

Crystal structure of (N[^]C) cyclometalated Au^{III} diazide at 100 K

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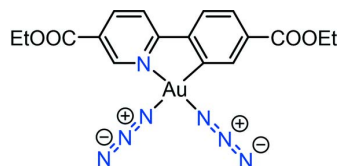
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The title compound, an (N[^]C)-cyclometalated gold(III) diazide, namely, diazido[5-ethoxycarbonyl-2-(5-ethoxycarbonylpyridin-2-yl)phenyl- κ^2 C¹,N]-gold(III), [Au(C₁₇H₁₆NO₄)(N₃)₂] or Au(ppy^{Et})(N₃)₂, was synthesized by reacting Au(ppy^{Et})Cl₂ with NaN₃ in water for 24 h. The complex has been structurally characterized and features a gold center with a square-planar environment. The Au–N(azide) bond lengths are significantly different depending on the influence of the atom *trans* to the azide group [Au–N(*trans* to C) of 2.067 (2) Å versus Au–N(*trans* to N) of 2.042 (2) Å]. The azide groups are twisted in-and-out of plane by 56.2 (2)°.

1. Chemical context

Among gold azide complexes, Au^I have dominated over Au^{III} azides (Del Castillo *et al.*, 2011; Powers *et al.*, 2015; Partyka *et al.*, 2007). Until now, only three examples of Au^{III} azide complexes have been reported (Fig. 1). The reported compounds feature the N-heterocyclic carbene complex and pyridine coordinated Au–triazide groups (Schuh *et al.*, 2016; Peng *et al.*, 2019) as well as cationic cyclometalated monoazide (Roth *et al.*, 2016). To the best of our knowledge, a cyclometalated phenyl pyridine Au^{III} azide complex has not been reported before.



2. Structural commentary

The molecular structure of Au(ppy^{Et})(N₃)₂ (**2**) is shown in Fig. 2. The complex forms monoclinic crystals belonging to the space group *P*2₁/*c* and crystallizes with one molecule in the asymmetric unit. The solid-state structure of **2** displays a

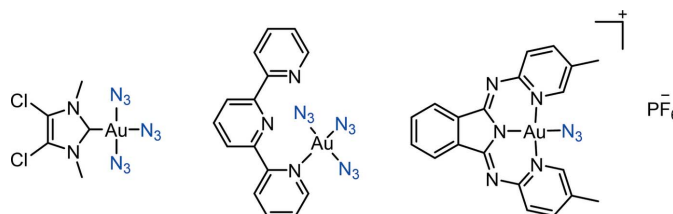
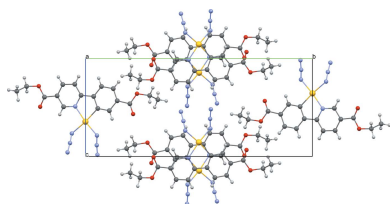


Figure 1
Au^{III}-azide complexes reported in the literature

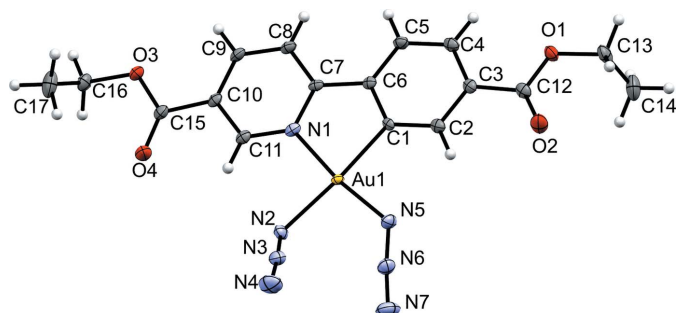


Figure 2
Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

square-planar coordination geometry, as expected for the d^8 electron configuration of the Au^{III} center. The Au–N bond length *trans* to the pyridine N atom [2.042 (2) Å] is shorter than the one *trans* to the C atom [2.067 (2) Å], indicating the stronger *trans* influence of the phenyl carbon atom. N–N bond distances in the azide ligands are in line with reported literature values (Dori *et al.*, 1973) with shorter terminal N–N bond lengths compared to the internal ones (1.150 vs 1.200 Å, on average). The N–N–N angles [174.7 (3) and 173.8 (3)°] deviate only slightly from the expected linear arrangement and the Au–N–N angles of 118.7 (2)° and 119.2 (2)° for the azide groups *trans* to N and C, respectively, indicate the expected bent coordination of these ligands. The azide groups are twisted by 56.2 (2)° with respect to each other, and point in-and-out of the plane with distances of 1.092 (2) Å for the terminal N atom *trans* to C and 0.975 (2) Å for the terminal N atom *trans* to the pyridine N atom (Fig. 3). The pyridine and benzene rings are essentially coplanar, the angle formed by their mean planes being 3.64 (10)°.

3. Supramolecular features

The title crystal structure features infinite stacking chains along the [100] direction. The neighboring molecules within the stack are related by inversion. The mean plane of the core of the complex molecule including the Au atom, both aromatic rings and two N atoms of azide groups attached to the Au

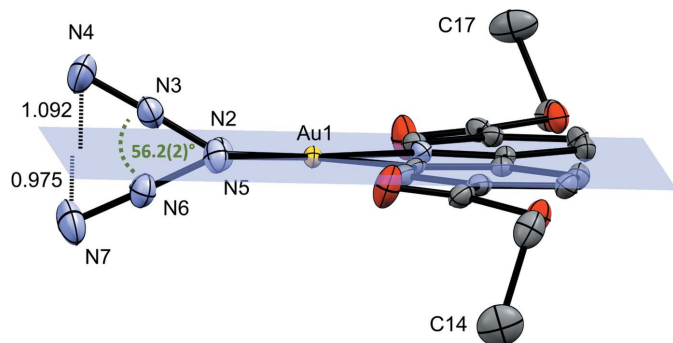


Figure 3
Mutual orientation of the azide groups with respect to the metalacycle plane.

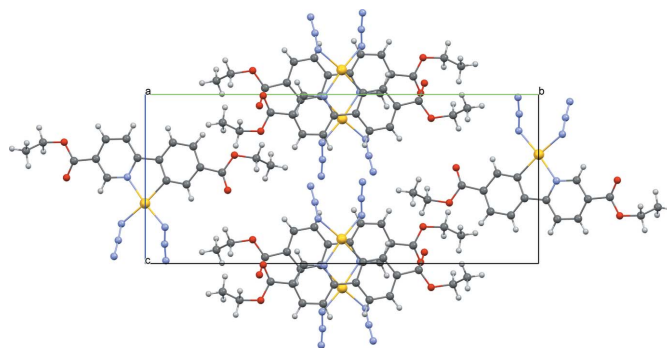


Figure 4
Crystal packing of the title compound viewed along the *a* axis.

atom form an angle with the *a*-axis direction of 69.53 (2)°. The distances between these planes of neighboring molecules within the stack are 3.331 (1) and 3.314 (1) Å (Fig. 4).

4. Database survey

A search was performed in the Cambridge Structural Database (CSD version 5.41; Groom *et al.*, 2016) with the following constraints: an Au^{III} complex featuring a phenylpyridine backbone and two additional non-cyclic ligands bonding to Au through N or C. Fourteen structures were found to match this motif. The features of the title structure resemble those observed in the structures found in this database survey, *e.g.* an observable *trans* effect (distance Au–*L trans* to N is always shorter than that *trans* to C), Au–C bond lengths are shorter than the Au–N ones and angles around the Au^{III} center are close to 90°.

5. Synthesis and crystallization

The reaction scheme for the synthesis of the title compound is provided in Fig. 5. The gold complex $\text{Au}(\text{ppy}^{\text{Et}})\text{Cl}_2$ (**1**) was prepared according to previously published procedure (Levchenko *et al.*, 2020). Complex **1** (70 mg, 0.124 mmol, 1 equiv.) was stirred with sodium azide (64.5 mg, 1 mmol, 8 equiv.) in water for 24 h at room temperature. The solids were recovered by filtration, washed with large excess of water and dried in air giving 50 mg (70%) of **2** as a white solid. Needle-like crystals were obtained by slow diffusion of cyclohexane into a solution of the product in CH_2Cl_2 containing few drops of acetone. $^1\text{H NMR}$ (600 MHz, $\text{DMSO}-d_6$): δ_{H} 9.28 (s, 1H), 8.82 (d, $J = 8.4$ Hz, 1H), 8.61 (d, $J = 8.4$ Hz, 1H), 8.24 (d, $J = 8.2$ Hz, 1H), 8.07–8.02 (m, 2H), 4.45 (dd, $J = 12.5, 5.4$ Hz, 2H), 4.38 (q, $J = 7.0$ Hz, 2H), 1.37 (dt, $J = 13.8, 7.2$ Hz, 6H). $^{13}\text{C NMR}$ (151 MHz, $\text{DMSO}-d_6$): δ_{C} 165.1, 164.5,

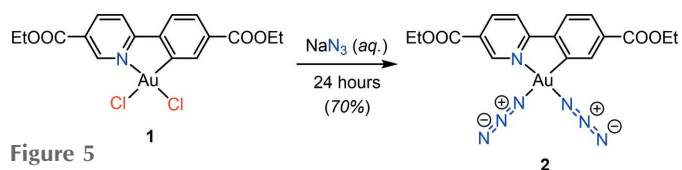


Figure 5
Synthesis of the title compound.

162.3, 148.9, 147.0, 146.3, 143.8, 132.5, 129.6, 128.2, 127.4, 127.1, 122.8, 62.3, 61.5, 14.1, 14.0. **MS** (ESI, CH₃OH): $m/z = 591.091$ ($[M - N_3 + OCH_3 + Na]^+$, 100), 602.082 ($[M + Na]^+$, 9). **HRMS** (CH₃OH): calculated for C₁₈H₁₉AuN₄O₅Na⁺ $[M - N_3 + OCH_3 + Na]^+$ 591.0913, found 591.0914 (Δ 0.00 ppm). Calculated for C₁₇H₁₆AuN₇O₄Na⁺ $[M + Na]^+$ 602.0822, found 602.0821 (Δ 0.10 ppm).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. *OLEX2* was used as user interface (Dolomanov *et al.*, 2009). All hydrogen atoms were placed in calculated positions with C–H = 0.95–0.99 Å and refined as riding with fixed isotropic displacement parameters [$U_{iso}(H) = 1.2$ – $1.5U_{eq}(C)$].

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Table 1

Experimental details.

Crystal data	
Chemical formula	[Au(C ₁₇ H ₁₆ NO ₄)(N ₃) ₂]
M_r	579.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	7.0788 (5), 24.6279 (16), 10.5840 (7)
β (°)	91.059 (1)
V (Å ³)	1844.9 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	8.02
Crystal size (mm)	0.2 × 0.03 × 0.01
Data collection	
Diffractometer	Bruker D8 Photon 100 area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2018)
T_{min} , T_{max}	0.554, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37671, 5655, 4677
R_{int}	0.023
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.036, 1.09
No. of reflections	5655
No. of parameters	264
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.92, -1.10

Computer programs: *APEX3* (Bruker, 2018), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020), *enCIFer* (Allen *et al.*, 2004).

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supporting information

Acta Cryst. (2020). E76, 1725-1727 [https://doi.org/10.1107/S2056989020012955]

Crystal structure of (N⁺C) cyclometalated Au^{III} diazide at 100 K

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Computing details

Data collection: *APEX3* (Bruker, 2018); cell refinement: *APEX3* (Bruker, 2018); data reduction: *APEX3* (Bruker, 2018); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

Diazido[5-ethoxycarbonyl-2-(5-ethoxycarbonylpyridin-2-yl)phenyl- κ^2 C¹,N]gold(III)

Crystal data

[Au(C₁₇H₁₆NO₄)(N₃)₂]

$M_r = 579.33$

Monoclinic, *P2₁/c*

$a = 7.0788$ (5) Å

$b = 24.6279$ (16) Å

$c = 10.5840$ (7) Å

$\beta = 91.059$ (1)°

$V = 1844.9$ (2) Å³

$Z = 4$

$F(000) = 1112$

$D_x = 2.086$ Mg m⁻³

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

Cell parameters from 9519 reflections

$\theta = 2.5$ – 30.6 °

$\mu = 8.02$ mm⁻¹

$T = 100$ K

Needle, colorless

$0.2 \times 0.03 \times 0.01$ mm

Data collection

Bruker D8 Photon 100 area detector
diffractometer

Radiation source: microfocus sealed X-ray tube,
Incoatec I μ s

Mirror optics monochromator

Detector resolution: 10.42 pixels mm⁻¹

ω and φ shutterless scans

Absorption correction: multi-scan
(SADABS; Bruker, 2018)

$T_{\min} = 0.554$, $T_{\max} = 0.746$

37671 measured reflections

5655 independent reflections

4677 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 30.6$ °, $\theta_{\min} = 2.5$ °

$h = -10$ → 10

$k = -35$ → 35

$l = -14$ → 15

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.018$

$wR(F^2) = 0.036$

$S = 1.09$

5655 reflections

264 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

$w = 1/[\sigma^2(F_o^2) + (0.0071P)^2 + 3.5107P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.92$ e Å⁻³

$\Delta\rho_{\min} = -1.09$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.75297 (2)	−0.00058 (2)	0.64453 (2)	0.01001 (2)
O1	0.4872 (2)	0.22687 (7)	0.35894 (15)	0.0181 (3)
O4	1.0437 (3)	−0.20014 (8)	0.49251 (17)	0.0272 (4)
O3	0.9998 (2)	−0.20622 (7)	0.28226 (15)	0.0170 (3)
O2	0.4569 (3)	0.20965 (8)	0.56671 (17)	0.0271 (4)
N6	0.7546 (3)	0.04933 (9)	0.88472 (19)	0.0213 (4)
N1	0.8122 (3)	−0.04540 (8)	0.48884 (17)	0.0141 (4)
N5	0.6697 (3)	0.05028 (8)	0.78531 (18)	0.0180 (4)
N4	0.7094 (4)	−0.07941 (11)	0.9575 (2)	0.0327 (5)
N2	0.8539 (3)	−0.06048 (8)	0.76482 (18)	0.0173 (4)
N7	0.8264 (4)	0.05242 (11)	0.9828 (2)	0.0346 (6)
N3	0.7753 (3)	−0.06848 (9)	0.86238 (19)	0.0211 (4)
C1	0.6763 (3)	0.05386 (8)	0.50946 (19)	0.0097 (4)
C2	0.6095 (3)	0.10502 (9)	0.5321 (2)	0.0144 (4)
H2	0.591225	0.116874	0.616458	0.017*
C6	0.7021 (3)	0.03570 (9)	0.3866 (2)	0.0119 (4)
C7	0.7724 (3)	−0.01977 (9)	0.3753 (2)	0.0120 (4)
C10	0.9087 (3)	−0.12530 (9)	0.3809 (2)	0.0135 (4)
C12	0.4984 (3)	0.19541 (9)	0.4620 (2)	0.0164 (4)
C9	0.8673 (3)	−0.10048 (9)	0.2653 (2)	0.0156 (4)
H9	0.885418	−0.119718	0.188635	0.019*
C8	0.7995 (3)	−0.04760 (9)	0.2623 (2)	0.0152 (4)
H8	0.771619	−0.030465	0.183738	0.018*
C5	0.6615 (3)	0.07016 (9)	0.2849 (2)	0.0159 (4)
H5	0.679171	0.058026	0.200723	0.019*
C17	0.9570 (4)	−0.30317 (11)	0.3331 (3)	0.0324 (6)
H17A	0.835596	−0.301253	0.287316	0.049*
H17B	0.936999	−0.297241	0.423392	0.049*
H17C	1.013575	−0.339051	0.320534	0.049*
C4	0.5950 (3)	0.12224 (9)	0.3074 (2)	0.0161 (4)
H4	0.567987	0.145929	0.238554	0.019*
C3	0.5680 (3)	0.13978 (9)	0.4310 (2)	0.0139 (4)
C16	1.0875 (3)	−0.26013 (9)	0.2839 (2)	0.0194 (5)
H16A	1.203416	−0.259024	0.337608	0.023*
H16B	1.124940	−0.269813	0.197057	0.023*
C15	0.9899 (3)	−0.18128 (9)	0.3932 (2)	0.0156 (4)
C13	0.4230 (4)	0.28268 (10)	0.3779 (2)	0.0220 (5)
H13A	0.324410	0.283170	0.443070	0.026*
H13B	0.366153	0.296654	0.298177	0.026*

C11	0.8795 (3)	-0.09698 (9)	0.4924 (2)	0.0140 (4)
H11	0.906730	-0.113793	0.571430	0.017*
C14	0.5832 (4)	0.31882 (11)	0.4186 (3)	0.0338 (7)
H14A	0.678520	0.319531	0.352664	0.051*
H14B	0.640129	0.304889	0.497250	0.051*
H14C	0.535687	0.355673	0.432548	0.051*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01148 (3)	0.01142 (4)	0.00713 (3)	-0.00123 (3)	0.00055 (2)	-0.00031 (3)
O1	0.0228 (8)	0.0159 (8)	0.0156 (8)	0.0037 (6)	0.0019 (6)	0.0042 (6)
O4	0.0454 (12)	0.0202 (9)	0.0159 (8)	0.0049 (8)	-0.0039 (8)	-0.0024 (7)
O3	0.0211 (8)	0.0162 (8)	0.0137 (8)	0.0017 (6)	0.0006 (6)	-0.0042 (6)
O2	0.0426 (11)	0.0221 (9)	0.0171 (9)	0.0038 (8)	0.0093 (8)	0.0025 (7)
N6	0.0256 (11)	0.0225 (10)	0.0158 (9)	0.0013 (8)	0.0036 (8)	-0.0022 (8)
N1	0.0139 (8)	0.0166 (9)	0.0119 (8)	-0.0039 (7)	0.0014 (7)	-0.0030 (7)
N5	0.0201 (9)	0.0203 (9)	0.0138 (9)	0.0059 (8)	0.0011 (7)	-0.0039 (7)
N4	0.0417 (14)	0.0388 (14)	0.0178 (11)	-0.0078 (11)	0.0049 (10)	0.0061 (10)
N2	0.0197 (9)	0.0166 (9)	0.0155 (9)	0.0067 (7)	-0.0008 (7)	0.0008 (7)
N7	0.0392 (14)	0.0469 (15)	0.0175 (11)	0.0068 (12)	-0.0050 (10)	-0.0075 (10)
N3	0.0256 (10)	0.0210 (10)	0.0165 (10)	-0.0017 (8)	-0.0041 (8)	-0.0010 (8)
C1	0.0081 (8)	0.0102 (9)	0.0109 (9)	-0.0026 (7)	0.0006 (7)	0.0032 (7)
C2	0.0130 (9)	0.0158 (10)	0.0144 (10)	-0.0032 (8)	0.0007 (8)	0.0028 (8)
C6	0.0105 (9)	0.0132 (9)	0.0121 (9)	-0.0032 (7)	0.0002 (7)	0.0004 (7)
C7	0.0104 (9)	0.0162 (9)	0.0095 (9)	-0.0039 (7)	0.0004 (7)	-0.0005 (7)
C10	0.0131 (9)	0.0138 (9)	0.0136 (10)	-0.0046 (8)	0.0018 (7)	-0.0024 (8)
C12	0.0154 (10)	0.0174 (10)	0.0165 (10)	-0.0025 (8)	0.0022 (8)	0.0043 (8)
C9	0.0188 (10)	0.0164 (10)	0.0117 (9)	-0.0050 (8)	0.0019 (8)	-0.0048 (8)
C8	0.0176 (10)	0.0179 (10)	0.0100 (9)	-0.0046 (8)	0.0009 (8)	-0.0013 (8)
C5	0.0195 (10)	0.0173 (10)	0.0109 (9)	-0.0030 (8)	0.0002 (8)	0.0014 (8)
C17	0.0302 (14)	0.0163 (12)	0.0509 (18)	-0.0024 (10)	0.0096 (13)	-0.0062 (12)
C4	0.0165 (10)	0.0173 (10)	0.0146 (10)	-0.0035 (8)	0.0000 (8)	0.0044 (8)
C3	0.0119 (9)	0.0141 (9)	0.0157 (10)	-0.0026 (8)	0.0002 (7)	0.0021 (8)
C16	0.0200 (11)	0.0173 (11)	0.0209 (11)	0.0029 (9)	0.0033 (9)	-0.0052 (9)
C15	0.0175 (10)	0.0143 (10)	0.0150 (10)	-0.0036 (8)	0.0014 (8)	-0.0033 (8)
C13	0.0255 (12)	0.0182 (11)	0.0224 (12)	0.0100 (9)	0.0046 (10)	0.0049 (9)
C11	0.0127 (9)	0.0159 (10)	0.0135 (10)	-0.0039 (8)	0.0018 (7)	-0.0019 (8)
C14	0.0397 (16)	0.0146 (11)	0.0473 (18)	0.0045 (11)	0.0031 (14)	0.0010 (11)

Geometric parameters (Å, °)

Au1—C1	2.027 (2)	C10—C9	1.394 (3)
Au1—N1	2.0335 (18)	C10—C15	1.498 (3)
Au1—N5	2.0418 (19)	C12—C3	1.494 (3)
Au1—N2	2.0674 (19)	C9—C8	1.388 (3)
O1—C12	1.339 (3)	C9—H9	0.9500
O1—C13	1.463 (3)	C8—H8	0.9500

O4—C15	1.204 (3)	C5—C4	1.388 (3)
O3—C15	1.328 (3)	C5—H5	0.9500
O3—C16	1.466 (3)	C17—C16	1.505 (4)
O2—C12	1.205 (3)	C17—H17A	0.9800
N6—N7	1.150 (3)	C17—H17B	0.9800
N6—N5	1.202 (3)	C17—H17C	0.9800
N1—C11	1.357 (3)	C4—C3	1.395 (3)
N1—C7	1.382 (3)	C4—H4	0.9500
N4—N3	1.150 (3)	C16—H16A	0.9900
N2—N3	1.198 (3)	C16—H16B	0.9900
C1—C2	1.369 (3)	C13—C14	1.499 (4)
C1—C6	1.390 (3)	C13—H13A	0.9900
C2—C3	1.397 (3)	C13—H13B	0.9900
C2—H2	0.9500	C11—H11	0.9500
C6—C5	1.397 (3)	C14—H14A	0.9800
C6—C7	1.459 (3)	C14—H14B	0.9800
C7—C8	1.395 (3)	C14—H14C	0.9800
C10—C11	1.390 (3)		
C1—Au1—N1	81.03 (8)	C4—C5—C6	119.7 (2)
C1—Au1—N5	91.82 (8)	C4—C5—H5	120.2
N1—Au1—N5	172.30 (8)	C6—C5—H5	120.2
C1—Au1—N2	172.51 (8)	C16—C17—H17A	109.5
N1—Au1—N2	92.15 (8)	C16—C17—H17B	109.5
N5—Au1—N2	95.13 (8)	H17A—C17—H17B	109.5
C12—O1—C13	116.48 (18)	C16—C17—H17C	109.5
C15—O3—C16	115.97 (18)	H17A—C17—H17C	109.5
N7—N6—N5	173.8 (3)	H17B—C17—H17C	109.5
C11—N1—C7	121.18 (19)	C5—C4—C3	120.0 (2)
C11—N1—Au1	124.28 (15)	C5—C4—H4	120.0
C7—N1—Au1	114.51 (15)	C3—C4—H4	120.0
N6—N5—Au1	118.70 (16)	C4—C3—C2	119.9 (2)
N3—N2—Au1	119.17 (16)	C4—C3—C12	122.8 (2)
N4—N3—N2	174.7 (3)	C2—C3—C12	117.3 (2)
C2—C1—C6	120.80 (19)	O3—C16—C17	112.3 (2)
C2—C1—Au1	125.05 (16)	O3—C16—H16A	109.1
C6—C1—Au1	114.12 (15)	C17—C16—H16A	109.1
C1—C2—C3	119.9 (2)	O3—C16—H16B	109.1
C1—C2—H2	120.1	C17—C16—H16B	109.1
C3—C2—H2	120.1	H16A—C16—H16B	107.9
C1—C6—C5	119.8 (2)	O4—C15—O3	124.9 (2)
C1—C6—C7	115.39 (19)	O4—C15—C10	123.1 (2)
C5—C6—C7	124.8 (2)	O3—C15—C10	112.00 (19)
N1—C7—C8	119.5 (2)	O1—C13—C14	111.2 (2)
N1—C7—C6	114.87 (18)	O1—C13—H13A	109.4
C8—C7—C6	125.7 (2)	C14—C13—H13A	109.4
C11—C10—C9	119.5 (2)	O1—C13—H13B	109.4
C11—C10—C15	116.8 (2)	C14—C13—H13B	109.4

C9—C10—C15	123.7 (2)	H13A—C13—H13B	108.0
O2—C12—O1	124.7 (2)	N1—C11—C10	120.3 (2)
O2—C12—C3	123.8 (2)	N1—C11—H11	119.9
O1—C12—C3	111.5 (2)	C10—C11—H11	119.9
C8—C9—C10	119.9 (2)	C13—C14—H14A	109.5
C8—C9—H9	120.1	C13—C14—H14B	109.5
C10—C9—H9	120.1	H14A—C14—H14B	109.5
C9—C8—C7	119.7 (2)	C13—C14—H14C	109.5
C9—C8—H8	120.2	H14A—C14—H14C	109.5
C7—C8—H8	120.2	H14B—C14—H14C	109.5
C6—C1—C2—C3	-0.6 (3)	C7—C6—C5—C4	180.0 (2)
Au1—C1—C2—C3	177.50 (15)	C6—C5—C4—C3	-0.4 (3)
C2—C1—C6—C5	0.7 (3)	C5—C4—C3—C2	0.5 (3)
Au1—C1—C6—C5	-177.58 (16)	C5—C4—C3—C12	179.5 (2)
C2—C1—C6—C7	-179.42 (19)	C1—C2—C3—C4	0.0 (3)
Au1—C1—C6—C7	2.3 (2)	C1—C2—C3—C12	-179.05 (19)
C11—N1—C7—C8	0.9 (3)	O2—C12—C3—C4	172.6 (2)
Au1—N1—C7—C8	-177.14 (16)	O1—C12—C3—C4	-7.0 (3)
C11—N1—C7—C6	-179.65 (18)	O2—C12—C3—C2	-8.4 (3)
Au1—N1—C7—C6	2.4 (2)	O1—C12—C3—C2	171.98 (19)
C1—C6—C7—N1	-3.1 (3)	C15—O3—C16—C17	76.9 (3)
C5—C6—C7—N1	176.8 (2)	C16—O3—C15—O4	-1.5 (3)
C1—C6—C7—C8	176.4 (2)	C16—O3—C15—C10	176.64 (18)
C5—C6—C7—C8	-3.8 (3)	C11—C10—C15—O4	-6.3 (3)
C13—O1—C12—O2	1.2 (3)	C9—C10—C15—O4	171.9 (2)
C13—O1—C12—C3	-179.18 (19)	C11—C10—C15—O3	175.56 (19)
C11—C10—C9—C8	0.8 (3)	C9—C10—C15—O3	-6.3 (3)
C15—C10—C9—C8	-177.4 (2)	C12—O1—C13—C14	84.2 (3)
C10—C9—C8—C7	-0.3 (3)	C7—N1—C11—C10	-0.4 (3)
N1—C7—C8—C9	-0.5 (3)	Au1—N1—C11—C10	177.39 (15)
C6—C7—C8—C9	-179.9 (2)	C9—C10—C11—N1	-0.4 (3)
C1—C6—C5—C4	-0.2 (3)	C15—C10—C11—N1	177.85 (19)
