E	0.8296 (6)	−0.1755 (8)	0.9634 (4)	0.084 (4)*	0.65
H2E	0.834207	−0.119077	0.950915	0.101*	0.65
C2F	0.8450 (6)	−0.1893 (9)	1.0045 (4)	0.097 (4)*	0.65
H2F	0.861197	−0.140917	1.022025	0.117*	0.65

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.02753 (13)	0.02967 (15)	0.03938 (15)	0.00434 (11)	0.01229 (10)	0.00096 (12)
O1	0.041 (3)	0.039 (3)	0.060 (3)	0.002 (2)	0.002 (2)	−0.006 (2)
O2	0.036 (3)	0.063 (4)	0.107 (5)	0.015 (3)	−0.003 (3)	−0.028 (3)
O3	0.056 (3)	0.043 (3)	0.060 (3)	0.005 (2)	0.025 (3)	0.013 (2)
O4	0.070 (4)	0.061 (4)	0.120 (5)	0.030 (3)	0.069 (4)	0.038 (3)
N1	0.027 (3)	0.028 (3)	0.044 (3)	0.004 (2)	0.012 (2)	−0.002 (2)
N2	0.026 (3)	0.033 (3)	0.042 (3)	0.007 (2)	0.008 (2)	0.000 (2)
N3	0.033 (3)	0.024 (3)	0.040 (3)	0.002 (2)	0.013 (2)	0.003 (2)
N4	0.031 (3)	0.024 (3)	0.044 (3)	0.008 (2)	0.014 (2)	0.005 (2)
C1	0.030 (3)	0.034 (4)	0.041 (4)	0.006 (3)	0.014 (3)	0.006 (3)
C2	0.031 (3)	0.031 (4)	0.047 (4)	0.002 (3)	0.014 (3)	−0.002 (3)
C3	0.036 (4)	0.052 (5)	0.062 (5)	0.014 (3)	0.006 (4)	−0.010 (4)
C4	0.041 (4)	0.038 (4)	0.058 (5)	0.013 (3)	0.012 (4)	−0.004 (3)
C5	0.048 (5)	0.043 (5)	0.084 (6)	0.021 (4)	0.012 (4)	−0.008 (4)
C6	0.070 (6)	0.049 (5)	0.088 (6)	0.028 (4)	0.025 (5)	−0.001 (5)
C7	0.068 (6)	0.028 (4)	0.082 (6)	0.015 (4)	0.018 (5)	−0.003 (4)
C8	0.053 (4)	0.035 (4)	0.056 (4)	0.003 (3)	0.016 (4)	−0.002 (4)
C9	0.043 (4)	0.032 (4)	0.051 (4)	0.005 (3)	0.016 (3)	0.002 (3)
C10	0.044 (4)	0.036 (4)	0.041 (4)	0.000 (3)	0.009 (3)	0.002 (3)
C11	0.029 (3)	0.032 (4)	0.042 (4)	0.005 (3)	0.009 (3)	0.002 (3)
C12	0.025 (3)	0.027 (3)	0.044 (4)	0.003 (3)	0.004 (3)	0.001 (3)
C13	0.049 (4)	0.032 (4)	0.042 (4)	0.007 (3)	0.006 (3)	−0.006 (3)
C14	0.057 (5)	0.044 (4)	0.042 (4)	0.005 (4)	−0.002 (4)	−0.004 (3)
C15	0.040 (4)	0.032 (4)	0.059 (5)	0.003 (3)	−0.010 (4)	−0.008 (3)
C16	0.033 (4)	0.035 (4)	0.062 (5)	0.001 (3)	0.004 (3)	0.001 (3)
C17	0.040 (4)	0.028 (4)	0.049 (4)	0.000 (3)	0.007 (3)	0.002 (3)
C18	0.065 (5)	0.079 (6)	0.044 (5)	0.002 (4)	0.018 (4)	0.009 (4)
C19	0.055 (5)	0.047 (5)	0.090 (6)	0.007 (4)	−0.023 (5)	−0.003 (4)
C20	0.034 (4)	0.066 (5)	0.064 (5)	0.008 (4)	0.012 (4)	0.017 (4)
C21	0.022 (3)	0.034 (4)	0.057 (4)	0.006 (3)	0.004 (3)	−0.007 (3)
C22	0.029 (4)	0.048 (5)	0.059 (5)	0.012 (3)	0.008 (3)	−0.007 (4)
C23	0.034 (4)	0.074 (6)	0.072 (5)	0.004 (4)	0.001 (4)	−0.031 (5)

C24	0.033 (4)	0.060 (6)	0.127 (9)	−0.008 (4)	0.019 (5)	−0.045 (6)
C25	0.035 (4)	0.043 (5)	0.123 (8)	−0.004 (4)	0.027 (5)	−0.007 (5)
C26	0.030 (4)	0.031 (4)	0.081 (6)	0.001 (3)	0.021 (4)	−0.004 (4)
C27	0.048 (5)	0.076 (6)	0.049 (5)	0.007 (4)	0.013 (4)	−0.001 (4)
C28	0.039 (5)	0.099 (8)	0.175 (11)	−0.006 (5)	0.000 (6)	−0.075 (8)
C29	0.056 (5)	0.059 (6)	0.083 (6)	0.002 (4)	0.026 (5)	0.011 (4)
C30	0.026 (3)	0.042 (4)	0.031 (3)	0.006 (3)	0.012 (3)	−0.001 (3)
C31	0.033 (4)	0.034 (4)	0.040 (4)	0.008 (3)	0.015 (3)	0.003 (3)
C32	0.044 (4)	0.041 (4)	0.071 (5)	0.013 (3)	0.028 (4)	0.010 (4)
C33	0.038 (4)	0.035 (4)	0.065 (5)	0.013 (3)	0.019 (4)	0.001 (3)
C34	0.053 (5)	0.043 (5)	0.104 (7)	0.013 (4)	0.034 (5)	0.014 (4)
C35	0.071 (6)	0.051 (5)	0.108 (8)	0.022 (4)	0.035 (6)	0.010 (5)
C36	0.067 (5)	0.030 (4)	0.085 (6)	0.021 (4)	0.019 (5)	0.020 (4)
C37	0.052 (5)	0.038 (4)	0.070 (5)	0.004 (4)	0.005 (4)	0.015 (4)
C38	0.040 (4)	0.029 (4)	0.048 (4)	0.000 (3)	0.002 (3)	0.004 (3)
C39	0.037 (4)	0.035 (4)	0.043 (4)	−0.001 (3)	0.011 (3)	0.002 (3)
C40	0.034 (3)	0.027 (4)	0.049 (4)	0.005 (3)	0.017 (3)	0.002 (3)
C41	0.041 (4)	0.027 (4)	0.050 (4)	0.006 (3)	0.027 (3)	0.003 (3)
C42	0.037 (4)	0.030 (4)	0.054 (4)	0.001 (3)	0.022 (3)	0.003 (3)
C43	0.043 (4)	0.041 (4)	0.074 (5)	−0.003 (3)	0.033 (4)	0.002 (4)
C44	0.067 (5)	0.036 (4)	0.070 (5)	0.006 (4)	0.048 (5)	0.009 (4)
C45	0.091 (7)	0.042 (5)	0.048 (5)	0.006 (4)	0.036 (5)	0.000 (4)
C46	0.056 (5)	0.036 (4)	0.041 (4)	−0.006 (3)	0.019 (4)	0.003 (3)
C47	0.049 (5)	0.063 (5)	0.065 (5)	−0.006 (4)	0.020 (4)	−0.008 (4)
C48	0.095 (7)	0.059 (6)	0.100 (7)	0.006 (5)	0.075 (6)	0.004 (5)
C49	0.067 (6)	0.076 (6)	0.047 (5)	−0.008 (4)	0.010 (4)	−0.013 (4)
C50	0.039 (4)	0.022 (3)	0.053 (4)	0.013 (3)	0.022 (3)	0.013 (3)
C51	0.037 (4)	0.031 (4)	0.057 (4)	0.007 (3)	0.016 (3)	0.004 (3)
C52	0.038 (4)	0.032 (4)	0.081 (6)	0.000 (3)	0.023 (4)	0.008 (4)
C53	0.039 (4)	0.046 (5)	0.092 (6)	0.017 (4)	0.038 (4)	0.026 (5)
C54	0.056 (5)	0.058 (5)	0.051 (4)	0.020 (4)	0.029 (4)	0.020 (4)
C55	0.040 (4)	0.043 (4)	0.050 (4)	0.013 (3)	0.019 (3)	0.009 (3)
C56	0.052 (5)	0.043 (5)	0.059 (5)	0.000 (3)	0.009 (4)	0.001 (3)
C57	0.071 (6)	0.066 (6)	0.129 (8)	0.015 (5)	0.062 (6)	0.046 (6)
C58	0.067 (5)	0.056 (5)	0.053 (5)	0.012 (4)	0.021 (4)	−0.001 (4)
Cl1	0.0436 (11)	0.0410 (12)	0.163 (2)	−0.0029 (9)	0.0434 (14)	−0.0022 (13)

Geometric parameters (Å, °)

Au1—C1	2.016 (6)	C33—C34	1.383 (9)
Au1—C30	2.021 (6)	C33—C38	1.416 (9)
O1—C10	1.215 (8)	C34—C35	1.381 (11)
O2—C3	1.219 (8)	C34—H34	0.9500
O3—C39	1.210 (7)	C35—C36	1.368 (11)
O4—C32	1.210 (8)	C35—H35	0.9500
N1—C1	1.360 (8)	C36—C37	1.373 (10)
N1—C11	1.384 (7)	C36—H36	0.9500
N1—C12	1.463 (7)	C37—C38	1.386 (9)

N2—C1	1.364 (7)	C37—H37	0.9500
N2—C2	1.385 (8)	C38—C39	1.488 (9)
N2—C21	1.457 (8)	C39—C40	1.468 (9)
N3—C30	1.360 (7)	C41—C46	1.381 (9)
N3—C40	1.380 (7)	C41—C42	1.396 (9)
N3—C41	1.462 (7)	C42—C43	1.385 (8)
N4—C30	1.347 (7)	C42—C47	1.506 (9)
N4—C31	1.372 (7)	C43—C44	1.395 (10)
N4—C50	1.470 (7)	C43—H43	0.9500
C2—C11	1.348 (8)	C44—C45	1.374 (11)
C2—C3	1.471 (9)	C44—C48	1.520 (9)
C3—C4	1.475 (10)	C45—C46	1.394 (9)
C4—C5	1.393 (9)	C45—H45	0.9500
C4—C9	1.415 (9)	C46—C49	1.495 (10)
C5—C6	1.392 (11)	C47—H47A	0.9800
C5—H5	0.9500	C47—H47B	0.9800
C6—C7	1.369 (11)	C47—H47C	0.9800
C6—H6	0.9500	C48—H48A	0.9800
C7—C8	1.382 (10)	C48—H48B	0.9800
C7—H7	0.9500	C48—H48C	0.9800
C8—C9	1.401 (9)	C49—H49A	0.9800
C8—H8	0.9500	C49—H49B	0.9800
C9—C10	1.492 (9)	C49—H49C	0.9800
C10—C11	1.464 (9)	C50—C55	1.389 (9)
C12—C13	1.373 (9)	C50—C51	1.390 (9)
C12—C17	1.383 (8)	C51—C52	1.388 (9)
C13—C14	1.395 (9)	C51—C56	1.499 (10)
C13—C18	1.500 (9)	C52—C53	1.388 (10)
C14—C15	1.379 (10)	C52—H52	0.9500
C14—H14	0.9500	C53—C54	1.384 (11)
C15—C16	1.370 (9)	C53—C57	1.533 (9)
C15—C19	1.521 (9)	C54—C55	1.405 (9)
C16—C17	1.410 (9)	C54—H54	0.9500
C16—H16	0.9500	C55—C58	1.498 (10)
C17—C20	1.498 (9)	C56—H56A	0.9800
C18—H18A	0.9800	C56—H56B	0.9800
C18—H18B	0.9800	C56—H56C	0.9800
C18—H18C	0.9800	C57—H57A	0.9800
C19—H19A	0.9800	C57—H57B	0.9800
C19—H19B	0.9800	C57—H57C	0.9800
C19—H19C	0.9800	C58—H58A	0.9800
C20—H20A	0.9800	C58—H58B	0.9800
C20—H20B	0.9800	C58—H58C	0.9800
C20—H20C	0.9800	C1A—C1F	1.397 (7)
C21—C26	1.379 (9)	C1A—C1B	1.406 (7)
C21—C22	1.401 (9)	C1A—H1A	0.9500
C22—C23	1.413 (10)	C1B—C1C	1.362 (7)
C22—C27	1.493 (10)	C1B—H1B	0.9500

C23—C24	1.393 (12)	C1C—C1D	1.424 (8)
C23—H23	0.9500	C1C—H1C	0.9500
C24—C25	1.396 (13)	C1D—C1E	1.422 (8)
C24—C28	1.524 (11)	C1D—H1D	0.9500
C25—C26	1.392 (11)	C1E—C1F	1.363 (7)
C25—H25	0.9500	C1E—H1E	0.9500
C26—C29	1.493 (10)	C1F—H1F	0.9500
C27—H27A	0.9800	C2A—C2F	1.400 (11)
C27—H27B	0.9800	C2A—C2B	1.413 (10)
C27—H27C	0.9800	C2A—H2A	0.9500
C28—H28A	0.9800	C2B—C2C	1.350 (10)
C28—H28B	0.9800	C2B—H2B	0.9500
C28—H28C	0.9800	C2C—C2D	1.440 (11)
C29—H29A	0.9800	C2C—H2C	0.9500
C29—H29B	0.9800	C2D—C2E	1.460 (11)
C29—H29C	0.9800	C2D—H2D	0.9500
C31—C40	1.363 (8)	C2E—C2F	1.348 (10)
C31—C32	1.478 (8)	C2E—H2E	0.9500
C32—C33	1.491 (9)	C2F—H2F	0.9500
C1—Au1—C30	174.2 (2)	C35—C34—C33	121.0 (7)
C1—N1—C11	109.2 (5)	C35—C34—H34	119.5
C1—N1—C12	121.9 (5)	C33—C34—H34	119.5
C11—N1—C12	128.4 (5)	C36—C35—C34	119.6 (7)
C1—N2—C2	109.6 (5)	C36—C35—H35	120.2
C1—N2—C21	122.0 (5)	C34—C35—H35	120.2
C2—N2—C21	128.4 (5)	C35—C36—C37	121.0 (7)
C30—N3—C40	109.6 (5)	C35—C36—H36	119.5
C30—N3—C41	122.1 (5)	C37—C36—H36	119.5
C40—N3—C41	127.9 (5)	C36—C37—C38	120.4 (7)
C30—N4—C31	110.1 (5)	C36—C37—H37	119.8
C30—N4—C50	122.1 (5)	C38—C37—H37	119.8
C31—N4—C50	127.5 (5)	C37—C38—C33	119.1 (6)
N1—C1—N2	106.2 (5)	C37—C38—C39	118.8 (6)
N1—C1—Au1	123.5 (4)	C33—C38—C39	122.1 (6)
N2—C1—Au1	130.1 (5)	O3—C39—C40	122.4 (6)
C11—C2—N2	107.0 (5)	O3—C39—C38	123.7 (6)
C11—C2—C3	124.0 (6)	C40—C39—C38	113.9 (5)
N2—C2—C3	128.9 (6)	C31—C40—N3	106.7 (5)
O2—C3—C2	122.5 (7)	C31—C40—C39	124.4 (5)
O2—C3—C4	123.6 (6)	N3—C40—C39	128.9 (5)
C2—C3—C4	113.9 (6)	C46—C41—C42	123.2 (6)
C5—C4—C9	118.8 (6)	C46—C41—N3	117.8 (6)
C5—C4—C3	118.9 (7)	C42—C41—N3	118.9 (6)
C9—C4—C3	122.3 (6)	C43—C42—C41	118.1 (6)
C6—C5—C4	120.3 (7)	C43—C42—C47	120.0 (6)
C6—C5—H5	119.8	C41—C42—C47	121.9 (5)
C4—C5—H5	119.8	C42—C43—C44	120.6 (7)

C7—C6—C5	120.0 (7)	C42—C43—H43	119.7
C7—C6—H6	120.0	C44—C43—H43	119.7
C5—C6—H6	120.0	C45—C44—C43	118.9 (6)
C6—C7—C8	121.8 (7)	C45—C44—C48	121.2 (7)
C6—C7—H7	119.1	C43—C44—C48	119.7 (7)
C8—C7—H7	119.1	C44—C45—C46	122.9 (7)
C7—C8—C9	118.7 (7)	C44—C45—H45	118.6
C7—C8—H8	120.7	C46—C45—H45	118.6
C9—C8—H8	120.7	C41—C46—C45	116.2 (7)
C8—C9—C4	120.4 (6)	C41—C46—C49	122.1 (6)
C8—C9—C10	117.8 (6)	C45—C46—C49	121.6 (7)
C4—C9—C10	121.9 (6)	C42—C47—H47A	109.5
O1—C10—C11	122.7 (6)	C42—C47—H47B	109.5
O1—C10—C9	123.5 (6)	H47A—C47—H47B	109.5
C11—C10—C9	113.8 (6)	C42—C47—H47C	109.5
C2—C11—N1	107.9 (5)	H47A—C47—H47C	109.5
C2—C11—C10	124.0 (6)	H47B—C47—H47C	109.5
N1—C11—C10	128.0 (6)	C44—C48—H48A	109.5
C13—C12—C17	124.0 (6)	C44—C48—H48B	109.5
C13—C12—N1	117.6 (5)	H48A—C48—H48B	109.5
C17—C12—N1	118.4 (5)	C44—C48—H48C	109.5
C12—C13—C14	116.5 (6)	H48A—C48—H48C	109.5
C12—C13—C18	122.1 (6)	H48B—C48—H48C	109.5
C14—C13—C18	121.4 (6)	C46—C49—H49A	109.5
C15—C14—C13	122.3 (7)	C46—C49—H49B	109.5
C15—C14—H14	118.9	H49A—C49—H49B	109.5
C13—C14—H14	118.9	C46—C49—H49C	109.5
C16—C15—C14	119.1 (6)	H49A—C49—H49C	109.5
C16—C15—C19	119.6 (7)	H49B—C49—H49C	109.5
C14—C15—C19	121.2 (7)	C55—C50—C51	124.7 (6)
C15—C16—C17	121.3 (6)	C55—C50—N4	118.7 (6)
C15—C16—H16	119.4	C51—C50—N4	116.6 (6)
C17—C16—H16	119.4	C52—C51—C50	117.1 (7)
C12—C17—C16	116.8 (6)	C52—C51—C56	120.6 (7)
C12—C17—C20	122.6 (6)	C50—C51—C56	122.3 (6)
C16—C17—C20	120.6 (6)	C53—C52—C51	121.1 (7)
C13—C18—H18A	109.5	C53—C52—H52	119.4
C13—C18—H18B	109.5	C51—C52—H52	119.4
H18A—C18—H18B	109.5	C54—C53—C52	119.3 (6)
C13—C18—H18C	109.5	C54—C53—C57	120.5 (8)
H18A—C18—H18C	109.5	C52—C53—C57	120.2 (8)
H18B—C18—H18C	109.5	C53—C54—C55	122.4 (7)
C15—C19—H19A	109.5	C53—C54—H54	118.8
C15—C19—H19B	109.5	C55—C54—H54	118.8
H19A—C19—H19B	109.5	C50—C55—C54	115.3 (7)
C15—C19—H19C	109.5	C50—C55—C58	122.6 (6)
H19A—C19—H19C	109.5	C54—C55—C58	122.1 (7)
H19B—C19—H19C	109.5	C51—C56—H56A	109.5

C17—C20—H20A	109.5	C51—C56—H56B	109.5
C17—C20—H20B	109.5	H56A—C56—H56B	109.5
H20A—C20—H20B	109.5	C51—C56—H56C	109.5
C17—C20—H20C	109.5	H56A—C56—H56C	109.5
H20A—C20—H20C	109.5	H56B—C56—H56C	109.5
H20B—C20—H20C	109.5	C53—C57—H57A	109.5
C26—C21—C22	124.0 (6)	C53—C57—H57B	109.5
C26—C21—N2	117.5 (6)	H57A—C57—H57B	109.5
C22—C21—N2	118.5 (6)	C53—C57—H57C	109.5
C21—C22—C23	116.4 (7)	H57A—C57—H57C	109.5
C21—C22—C27	122.2 (6)	H57B—C57—H57C	109.5
C23—C22—C27	121.4 (7)	C55—C58—H58A	109.5
C24—C23—C22	121.6 (8)	C55—C58—H58B	109.5
C24—C23—H23	119.2	H58A—C58—H58B	109.5
C22—C23—H23	119.2	C55—C58—H58C	109.5
C23—C24—C25	118.6 (7)	H58A—C58—H58C	109.5
C23—C24—C28	119.2 (10)	H58B—C58—H58C	109.5
C25—C24—C28	122.2 (9)	C1F—C1A—C1B	119.5 (5)
C26—C25—C24	122.1 (8)	C1F—C1A—H1A	120.3
C26—C25—H25	118.9	C1B—C1A—H1A	120.3
C24—C25—H25	118.9	C1C—C1B—C1A	121.4 (5)
C21—C26—C25	117.2 (8)	C1C—C1B—H1B	119.3
C21—C26—C29	121.6 (7)	C1A—C1B—H1B	119.3
C25—C26—C29	121.2 (7)	C1B—C1C—C1D	118.6 (5)
C22—C27—H27A	109.5	C1B—C1C—H1C	120.7
C22—C27—H27B	109.5	C1D—C1C—H1C	120.7
H27A—C27—H27B	109.5	C1E—C1D—C1C	120.3 (5)
C22—C27—H27C	109.5	C1E—C1D—H1D	119.8
H27A—C27—H27C	109.5	C1C—C1D—H1D	119.8
H27B—C27—H27C	109.5	C1F—C1E—C1D	119.1 (5)
C24—C28—H28A	109.5	C1F—C1E—H1E	120.5
C24—C28—H28B	109.5	C1D—C1E—H1E	120.5
H28A—C28—H28B	109.5	C1E—C1F—C1A	121.1 (5)
C24—C28—H28C	109.5	C1E—C1F—H1F	119.4
H28A—C28—H28C	109.5	C1A—C1F—H1F	119.4
H28B—C28—H28C	109.5	C2F—C2A—C2B	122.8 (11)
C26—C29—H29A	109.5	C2F—C2A—H2A	118.6
C26—C29—H29B	109.5	C2B—C2A—H2A	118.6
H29A—C29—H29B	109.5	C2C—C2B—C2A	120.5 (10)
C26—C29—H29C	109.5	C2C—C2B—H2B	119.8
H29A—C29—H29C	109.5	C2A—C2B—H2B	119.8
H29B—C29—H29C	109.5	C2B—C2C—C2D	115.0 (10)
N4—C30—N3	106.3 (5)	C2B—C2C—H2C	122.5
N4—C30—Au1	130.0 (4)	C2D—C2C—H2C	122.5
N3—C30—Au1	123.5 (4)	C2C—C2D—C2E	126.1 (10)
C40—C31—N4	107.2 (5)	C2C—C2D—H2D	116.9
C40—C31—C32	123.2 (6)	C2E—C2D—H2D	116.9
N4—C31—C32	129.5 (5)	C2F—C2E—C2D	114.0 (10)

O4—C32—C31	122.6 (6)	C2F—C2E—H2E	123.0
O4—C32—C33	123.3 (6)	C2D—C2E—H2E	123.0
C31—C32—C33	114.1 (5)	C2E—C2F—C2A	121.6 (11)
C34—C33—C38	118.9 (6)	C2E—C2F—H2F	119.2
C34—C33—C32	118.9 (6)	C2A—C2F—H2F	119.2
C38—C33—C32	122.2 (6)		
C11—N1—C1—N2	−0.1 (6)	C40—N3—C30—Au1	175.4 (4)
C12—N1—C1—N2	−173.3 (5)	C41—N3—C30—Au1	1.4 (8)
C11—N1—C1—Au1	175.8 (4)	C30—N4—C31—C40	0.2 (7)
C12—N1—C1—Au1	2.6 (8)	C50—N4—C31—C40	−173.8 (6)
C2—N2—C1—N1	−0.4 (6)	C30—N4—C31—C32	177.4 (7)
C21—N2—C1—N1	178.5 (5)	C50—N4—C31—C32	3.4 (11)
C2—N2—C1—Au1	−176.0 (4)	C40—C31—C32—O4	178.9 (8)
C21—N2—C1—Au1	3.0 (8)	N4—C31—C32—O4	2.1 (13)
C1—N2—C2—C11	0.8 (7)	C40—C31—C32—C33	−2.8 (10)
C21—N2—C2—C11	−178.1 (6)	N4—C31—C32—C33	−179.6 (7)
C1—N2—C2—C3	177.2 (6)	O4—C32—C33—C34	−0.5 (12)
C21—N2—C2—C3	−1.7 (11)	C31—C32—C33—C34	−178.8 (7)
C11—C2—C3—O2	175.7 (7)	O4—C32—C33—C38	179.1 (8)
N2—C2—C3—O2	−0.1 (12)	C31—C32—C33—C38	0.8 (10)
C11—C2—C3—C4	−4.4 (10)	C38—C33—C34—C35	−2.4 (13)
N2—C2—C3—C4	179.8 (6)	C32—C33—C34—C35	177.3 (8)
O2—C3—C4—C5	1.4 (12)	C33—C34—C35—C36	4.3 (14)
C2—C3—C4—C5	−178.5 (7)	C34—C35—C36—C37	−4.7 (14)
O2—C3—C4—C9	−177.4 (7)	C35—C36—C37—C38	3.3 (13)
C2—C3—C4—C9	2.7 (10)	C36—C37—C38—C33	−1.3 (11)
C9—C4—C5—C6	−2.1 (11)	C36—C37—C38—C39	178.8 (7)
C3—C4—C5—C6	179.0 (7)	C34—C33—C38—C37	0.9 (11)
C4—C5—C6—C7	1.9 (13)	C32—C33—C38—C37	−178.8 (7)
C5—C6—C7—C8	−0.5 (13)	C34—C33—C38—C39	−179.3 (7)
C6—C7—C8—C9	−0.4 (12)	C32—C33—C38—C39	1.1 (11)
C7—C8—C9—C4	0.1 (10)	C37—C38—C39—O3	−1.2 (10)
C7—C8—C9—C10	−179.1 (6)	C33—C38—C39—O3	178.9 (7)
C5—C4—C9—C8	1.2 (10)	C37—C38—C39—C40	178.7 (6)
C3—C4—C9—C8	179.9 (6)	C33—C38—C39—C40	−1.2 (9)
C5—C4—C9—C10	−179.6 (6)	N4—C31—C40—N3	−0.4 (7)
C3—C4—C9—C10	−0.8 (10)	C32—C31—C40—N3	−177.8 (6)
C8—C9—C10—O1	−1.2 (10)	N4—C31—C40—C39	−179.7 (6)
C4—C9—C10—O1	179.6 (6)	C32—C31—C40—C39	2.9 (11)
C8—C9—C10—C11	179.4 (6)	C30—N3—C40—C31	0.4 (7)
C4—C9—C10—C11	0.2 (9)	C41—N3—C40—C31	174.0 (6)
N2—C2—C11—N1	−0.8 (7)	C30—N3—C40—C39	179.7 (6)
C3—C2—C11—N1	−177.4 (6)	C41—N3—C40—C39	−6.7 (11)
N2—C2—C11—C10	−179.2 (5)	O3—C39—C40—C31	179.1 (7)
C3—C2—C11—C10	4.2 (10)	C38—C39—C40—C31	−0.8 (9)
C1—N1—C11—C2	0.6 (7)	O3—C39—C40—N3	0.0 (11)
C12—N1—C11—C2	173.2 (5)	C38—C39—C40—N3	−179.9 (6)

C1—N1—C11—C10	178.9 (6)	C30—N3—C41—C46	85.7 (7)
C12—N1—C11—C10	−8.5 (10)	C40—N3—C41—C46	−87.2 (8)
O1—C10—C11—C2	178.8 (6)	C30—N3—C41—C42	−91.5 (7)
C9—C10—C11—C2	−1.8 (9)	C40—N3—C41—C42	95.6 (8)
O1—C10—C11—N1	0.7 (10)	C46—C41—C42—C43	−1.2 (10)
C9—C10—C11—N1	−179.9 (6)	N3—C41—C42—C43	175.8 (6)
C1—N1—C12—C13	84.2 (7)	C46—C41—C42—C47	−179.9 (6)
C11—N1—C12—C13	−87.5 (8)	N3—C41—C42—C47	−2.9 (9)
C1—N1—C12—C17	−94.1 (7)	C41—C42—C43—C44	−0.5 (10)
C11—N1—C12—C17	94.1 (7)	C47—C42—C43—C44	178.2 (6)
C17—C12—C13—C14	1.0 (10)	C42—C43—C44—C45	1.6 (10)
N1—C12—C13—C14	−177.2 (5)	C42—C43—C44—C48	−173.8 (6)
C17—C12—C13—C18	−179.7 (6)	C43—C44—C45—C46	−1.0 (11)
N1—C12—C13—C18	2.1 (9)	C48—C44—C45—C46	174.3 (7)
C12—C13—C14—C15	1.0 (10)	C42—C41—C46—C45	1.7 (10)
C18—C13—C14—C15	−178.3 (7)	N3—C41—C46—C45	−175.3 (6)
C13—C14—C15—C16	−2.4 (11)	C42—C41—C46—C49	179.8 (7)
C13—C14—C15—C19	175.7 (6)	N3—C41—C46—C49	2.7 (10)
C14—C15—C16—C17	1.9 (10)	C44—C45—C46—C41	−0.6 (10)
C19—C15—C16—C17	−176.2 (6)	C44—C45—C46—C49	−178.7 (7)
C13—C12—C17—C16	−1.4 (10)	C30—N4—C50—C55	104.7 (7)
N1—C12—C17—C16	176.8 (5)	C31—N4—C50—C55	−82.0 (8)
C13—C12—C17—C20	179.7 (6)	C30—N4—C50—C51	−74.2 (8)
N1—C12—C17—C20	−2.2 (9)	C31—N4—C50—C51	99.1 (7)
C15—C16—C17—C12	−0.1 (10)	C55—C50—C51—C52	−4.5 (10)
C15—C16—C17—C20	178.9 (7)	N4—C50—C51—C52	174.3 (5)
C1—N2—C21—C26	−75.9 (7)	C55—C50—C51—C56	174.3 (6)
C2—N2—C21—C26	102.8 (7)	N4—C50—C51—C56	−6.9 (9)
C1—N2—C21—C22	102.3 (7)	C50—C51—C52—C53	2.2 (10)
C2—N2—C21—C22	−78.9 (8)	C56—C51—C52—C53	−176.7 (6)
C26—C21—C22—C23	3.5 (9)	C51—C52—C53—C54	1.3 (10)
N2—C21—C22—C23	−174.6 (5)	C51—C52—C53—C57	−177.7 (6)
C26—C21—C22—C27	−177.0 (6)	C52—C53—C54—C55	−2.8 (11)
N2—C21—C22—C27	4.9 (9)	C57—C53—C54—C55	176.2 (6)
C21—C22—C23—C24	−0.9 (10)	C51—C50—C55—C54	3.1 (9)
C27—C22—C23—C24	179.6 (7)	N4—C50—C55—C54	−175.7 (5)
C22—C23—C24—C25	−1.3 (11)	C51—C50—C55—C58	−175.0 (6)
C22—C23—C24—C28	176.4 (7)	N4—C50—C55—C58	6.2 (9)
C23—C24—C25—C26	1.2 (12)	C53—C54—C55—C50	0.7 (10)
C28—C24—C25—C26	−176.5 (7)	C53—C54—C55—C58	178.8 (6)
C22—C21—C26—C25	−3.6 (10)	C1F—C1A—C1B—C1C	0.0 (3)
N2—C21—C26—C25	174.5 (6)	C1A—C1B—C1C—C1D	0.1 (3)
C22—C21—C26—C29	173.9 (6)	C1B—C1C—C1D—C1E	−0.2 (6)
N2—C21—C26—C29	−7.9 (9)	C1C—C1D—C1E—C1F	0.2 (9)
C24—C25—C26—C21	1.2 (11)	C1D—C1E—C1F—C1A	0.0 (9)
C24—C25—C26—C29	−176.4 (7)	C1B—C1A—C1F—C1E	−0.1 (7)
C31—N4—C30—N3	0.1 (7)	C2F—C2A—C2B—C2C	0.0 (3)
C50—N4—C30—N3	174.4 (5)	C2A—C2B—C2C—C2D	0.1 (3)

C31—N4—C30—Au1	−175.3 (5)	C2B—C2C—C2D—C2E	−0.2 (6)
C50—N4—C30—Au1	−0.9 (9)	C2C—C2D—C2E—C2F	0.2 (8)
C40—N3—C30—N4	−0.3 (7)	C2D—C2E—C2F—C2A	−0.1 (8)
C41—N3—C30—N4	−174.3 (5)	C2B—C2A—C2F—C2E	0.0 (7)

Bis(1,3-dimesityl-4,5-naphthoquinoimidazol-2-ylidene)gold(I) dichloridaurate(I) dichloromethane disolvate
(shelx_p-1)

Crystal data

[Au(C₂₉H₂₆N₂O₂)₂][AuCl₂]·2CH₂Cl₂

M_r = 1503.72

Triclinic, *P*1̄

a = 11.9236 (11) Å

b = 15.1244 (14) Å

c = 18.4014 (16) Å

α = 100.460 (3)°

β = 105.164 (3)°

γ = 103.994 (3)°

V = 2999.8 (5) Å³

Z = 2

F(000) = 1472

D_x = 1.665 Mg m^{−3}

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 9938 reflections

θ = 2.2–24.8°

μ = 5.20 mm^{−1}

T = 183 K

Block, yellow

0.74 × 0.50 × 0.25 mm

Data collection

Bruker SMART X2S benchtop
diffractometer

Radiation source: XOS X-beam microfocus
source

Doubly curved silicon crystal monochromator
ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2014)

T_{min} = 0.413, *T_{max}* = 1.000

53862 measured reflections

10522 independent reflections

7802 reflections with *I* > 2σ(*I*)

R_{int} = 0.105

θ_{max} = 25.1°, θ_{min} = 2.0°

h = −14→14

k = −18→17

l = −21→21

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.052

wR(*F*²) = 0.138

S = 0.99

10522 reflections

697 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0788*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.001

Δρ_{max} = 2.29 e Å^{−3}

Δρ_{min} = −2.27 e Å^{−3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i> */ <i>U_{eq}</i>
Au1	0.29603 (3)	0.46949 (2)	0.28062 (2)	0.01952 (11)
O1	0.4592 (5)	0.3022 (4)	0.0258 (3)	0.0298 (14)

O2	0.1641 (6)	0.0544 (4)	0.1236 (3)	0.0394 (16)
O3	0.4847 (5)	0.8511 (4)	0.5106 (4)	0.0351 (15)
O4	0.0051 (5)	0.7269 (4)	0.3426 (4)	0.0366 (15)
N1	0.3758 (5)	0.3620 (4)	0.1619 (3)	0.0182 (14)
N2	0.2468 (5)	0.2630 (5)	0.1951 (4)	0.0211 (15)
N3	0.3673 (5)	0.6637 (4)	0.3928 (3)	0.0189 (14)
N4	0.1750 (5)	0.6133 (4)	0.3269 (4)	0.0198 (14)
C1	0.3086 (7)	0.3549 (6)	0.2121 (5)	0.0255 (19)
C2	0.3548 (7)	0.2724 (6)	0.1148 (4)	0.0215 (17)
C3	0.4000 (6)	0.2454 (6)	0.0506 (4)	0.0215 (18)
C4	0.3639 (7)	0.1438 (6)	0.0168 (5)	0.0275 (19)
C5	0.4091 (7)	0.1112 (7)	−0.0415 (5)	0.035 (2)
H5	0.462325	0.154880	−0.058066	0.042*
C6	0.3774 (8)	0.0158 (7)	−0.0756 (5)	0.041 (2)
H6	0.408684	−0.005650	−0.115585	0.049*
C7	0.3005 (9)	−0.0488 (7)	−0.0522 (5)	0.042 (2)
H7	0.280749	−0.114465	−0.075104	0.051*
C8	0.2522 (8)	−0.0173 (7)	0.0051 (5)	0.038 (2)
H8	0.195651	−0.061207	0.019299	0.046*
C9	0.2865 (7)	0.0774 (6)	0.0409 (5)	0.031 (2)
C10	0.2327 (7)	0.1093 (6)	0.1024 (4)	0.0265 (19)
C11	0.2749 (6)	0.2108 (5)	0.1371 (4)	0.0187 (17)
C12	0.4614 (6)	0.4492 (5)	0.1635 (4)	0.0195 (17)
C13	0.5738 (7)	0.4812 (6)	0.2202 (5)	0.0240 (18)
C14	0.6586 (7)	0.5631 (6)	0.2180 (5)	0.0261 (19)
H14	0.737018	0.586861	0.256443	0.031*
C15	0.6295 (8)	0.6088 (7)	0.1611 (5)	0.035 (2)
C16	0.5136 (8)	0.5764 (7)	0.1074 (5)	0.036 (2)
H16	0.492381	0.610501	0.070027	0.043*
C17	0.4276 (7)	0.4959 (6)	0.1063 (5)	0.0252 (19)
C18	0.6072 (8)	0.4346 (7)	0.2850 (5)	0.033 (2)
H18A	0.565213	0.449151	0.322726	0.050*
H18B	0.695597	0.458235	0.311178	0.050*
H18C	0.582474	0.366106	0.263260	0.050*
C19	0.7213 (9)	0.6977 (7)	0.1608 (6)	0.049 (3)
H19A	0.793207	0.715731	0.207294	0.073*
H19B	0.684197	0.748916	0.160887	0.073*
H19C	0.745766	0.686023	0.113944	0.073*
C20	0.3009 (8)	0.4599 (7)	0.0463 (5)	0.041 (2)
H20A	0.286808	0.395348	0.016494	0.062*
H20B	0.294424	0.500838	0.010754	0.062*
H20C	0.239696	0.460333	0.072914	0.062*
C21	0.1614 (7)	0.2238 (6)	0.2338 (5)	0.0237 (18)
C22	0.0406 (7)	0.2243 (6)	0.2048 (5)	0.0273 (19)
C23	−0.0389 (7)	0.1821 (7)	0.2419 (5)	0.036 (2)
H23	−0.122055	0.179927	0.223908	0.043*
C24	−0.0028 (8)	0.1439 (6)	0.3025 (5)	0.034 (2)
C25	0.1175 (8)	0.1453 (7)	0.3284 (5)	0.035 (2)

H25	0.142681	0.117850	0.369988	0.042*
C26	0.2022 (7)	0.1857 (6)	0.2955 (5)	0.0262 (19)
C27	0.0015 (8)	0.2629 (7)	0.1377 (5)	0.038 (2)
H27A	0.041315	0.331273	0.152590	0.058*
H27B	−0.087226	0.250050	0.121569	0.058*
H27C	0.024470	0.233136	0.094222	0.058*
C28	−0.0953 (9)	0.0942 (8)	0.3366 (6)	0.052 (3)
H28A	−0.067757	0.045342	0.357756	0.077*
H28B	−0.174563	0.065091	0.295730	0.077*
H28C	−0.103155	0.140213	0.378502	0.077*
C29	0.3313 (8)	0.1828 (7)	0.3217 (5)	0.041 (2)
H29A	0.345742	0.141535	0.279786	0.062*
H29B	0.344769	0.158214	0.367996	0.062*
H29C	0.387668	0.246605	0.334530	0.062*
C30	0.2800 (7)	0.5889 (6)	0.3388 (4)	0.0210 (17)
C31	0.3195 (6)	0.7345 (5)	0.4143 (4)	0.0188 (17)
C32	0.3805 (8)	0.8269 (6)	0.4731 (5)	0.0265 (19)
C33	0.2967 (7)	0.8868 (6)	0.4774 (5)	0.0270 (19)
C34	0.3460 (8)	0.9758 (6)	0.5277 (6)	0.038 (2)
H34	0.429280	0.997274	0.559362	0.045*
C35	0.2721 (9)	1.0339 (6)	0.5316 (6)	0.043 (3)
H35	0.306307	1.095641	0.565860	0.051*
C36	0.1537 (9)	1.0051 (7)	0.4882 (5)	0.039 (2)
H36	0.105448	1.046466	0.490740	0.046*
C37	0.1023 (8)	0.9135 (7)	0.4391 (5)	0.033 (2)
H37	0.018040	0.892177	0.409635	0.040*
C38	0.1722 (7)	0.8534 (6)	0.4330 (4)	0.0226 (18)
C39	0.1139 (7)	0.7577 (6)	0.3786 (4)	0.0219 (18)
C40	0.1980 (7)	0.7029 (6)	0.3732 (4)	0.0224 (18)
C41	0.4967 (6)	0.6691 (6)	0.4173 (4)	0.0203 (17)
C42	0.5662 (7)	0.6989 (6)	0.3732 (4)	0.0234 (18)
C43	0.6901 (7)	0.7041 (6)	0.3983 (5)	0.028 (2)
H43	0.740491	0.725578	0.368725	0.034*
C44	0.7395 (7)	0.6789 (6)	0.4642 (5)	0.032 (2)
C45	0.6652 (7)	0.6484 (6)	0.5072 (5)	0.031 (2)
H45	0.699732	0.631741	0.553432	0.038*
C46	0.5407 (7)	0.6413 (6)	0.4847 (5)	0.027 (2)
C47	0.5128 (8)	0.7258 (7)	0.2996 (5)	0.036 (2)
H47A	0.454534	0.669544	0.260164	0.055*
H47B	0.578415	0.753106	0.279873	0.055*
H47C	0.470891	0.772358	0.311011	0.055*
C48	0.8722 (8)	0.6812 (8)	0.4886 (6)	0.047 (3)
H48A	0.908672	0.706939	0.545229	0.070*
H48B	0.916522	0.721031	0.462386	0.070*
H48C	0.877158	0.616931	0.473954	0.070*
C49	0.4614 (8)	0.6079 (7)	0.5317 (5)	0.037 (2)
H49A	0.430839	0.658693	0.551602	0.056*
H49B	0.509134	0.590093	0.575524	0.056*

H49C	0.392328	0.553032	0.498584	0.056*
C50	0.0592 (6)	0.5502 (5)	0.2712 (5)	0.0209 (17)
C51	0.0266 (8)	0.5635 (7)	0.1971 (5)	0.033 (2)
C52	−0.0810 (9)	0.5005 (8)	0.1448 (6)	0.047 (3)
H52	−0.106613	0.507695	0.093344	0.056*
C53	−0.1530 (8)	0.4279 (7)	0.1635 (6)	0.043 (3)
C54	−0.1160 (7)	0.4200 (6)	0.2387 (6)	0.037 (2)
H54	−0.164543	0.370884	0.253210	0.044*
C55	−0.0095 (8)	0.4819 (7)	0.2939 (5)	0.033 (2)
C56	0.1050 (10)	0.6421 (7)	0.1750 (6)	0.057 (3)
H56A	0.104507	0.703186	0.203892	0.085*
H56B	0.072429	0.635259	0.118906	0.085*
H56C	0.188766	0.638926	0.188084	0.085*
C57	−0.2700 (9)	0.3621 (8)	0.1048 (7)	0.068 (4)
H57A	−0.308216	0.315226	0.128522	0.102*
H57B	−0.252795	0.329826	0.059645	0.102*
H57C	−0.325462	0.398149	0.087830	0.102*
C58	0.0306 (9)	0.4704 (8)	0.3759 (6)	0.051 (3)
H58A	0.107137	0.454421	0.385322	0.077*
H58B	−0.032453	0.419700	0.381938	0.077*
H58C	0.042989	0.529566	0.413583	0.077*
Au2	0.32100 (3)	0.77171 (3)	0.67602 (2)	0.03643 (13)
Cl1	0.4481 (3)	0.8454 (2)	0.79868 (15)	0.0602 (8)
Cl2	0.1922 (2)	0.6923 (2)	0.55543 (14)	0.0475 (6)
Cl3	0.0096 (3)	−0.1064 (2)	0.22955 (17)	0.0683 (8)
Cl4	−0.0574 (3)	−0.1727 (2)	0.06283 (16)	0.0634 (8)
C59	−0.0624 (9)	−0.0909 (7)	0.1407 (6)	0.048 (3)
H59A	−0.022872	−0.026446	0.138168	0.058*
H59B	−0.148568	−0.096647	0.136127	0.058*
Cl5	0.3382 (3)	−0.0834 (3)	0.3000 (2)	0.0777 (10)
Cl6	0.3542 (4)	−0.1655 (3)	0.1487 (2)	0.1018 (13)
C60	0.3338 (13)	−0.0711 (10)	0.2067 (8)	0.084 (4)
H60A	0.254123	−0.063579	0.180585	0.101*
H60B	0.398200	−0.012867	0.211722	0.101*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01953 (18)	0.01883 (18)	0.02378 (19)	0.00784 (14)	0.00909 (14)	0.00830 (14)
O1	0.027 (3)	0.036 (4)	0.026 (3)	0.003 (3)	0.012 (3)	0.010 (3)
O2	0.061 (4)	0.013 (3)	0.040 (4)	−0.004 (3)	0.029 (3)	0.000 (3)
O3	0.023 (3)	0.030 (4)	0.049 (4)	0.011 (3)	0.005 (3)	0.008 (3)
O4	0.030 (4)	0.035 (4)	0.046 (4)	0.016 (3)	0.011 (3)	0.008 (3)
N1	0.021 (3)	0.015 (4)	0.022 (3)	0.005 (3)	0.011 (3)	0.009 (3)
N2	0.019 (3)	0.024 (4)	0.023 (4)	0.003 (3)	0.009 (3)	0.012 (3)
N3	0.018 (3)	0.023 (4)	0.023 (4)	0.012 (3)	0.007 (3)	0.015 (3)
N4	0.016 (3)	0.022 (4)	0.025 (4)	0.006 (3)	0.009 (3)	0.011 (3)
C1	0.024 (4)	0.024 (5)	0.031 (5)	0.011 (4)	0.008 (4)	0.006 (4)

C2	0.020 (4)	0.021 (5)	0.019 (4)	0.003 (4)	0.002 (3)	0.004 (4)
C3	0.016 (4)	0.029 (5)	0.015 (4)	0.003 (4)	0.002 (3)	0.005 (4)
C4	0.023 (4)	0.035 (5)	0.025 (5)	0.011 (4)	0.005 (4)	0.010 (4)
C5	0.030 (5)	0.045 (6)	0.028 (5)	0.011 (4)	0.015 (4)	0.000 (4)
C6	0.046 (6)	0.039 (6)	0.032 (5)	0.011 (5)	0.016 (5)	−0.005 (5)
C7	0.055 (6)	0.034 (6)	0.030 (5)	0.016 (5)	0.009 (5)	−0.008 (4)
C8	0.040 (5)	0.046 (6)	0.030 (5)	0.013 (5)	0.013 (4)	0.008 (5)
C9	0.035 (5)	0.021 (5)	0.032 (5)	0.002 (4)	0.016 (4)	−0.003 (4)
C10	0.026 (4)	0.033 (5)	0.023 (4)	0.010 (4)	0.008 (4)	0.012 (4)
C11	0.020 (4)	0.017 (4)	0.023 (4)	0.005 (3)	0.013 (3)	0.007 (3)
C12	0.019 (4)	0.013 (4)	0.029 (4)	0.003 (3)	0.013 (4)	0.008 (4)
C13	0.031 (5)	0.019 (4)	0.027 (5)	0.008 (4)	0.014 (4)	0.010 (4)
C14	0.026 (4)	0.022 (5)	0.023 (4)	0.000 (4)	0.009 (4)	−0.004 (4)
C15	0.038 (5)	0.034 (6)	0.032 (5)	−0.001 (4)	0.019 (5)	0.012 (4)
C16	0.043 (6)	0.032 (6)	0.030 (5)	0.002 (5)	0.011 (4)	0.017 (4)
C17	0.029 (5)	0.022 (5)	0.025 (4)	0.005 (4)	0.007 (4)	0.012 (4)
C18	0.034 (5)	0.037 (6)	0.029 (5)	0.013 (4)	0.004 (4)	0.014 (4)
C19	0.051 (6)	0.040 (6)	0.050 (6)	−0.006 (5)	0.020 (5)	0.020 (5)
C20	0.049 (6)	0.040 (6)	0.040 (6)	0.015 (5)	0.009 (5)	0.030 (5)
C21	0.026 (4)	0.022 (5)	0.028 (5)	0.004 (4)	0.019 (4)	0.005 (4)
C22	0.032 (5)	0.028 (5)	0.030 (5)	0.016 (4)	0.014 (4)	0.013 (4)
C23	0.020 (4)	0.042 (6)	0.046 (6)	0.008 (4)	0.016 (4)	0.010 (5)
C24	0.047 (6)	0.029 (5)	0.047 (6)	0.016 (4)	0.036 (5)	0.021 (5)
C25	0.047 (6)	0.042 (6)	0.029 (5)	0.020 (5)	0.023 (4)	0.019 (4)
C26	0.027 (4)	0.024 (5)	0.032 (5)	0.009 (4)	0.012 (4)	0.012 (4)
C27	0.032 (5)	0.050 (6)	0.045 (6)	0.019 (5)	0.018 (5)	0.023 (5)
C28	0.059 (7)	0.052 (7)	0.068 (7)	0.017 (6)	0.046 (6)	0.037 (6)
C29	0.034 (5)	0.062 (7)	0.026 (5)	0.015 (5)	0.007 (4)	0.010 (5)
C30	0.020 (4)	0.022 (5)	0.019 (4)	0.005 (4)	0.004 (4)	0.007 (4)
C31	0.021 (4)	0.018 (4)	0.025 (4)	0.012 (4)	0.011 (4)	0.007 (3)
C32	0.028 (5)	0.019 (5)	0.034 (5)	0.005 (4)	0.015 (4)	0.007 (4)
C33	0.028 (5)	0.030 (5)	0.035 (5)	0.010 (4)	0.019 (4)	0.024 (4)
C34	0.037 (5)	0.021 (5)	0.060 (6)	0.007 (4)	0.025 (5)	0.011 (5)
C35	0.051 (6)	0.016 (5)	0.065 (7)	0.011 (5)	0.031 (6)	0.003 (5)
C36	0.049 (6)	0.034 (6)	0.053 (6)	0.027 (5)	0.033 (5)	0.018 (5)
C37	0.032 (5)	0.041 (6)	0.045 (6)	0.022 (5)	0.022 (4)	0.026 (5)
C38	0.032 (5)	0.027 (5)	0.022 (4)	0.019 (4)	0.016 (4)	0.016 (4)
C39	0.024 (5)	0.021 (5)	0.024 (4)	0.010 (4)	0.010 (4)	0.008 (4)
C40	0.027 (4)	0.025 (5)	0.019 (4)	0.009 (4)	0.010 (4)	0.009 (4)
C41	0.018 (4)	0.023 (5)	0.023 (4)	0.013 (4)	0.006 (3)	0.007 (4)
C42	0.018 (4)	0.032 (5)	0.026 (4)	0.015 (4)	0.007 (4)	0.012 (4)
C43	0.028 (5)	0.029 (5)	0.028 (5)	0.008 (4)	0.013 (4)	0.006 (4)
C44	0.025 (5)	0.033 (5)	0.038 (5)	0.015 (4)	0.011 (4)	0.005 (4)
C45	0.032 (5)	0.045 (6)	0.027 (5)	0.025 (5)	0.006 (4)	0.023 (4)
C46	0.022 (4)	0.037 (5)	0.029 (5)	0.014 (4)	0.011 (4)	0.012 (4)
C47	0.036 (5)	0.043 (6)	0.043 (6)	0.017 (5)	0.018 (5)	0.027 (5)
C48	0.027 (5)	0.071 (8)	0.051 (6)	0.025 (5)	0.013 (5)	0.022 (6)
C49	0.041 (5)	0.048 (6)	0.040 (5)	0.024 (5)	0.017 (5)	0.032 (5)

C50	0.014 (4)	0.018 (4)	0.030 (5)	0.006 (3)	0.006 (4)	0.007 (4)
C51	0.031 (5)	0.040 (6)	0.030 (5)	0.016 (5)	0.005 (4)	0.013 (4)
C52	0.042 (6)	0.054 (7)	0.033 (6)	0.022 (6)	−0.009 (5)	0.006 (5)
C53	0.018 (5)	0.039 (6)	0.060 (7)	0.010 (4)	−0.001 (5)	−0.002 (5)
C54	0.019 (5)	0.027 (5)	0.058 (7)	0.001 (4)	0.013 (5)	0.003 (5)
C55	0.031 (5)	0.038 (6)	0.040 (5)	0.018 (4)	0.020 (4)	0.015 (5)
C56	0.081 (8)	0.043 (7)	0.049 (7)	0.012 (6)	0.019 (6)	0.032 (6)
C57	0.030 (6)	0.055 (8)	0.083 (9)	0.004 (6)	−0.013 (6)	−0.011 (7)
C58	0.045 (6)	0.054 (7)	0.059 (7)	0.002 (5)	0.025 (5)	0.032 (6)
Au2	0.0391 (2)	0.0412 (3)	0.0397 (2)	0.02189 (19)	0.01651 (18)	0.01764 (19)
Cl1	0.0633 (17)	0.070 (2)	0.0447 (16)	0.0420 (16)	0.0053 (13)	−0.0017 (14)
Cl2	0.0388 (13)	0.0661 (19)	0.0400 (14)	0.0124 (13)	0.0151 (11)	0.0210 (13)
Cl3	0.081 (2)	0.061 (2)	0.0505 (17)	0.0179 (17)	0.0020 (16)	0.0172 (15)
Cl4	0.0630 (18)	0.077 (2)	0.0490 (16)	0.0199 (16)	0.0185 (14)	0.0144 (15)
C59	0.042 (6)	0.050 (7)	0.054 (6)	0.007 (5)	0.016 (5)	0.028 (6)
Cl5	0.081 (2)	0.088 (3)	0.078 (2)	0.037 (2)	0.0255 (19)	0.039 (2)
Cl6	0.142 (3)	0.107 (3)	0.111 (3)	0.063 (3)	0.082 (3)	0.065 (3)
C60	0.108 (11)	0.089 (11)	0.091 (10)	0.041 (9)	0.054 (9)	0.062 (9)

Geometric parameters (Å, °)

Au1—C30	2.004 (8)	C28—H28C	0.9800
Au1—C1	2.013 (8)	C29—H29A	0.9800
O1—C3	1.210 (9)	C29—H29B	0.9800
O2—C10	1.212 (9)	C29—H29C	0.9800
O3—C32	1.181 (9)	C31—C40	1.363 (10)
O4—C39	1.218 (9)	C31—C32	1.484 (11)
N1—C1	1.372 (9)	C32—C33	1.509 (11)
N1—C2	1.396 (10)	C33—C34	1.376 (12)
N1—C12	1.450 (9)	C33—C38	1.408 (11)
N2—C1	1.341 (10)	C34—C35	1.392 (12)
N2—C11	1.373 (9)	C34—H34	0.9500
N2—C21	1.461 (9)	C35—C36	1.345 (13)
N3—C30	1.353 (10)	C35—H35	0.9500
N3—C31	1.375 (9)	C36—C37	1.398 (12)
N3—C41	1.467 (9)	C36—H36	0.9500
N4—C30	1.364 (9)	C37—C38	1.383 (10)
N4—C40	1.384 (10)	C37—H37	0.9500
N4—C50	1.462 (9)	C38—C39	1.484 (11)
C2—C11	1.364 (10)	C39—C40	1.459 (10)
C2—C3	1.454 (10)	C41—C42	1.360 (10)
C3—C4	1.457 (11)	C41—C46	1.395 (11)
C4—C5	1.388 (10)	C42—C43	1.405 (10)
C4—C9	1.410 (11)	C42—C47	1.511 (11)
C5—C6	1.379 (12)	C43—C44	1.366 (12)
C5—H5	0.9500	C43—H43	0.9500
C6—C7	1.380 (13)	C44—C45	1.388 (11)
C6—H6	0.9500	C44—C48	1.518 (11)

C7—C8	1.392 (11)	C45—C46	1.405 (10)
C7—H7	0.9500	C45—H45	0.9500
C8—C9	1.374 (12)	C46—C49	1.501 (11)
C8—H8	0.9500	C47—H47A	0.9800
C9—C10	1.502 (10)	C47—H47B	0.9800
C10—C11	1.455 (11)	C47—H47C	0.9800
C12—C13	1.375 (11)	C48—H48A	0.9800
C12—C17	1.398 (11)	C48—H48B	0.9800
C13—C14	1.411 (11)	C48—H48C	0.9800
C13—C18	1.507 (11)	C49—H49A	0.9800
C14—C15	1.372 (12)	C49—H49B	0.9800
C14—H14	0.9500	C49—H49C	0.9800
C15—C16	1.382 (12)	C50—C55	1.356 (11)
C15—C19	1.517 (12)	C50—C51	1.383 (11)
C16—C17	1.383 (11)	C51—C52	1.382 (12)
C16—H16	0.9500	C51—C56	1.512 (13)
C17—C20	1.520 (11)	C52—C53	1.378 (14)
C18—H18A	0.9800	C52—H52	0.9500
C18—H18B	0.9800	C53—C54	1.375 (14)
C18—H18C	0.9800	C53—C57	1.501 (13)
C19—H19A	0.9800	C54—C55	1.389 (12)
C19—H19B	0.9800	C54—H54	0.9500
C19—H19C	0.9800	C55—C58	1.515 (13)
C20—H20A	0.9800	C56—H56A	0.9800
C20—H20B	0.9800	C56—H56B	0.9800
C20—H20C	0.9800	C56—H56C	0.9800
C21—C26	1.394 (11)	C57—H57A	0.9800
C21—C22	1.402 (11)	C57—H57B	0.9800
C22—C23	1.407 (11)	C57—H57C	0.9800
C22—C27	1.475 (12)	C58—H58A	0.9800
C23—C24	1.364 (12)	C58—H58B	0.9800
C23—H23	0.9500	C58—H58C	0.9800
C24—C25	1.382 (12)	Au2—Cl2	2.254 (3)
C24—C28	1.520 (11)	Au2—Cl1	2.261 (3)
C25—C26	1.385 (11)	Cl3—C59	1.723 (10)
C25—H25	0.9500	Cl4—C59	1.739 (10)
C26—C29	1.502 (11)	C59—H59A	0.9900
C27—H27A	0.9800	C59—H59B	0.9900
C27—H27B	0.9800	Cl5—C60	1.748 (12)
C27—H27C	0.9800	Cl6—C60	1.729 (14)
C28—H28A	0.9800	C60—H60A	0.9900
C28—H28B	0.9800	C60—H60B	0.9900
C30—Au1—C1	173.9 (3)	N3—C30—N4	105.4 (6)
C1—N1—C2	109.4 (6)	N3—C30—Au1	129.3 (5)
C1—N1—C12	123.9 (6)	N4—C30—Au1	125.2 (6)
C2—N1—C12	126.5 (6)	C40—C31—N3	106.8 (7)
C1—N2—C11	111.1 (6)	C40—C31—C32	123.9 (7)

C1—N2—C21	124.4 (6)	N3—C31—C32	129.2 (7)
C11—N2—C21	124.5 (6)	O3—C32—C31	122.8 (7)
C30—N3—C31	110.9 (6)	O3—C32—C33	124.2 (8)
C30—N3—C41	122.8 (6)	C31—C32—C33	113.0 (7)
C31—N3—C41	126.1 (6)	C34—C33—C38	120.6 (8)
C30—N4—C40	110.1 (6)	C34—C33—C32	117.5 (8)
C30—N4—C50	121.9 (6)	C38—C33—C32	121.9 (8)
C40—N4—C50	128.0 (6)	C33—C34—C35	119.0 (9)
N2—C1—N1	105.9 (6)	C33—C34—H34	120.5
N2—C1—Au1	131.4 (6)	C35—C34—H34	120.5
N1—C1—Au1	122.0 (6)	C36—C35—C34	121.8 (9)
C11—C2—N1	106.5 (6)	C36—C35—H35	119.1
C11—C2—C3	124.1 (7)	C34—C35—H35	119.1
N1—C2—C3	129.3 (7)	C35—C36—C37	119.3 (8)
O1—C3—C2	123.0 (8)	C35—C36—H36	120.4
O1—C3—C4	122.8 (7)	C37—C36—H36	120.4
C2—C3—C4	114.2 (7)	C38—C37—C36	121.0 (8)
C5—C4—C9	118.6 (8)	C38—C37—H37	119.5
C5—C4—C3	118.2 (8)	C36—C37—H37	119.5
C9—C4—C3	123.3 (7)	C37—C38—C33	118.2 (8)
C6—C5—C4	120.4 (9)	C37—C38—C39	118.9 (7)
C6—C5—H5	119.8	C33—C38—C39	122.9 (7)
C4—C5—H5	119.8	O4—C39—C40	122.9 (7)
C5—C6—C7	120.7 (8)	O4—C39—C38	123.1 (7)
C5—C6—H6	119.6	C40—C39—C38	114.0 (7)
C7—C6—H6	119.6	C31—C40—N4	106.8 (6)
C6—C7—C8	119.7 (9)	C31—C40—C39	124.2 (7)
C6—C7—H7	120.1	N4—C40—C39	129.0 (7)
C8—C7—H7	120.1	C42—C41—C46	123.7 (7)
C9—C8—C7	119.8 (9)	C42—C41—N3	119.1 (7)
C9—C8—H8	120.1	C46—C41—N3	117.1 (6)
C7—C8—H8	120.1	C41—C42—C43	118.0 (7)
C8—C9—C4	120.7 (7)	C41—C42—C47	121.4 (7)
C8—C9—C10	118.6 (8)	C43—C42—C47	120.6 (7)
C4—C9—C10	120.5 (7)	C44—C43—C42	121.3 (7)
O2—C10—C11	122.9 (7)	C44—C43—H43	119.3
O2—C10—C9	122.4 (8)	C42—C43—H43	119.3
C11—C10—C9	114.6 (7)	C43—C44—C45	118.8 (7)
C2—C11—N2	107.1 (7)	C43—C44—C48	120.7 (8)
C2—C11—C10	123.0 (7)	C45—C44—C48	120.5 (8)
N2—C11—C10	129.9 (6)	C44—C45—C46	122.3 (8)
C13—C12—C17	122.7 (7)	C44—C45—H45	118.9
C13—C12—N1	118.4 (7)	C46—C45—H45	118.9
C17—C12—N1	118.8 (7)	C41—C46—C45	115.8 (7)
C12—C13—C14	117.7 (7)	C41—C46—C49	122.5 (7)
C12—C13—C18	122.7 (7)	C45—C46—C49	121.7 (7)
C14—C13—C18	119.6 (7)	C42—C47—H47A	109.5
C15—C14—C13	120.9 (8)	C42—C47—H47B	109.5

C15—C14—H14	119.5	H47A—C47—H47B	109.5
C13—C14—H14	119.5	C42—C47—H47C	109.5
C14—C15—C16	119.3 (8)	H47A—C47—H47C	109.5
C14—C15—C19	120.1 (8)	H47B—C47—H47C	109.5
C16—C15—C19	120.5 (8)	C44—C48—H48A	109.5
C15—C16—C17	121.9 (8)	C44—C48—H48B	109.5
C15—C16—H16	119.0	H48A—C48—H48B	109.5
C17—C16—H16	119.0	C44—C48—H48C	109.5
C16—C17—C12	117.3 (7)	H48A—C48—H48C	109.5
C16—C17—C20	121.7 (7)	H48B—C48—H48C	109.5
C12—C17—C20	121.1 (7)	C46—C49—H49A	109.5
C13—C18—H18A	109.5	C46—C49—H49B	109.5
C13—C18—H18B	109.5	H49A—C49—H49B	109.5
H18A—C18—H18B	109.5	C46—C49—H49C	109.5
C13—C18—H18C	109.5	H49A—C49—H49C	109.5
H18A—C18—H18C	109.5	H49B—C49—H49C	109.5
H18B—C18—H18C	109.5	C55—C50—C51	123.6 (8)
C15—C19—H19A	109.5	C55—C50—N4	119.1 (7)
C15—C19—H19B	109.5	C51—C50—N4	117.3 (7)
H19A—C19—H19B	109.5	C52—C51—C50	115.9 (9)
C15—C19—H19C	109.5	C52—C51—C56	122.4 (9)
H19A—C19—H19C	109.5	C50—C51—C56	121.6 (8)
H19B—C19—H19C	109.5	C53—C52—C51	123.3 (9)
C17—C20—H20A	109.5	C53—C52—H52	118.4
C17—C20—H20B	109.5	C51—C52—H52	118.4
H20A—C20—H20B	109.5	C54—C53—C52	117.5 (8)
C17—C20—H20C	109.5	C54—C53—C57	121.2 (10)
H20A—C20—H20C	109.5	C52—C53—C57	121.2 (10)
H20B—C20—H20C	109.5	C53—C54—C55	121.6 (9)
C26—C21—C22	123.4 (7)	C53—C54—H54	119.2
C26—C21—N2	119.1 (7)	C55—C54—H54	119.2
C22—C21—N2	117.5 (7)	C50—C55—C54	117.9 (8)
C21—C22—C23	115.1 (8)	C50—C55—C58	121.5 (8)
C21—C22—C27	121.0 (7)	C54—C55—C58	120.6 (9)
C23—C22—C27	123.8 (7)	C51—C56—H56A	109.5
C24—C23—C22	123.4 (8)	C51—C56—H56B	109.5
C24—C23—H23	118.3	H56A—C56—H56B	109.5
C22—C23—H23	118.3	C51—C56—H56C	109.5
C23—C24—C25	118.8 (7)	H56A—C56—H56C	109.5
C23—C24—C28	120.5 (8)	H56B—C56—H56C	109.5
C25—C24—C28	120.5 (8)	C53—C57—H57A	109.5
C24—C25—C26	121.7 (8)	C53—C57—H57B	109.5
C24—C25—H25	119.2	H57A—C57—H57B	109.5
C26—C25—H25	119.2	C53—C57—H57C	109.5
C25—C26—C21	117.5 (7)	H57A—C57—H57C	109.5
C25—C26—C29	121.2 (8)	H57B—C57—H57C	109.5
C21—C26—C29	121.2 (7)	C55—C58—H58A	109.5
C22—C27—H27A	109.5	C55—C58—H58B	109.5

C22—C27—H27B	109.5	H58A—C58—H58B	109.5
H27A—C27—H27B	109.5	C55—C58—H58C	109.5
C22—C27—H27C	109.5	H58A—C58—H58C	109.5
H27A—C27—H27C	109.5	H58B—C58—H58C	109.5
H27B—C27—H27C	109.5	Cl2—Au2—Cl1	177.45 (11)
C24—C28—H28A	109.5	Cl3—C59—Cl4	112.3 (6)
C24—C28—H28B	109.5	Cl3—C59—H59A	109.1
H28A—C28—H28B	109.5	Cl4—C59—H59A	109.1
C24—C28—H28C	109.5	Cl3—C59—H59B	109.1
H28A—C28—H28C	109.5	Cl4—C59—H59B	109.1
H28B—C28—H28C	109.5	H59A—C59—H59B	107.9
C26—C29—H29A	109.5	Cl6—C60—Cl5	113.6 (7)
C26—C29—H29B	109.5	Cl6—C60—H60A	108.8
H29A—C29—H29B	109.5	Cl5—C60—H60A	108.8
C26—C29—H29C	109.5	Cl6—C60—H60B	108.8
H29A—C29—H29C	109.5	Cl5—C60—H60B	108.8
H29B—C29—H29C	109.5	H60A—C60—H60B	107.7
C11—N2—C1—N1	1.7 (9)	C31—N3—C30—N4	−0.6 (8)
C21—N2—C1—N1	−178.7 (6)	C41—N3—C30—N4	−174.8 (6)
C11—N2—C1—Au1	171.8 (6)	C31—N3—C30—Au1	175.4 (6)
C21—N2—C1—Au1	−8.6 (12)	C41—N3—C30—Au1	1.2 (10)
C2—N1—C1—N2	−0.8 (8)	C40—N4—C30—N3	0.3 (8)
C12—N1—C1—N2	−176.5 (6)	C50—N4—C30—N3	179.3 (6)
C2—N1—C1—Au1	−172.0 (5)	C40—N4—C30—Au1	−175.9 (5)
C12—N1—C1—Au1	12.3 (10)	C50—N4—C30—Au1	3.1 (10)
C1—N1—C2—C11	−0.4 (9)	C30—N3—C31—C40	0.7 (8)
C12—N1—C2—C11	175.1 (7)	C41—N3—C31—C40	174.6 (6)
C1—N1—C2—C3	176.3 (7)	C30—N3—C31—C32	177.7 (7)
C12—N1—C2—C3	−8.2 (13)	C41—N3—C31—C32	−8.4 (12)
C11—C2—C3—O1	171.0 (8)	C40—C31—C32—O3	176.4 (8)
N1—C2—C3—O1	−5.1 (13)	N3—C31—C32—O3	−0.1 (13)
C11—C2—C3—C4	−6.8 (11)	C40—C31—C32—C33	−5.5 (11)
N1—C2—C3—C4	177.0 (7)	N3—C31—C32—C33	177.9 (7)
O1—C3—C4—C5	6.1 (12)	O3—C32—C33—C34	0.9 (12)
C2—C3—C4—C5	−176.1 (7)	C31—C32—C33—C34	−177.1 (7)
O1—C3—C4—C9	−174.5 (8)	O3—C32—C33—C38	−178.1 (8)
C2—C3—C4—C9	3.3 (11)	C31—C32—C33—C38	3.9 (10)
C9—C4—C5—C6	0.9 (13)	C38—C33—C34—C35	−2.8 (13)
C3—C4—C5—C6	−179.7 (8)	C32—C33—C34—C35	178.3 (8)
C4—C5—C6—C7	−0.2 (14)	C33—C34—C35—C36	0.7 (14)
C5—C6—C7—C8	1.6 (15)	C34—C35—C36—C37	1.6 (14)
C6—C7—C8—C9	−3.6 (14)	C35—C36—C37—C38	−2.0 (13)
C7—C8—C9—C4	4.3 (14)	C36—C37—C38—C33	0.0 (12)
C7—C8—C9—C10	179.9 (8)	C36—C37—C38—C39	−178.5 (7)
C5—C4—C9—C8	−2.9 (13)	C34—C33—C38—C37	2.4 (11)
C3—C4—C9—C8	177.7 (8)	C32—C33—C38—C37	−178.7 (7)
C5—C4—C9—C10	−178.4 (7)	C34—C33—C38—C39	−179.2 (8)

C3—C4—C9—C10	2.2 (13)	C32—C33—C38—C39	−0.3 (11)
C8—C9—C10—O2	3.0 (13)	C37—C38—C39—O4	−4.9 (12)
C4—C9—C10—O2	178.6 (8)	C33—C38—C39—O4	176.7 (7)
C8—C9—C10—C11	179.8 (8)	C37—C38—C39—C40	176.2 (7)
C4—C9—C10—C11	−4.6 (11)	C33—C38—C39—C40	−2.2 (11)
N1—C2—C11—N2	1.4 (8)	N3—C31—C40—N4	−0.5 (8)
C3—C2—C11—N2	−175.5 (7)	C32—C31—C40—N4	−177.6 (7)
N1—C2—C11—C10	−178.5 (7)	N3—C31—C40—C39	−179.4 (7)
C3—C2—C11—C10	4.6 (12)	C32—C31—C40—C39	3.4 (12)
C1—N2—C11—C2	−2.0 (9)	C30—N4—C40—C31	0.1 (8)
C21—N2—C11—C2	178.4 (7)	C50—N4—C40—C31	−178.8 (7)
C1—N2—C11—C10	177.9 (8)	C30—N4—C40—C39	179.0 (7)
C21—N2—C11—C10	−1.6 (13)	C50—N4—C40—C39	0.1 (13)
O2—C10—C11—C2	178.2 (8)	O4—C39—C40—C31	−178.2 (8)
C9—C10—C11—C2	1.3 (11)	C38—C39—C40—C31	0.7 (11)
O2—C10—C11—N2	−1.8 (14)	O4—C39—C40—N4	3.1 (13)
C9—C10—C11—N2	−178.6 (7)	C38—C39—C40—N4	−178.0 (7)
C1—N1—C12—C13	77.4 (9)	C30—N3—C41—C42	82.9 (10)
C2—N1—C12—C13	−97.6 (9)	C31—N3—C41—C42	−90.4 (9)
C1—N1—C12—C17	−104.3 (9)	C30—N3—C41—C46	−95.9 (9)
C2—N1—C12—C17	80.8 (9)	C31—N3—C41—C46	90.8 (9)
C17—C12—C13—C14	−2.0 (11)	C46—C41—C42—C43	−1.7 (13)
N1—C12—C13—C14	176.2 (6)	N3—C41—C42—C43	179.6 (7)
C17—C12—C13—C18	175.8 (7)	C46—C41—C42—C47	178.4 (8)
N1—C12—C13—C18	−6.0 (11)	N3—C41—C42—C47	−0.3 (12)
C12—C13—C14—C15	−0.1 (11)	C41—C42—C43—C44	0.9 (13)
C18—C13—C14—C15	−178.0 (8)	C47—C42—C43—C44	−179.2 (8)
C13—C14—C15—C16	2.9 (12)	C42—C43—C44—C45	−0.5 (13)
C13—C14—C15—C19	178.8 (8)	C42—C43—C44—C48	177.5 (8)
C14—C15—C16—C17	−3.7 (13)	C43—C44—C45—C46	0.9 (14)
C19—C15—C16—C17	−179.7 (8)	C48—C44—C45—C46	−177.1 (8)
C15—C16—C17—C12	1.7 (13)	C42—C41—C46—C45	2.0 (13)
C15—C16—C17—C20	−179.1 (8)	N3—C41—C46—C45	−179.3 (7)
C13—C12—C17—C16	1.2 (12)	C42—C41—C46—C49	−179.4 (8)
N1—C12—C17—C16	−177.0 (7)	N3—C41—C46—C49	−0.7 (12)
C13—C12—C17—C20	−178.0 (7)	C44—C45—C46—C41	−1.6 (13)
N1—C12—C17—C20	3.8 (11)	C44—C45—C46—C49	179.8 (9)
C1—N2—C21—C26	−96.3 (10)	C30—N4—C50—C55	84.0 (9)
C11—N2—C21—C26	83.2 (10)	C40—N4—C50—C55	−97.2 (9)
C1—N2—C21—C22	85.4 (10)	C30—N4—C50—C51	−95.1 (9)
C11—N2—C21—C22	−95.0 (9)	C40—N4—C50—C51	83.6 (9)
C26—C21—C22—C23	−0.8 (12)	C55—C50—C51—C52	−1.6 (12)
N2—C21—C22—C23	177.4 (7)	N4—C50—C51—C52	177.6 (7)
C26—C21—C22—C27	−178.0 (8)	C55—C50—C51—C56	178.6 (8)
N2—C21—C22—C27	0.2 (12)	N4—C50—C51—C56	−2.2 (12)
C21—C22—C23—C24	0.8 (13)	C50—C51—C52—C53	−0.4 (14)
C27—C22—C23—C24	177.9 (9)	C56—C51—C52—C53	179.4 (9)
C22—C23—C24—C25	−1.0 (14)	C51—C52—C53—C54	1.5 (14)

C22—C23—C24—C28	−176.4 (9)	C51—C52—C53—C57	179.3 (9)
C23—C24—C25—C26	1.1 (14)	C52—C53—C54—C55	−0.7 (13)
C28—C24—C25—C26	176.5 (8)	C57—C53—C54—C55	−178.4 (8)
C24—C25—C26—C21	−1.1 (13)	C51—C50—C55—C54	2.4 (12)
C24—C25—C26—C29	−177.2 (8)	N4—C50—C55—C54	−176.8 (7)
C22—C21—C26—C25	1.0 (12)	C51—C50—C55—C58	179.9 (8)
N2—C21—C26—C25	−177.2 (7)	N4—C50—C55—C58	0.8 (12)
C22—C21—C26—C29	177.0 (8)	C53—C54—C55—C50	−1.2 (13)
N2—C21—C26—C29	−1.1 (12)	C53—C54—C55—C58	−178.8 (8)

Selected bond lengths (Å) and angles (°) for compounds 2 and 4

Please define Imi-1 and Imi-2. Do square brackets indicate averages?

Compound	[(NQMes) ₂ Au]Cl, 2	[(NQMes) ₂ Au][AuCl ₂], 4
Au—C(carbene)	2.017[5]	2.004[8]
C(carbene)—N1/C(carbene)—N2	1.356 (6)/1.364 (6)	1.369 (9)/1.347 (11)
N1—C11/N2—C2	1.385 (6)/1.388 (6)	1.400 (10)/1.374 (9)
C2—C11	1.384 (7)	1.366 (11)
C2—C3	1.468 (7)	1.454 (10)
C3—O2	1.214 (7)	1.212 (9)
Cl1—Au2		2.263 (3)
Au2—Cl2		2.255 (3)
C(carbene)—Au—C(carbene)	173.7[2]	173.8[3]
N1—C(carbene)—N2	106.4 (4)	105.8 (7)
C1—N2—C2	109.4 (4)	109.5 (6)
C1—N1—C11	109.3 (4)	111.2 (6)
Imi-1(plane)—Au—Imi-2(plane)	69.7	62.27