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Di-μ-acetato-bis{[3-benzyl-1-(2,4,6-trimethylphenyl)imidazol-2-ylidene]silver(I)}

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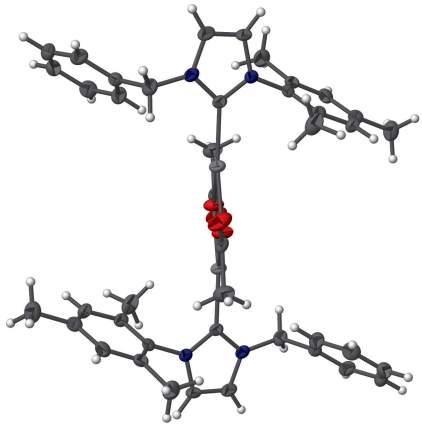
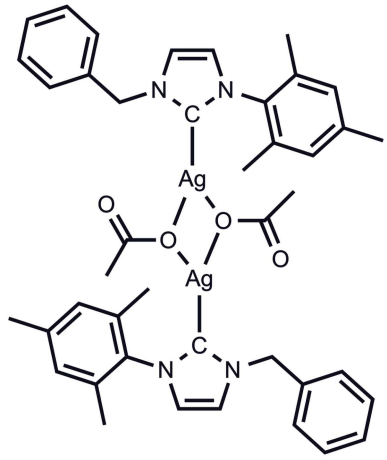
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Ag_2(C_2H_3O_2)_2(C_{19}H_{20}N_2)_2]$ (**2**), was readily synthesized by treatment of 3-benzyl-1-(2,4,6-trimethylphenyl)imidazolium chloride with silver acetate. The solution structure of the complex was analyzed by NMR spectroscopy, while the solid-state structure was confirmed by single-crystal X-ray diffraction studies. Compound **2** crystallizes in the triclinic space group $P\overline{1}$, with a silver-to-carbene bond length (Ag—C_{NHC}) of 2.084 (3) Å. The molecule resides on an inversion center, so that only half of the molecule is crystallographically unique. The planes defined by the two imidazole rings are parallel to each other, but not coplanar [interplanar distance is 0.662 (19) Å]. The dihedral angles between the imidazole ring and the benzyl and mesityl rings are 77.87 (12) and 72.86 (11)°, respectively. The crystal structure features π–π stacking interactions between the benzylic groups of inversion-related ($-x+1$, $-y+1$, $-z+1$) molecules and C—H$\cdots\pi$ interactions.

3D view



Chemical scheme



Structure description

The quest for new antibacterial drugs with different modes of action is necessary, as evident from recent bacterial outbreaks (Brown & Wright, 2016). Silver-based drugs are promising alternatives to current β-lactam drugs because of their higher antibacterial activity with minimal bacterial resistance and non-toxicity in small doses (Morones-Ramirez *et al.*, 2013; Clement & Jarrett, 1994). However, many silver-based antibacterial drugs release silver ions rapidly, limiting their bioavailability for a longer period of time (Johnson *et al.*, 2017). Recently, silver complexes containing N-heterocyclic carbenes (NHC) have become a popular subject of research because of their versatility and they may release silver ions slowly under biological conditions. Moreover, NHCs are highly desired owing to their facile synthetic modifications and strong affinity for transition-

metal centers, which ensures the delayed release of silver to the biological system over longer periods of time (Herrmann, 2002; Jafarpour *et al.*, 1999; Garrison & Youngs, 2005; Meng *et al.*, 2019). Several silver–NHC complexes have been synthesized and tested against several bacterial strains (gram-positive and gram-negative). In most instances, these complexes displayed outstanding antibacterial activity (Johnson *et al.*, 2017; Liang *et al.*, 2018; Patil *et al.*, 2011; Sim *et al.*, 2018). Recently, our group reported several dual-targeting redox-active N-heterocyclic carbene ligated gold(I) complexes as cancer therapeutic agents (Arambula *et al.*, 2016; McCall *et al.*, 2017). In a continuation of this effort, we are currently focusing on the development of dual-targeting redox-active N-heterocyclic carbene-ligated silver(I) complexes to combat drug-resistant bacteria strains. In relevance to this context, we prepared the title compound di-μ-acetato-bis[[3-benzyl-1-(2,4,6-trimethylphenyl)imidazol-2-yl]silver(I)] and studied its solid-state structural features. The results related to the synthesis and solid-state structural characterization are presented here.

The title compound was obtained as colorless crystalline needles by diffusing Et_2O into a saturated CH_2Cl_2 solution. The molecular structure of compound **2** is presented in Fig. 1. Compound **2** forms triclinic crystals, space group $P\overline{1}$. The Ag—C_{NHC} bond distance was found to be 2.084 (3) Å, which falls within the range reported for other Ag^I–NHC complexes (2.056 to 2.094 Å; Patil *et al.*, 2011). The solid-state structure of complex **2** reveals that the molecule resides on an inversion center ($\frac{1}{2}$, 1, $\frac{1}{2}$), so that only half of the molecule is crystallographically unique. This arrangement results in a four-membered centrosymmetric ring (two Ag^I and two O atoms) representing each corner of a parallelogram with Ag—O distances of 2.165 (2) and 2.525 (3) Å and O1—Ag—O1^i and Ag—O1—Ag^i [symmetry code: (i) $1-x, 2-y, 1-z$] bond angles of 70.65 (11) and 109.35 (11)°, respectively. The geometry at the silver atom is trigonal planar, but with significant deviation from idealized geometry because of the non-identical nature of the three groups attached to the silver atom. The O1—Ag—C1 bond angle is 127.22 (11)°, while the C1—Ag—O1^i bond angle is 161.35 (12)°. The dihedral angle between the plane of the imidazole ring (C2–N1–C1–N2–C3) and the parallelogram Ag1–O1–Ag1^i–O1^i is 69.71 (12)°. Similarly, the dihedral angles between the plane of the imidazole ring and the planes of the benzyl (C4–C10) and mesityl (C11–C16) rings are 77.87 (12) and 72.86 (11)°, respectively.

Table 1
Selected short interactions (Å).

H3···$\pi_{mesityl}$($2-x, 1-y, 2-z$)	2.642
H13···O2($x-1, 1+y, z$)	2.542
O2···H2($x-1, 1+y, z$)	2.376
O2···C2($x-1, 1+y, z$)	3.162 (5)
H17*C*···C20($1+x, y, z$)	2.820
π_{benzyl}···π_{benzyl}($1-x, 1-y, 1-z$)	3.968 (3)

The solid-state structure of compound **2** features C—H···π and π–π interactions, the parameters related to these interactions are presented in Table 1. Pictorial representations of the C—H···π and π–π interactions are presented in Fig. 2. As viewed along the *c* axis, molecules are interconnected *via* C—H···π interactions to give uni-directional strands, Fig. 2. These strands are held together by intermolecular π–π stacking

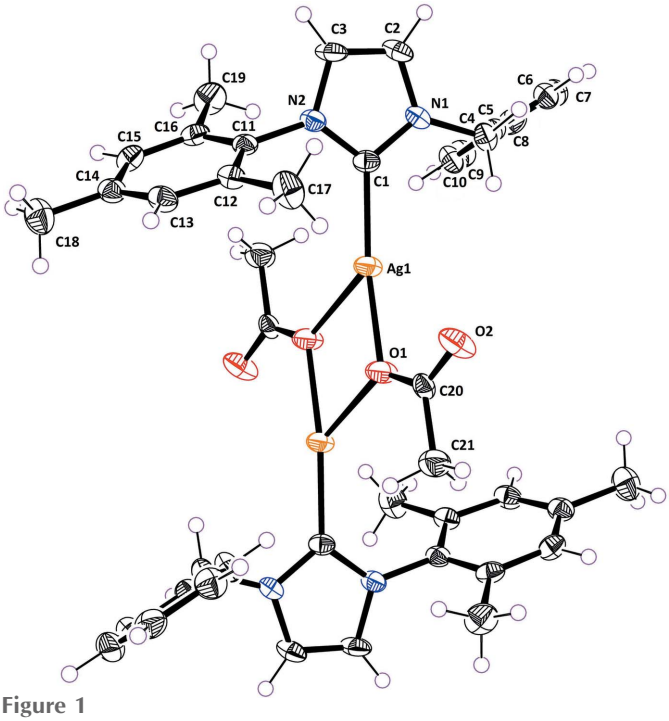


Figure 1
Molecular structure of **2**, with displacement ellipsoids drawn at the 50% probability level.

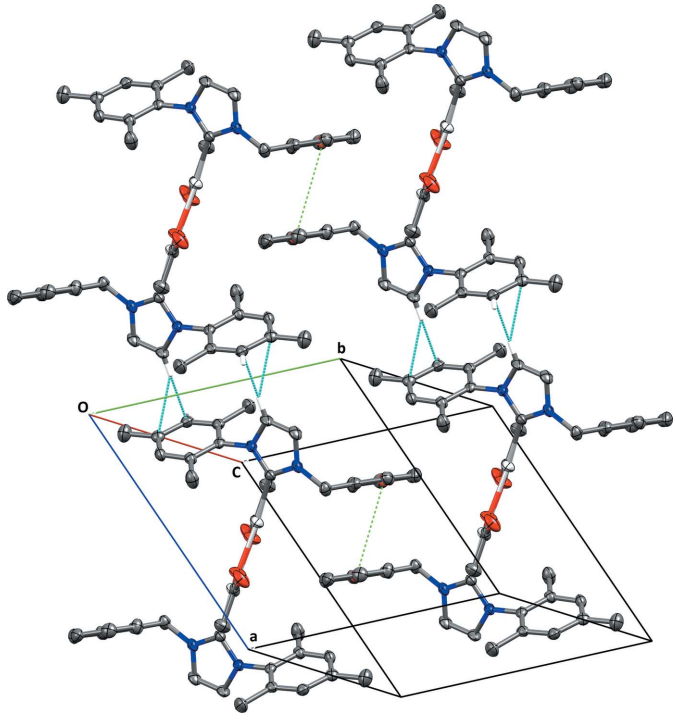


Figure 2
Intermolecular C—H···π interactions and π–π stacking interactions (shown as dotted lines) for compound **2**.

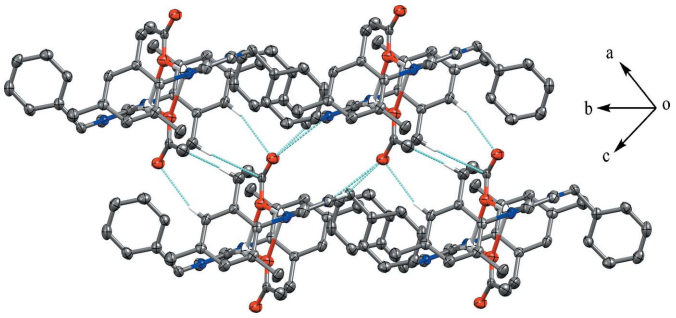


Figure 3
Intercalation of two-dimensional sheets *via* C—H···O and C—H···C short interactions in complex **2**.

interactions of inversion-related benzyl groups parallel to the *b* axis to yield two-dimensional sheets, Fig. 2. These two-dimensional sheets are stacked one over the other and are held in place by weak intersheet C—H···O interactions, Fig. 3. Short interactions of mesityl aryl H atoms with carbonyl oxygen, C—H···O, and short interactions of mesityl methyl H atoms with carbonyl carbon, C—H···C(O), are represented in Fig. 3.

A CSD (Groom *et al.*, 2016) structure search for the core NHC–Ag–O revealed 35 hits. A few of those results are summarized here. For more information regarding symmetrically and unsymmetrically substituted silver–NHC acetate complexes such as 1-methyl-3-(4-cyanobenzyl)imidazole-2-silver(I)acetate and 1,3-dibenzyl-4,5-diphenylimidazole-2-silver(I) acetate, see: Patil *et al.*, (2011). For silver(I)–N-heterocyclic carbene complexes derived from caffeine, see: Mohamed *et al.* (2015); Kascatan-Nebioglu *et al.* (2006). Bis(thiophene)-substituted silver acetate complexes have been prepared and used as monomers to make electroconducting polymers, for more information, see: Powell *et al.* (2010). For NHC–Ag acetate complexes bearing benzyl groups, see: Patil *et al.* (2010). In scanning the literature, the C_{NHC}—Ag, Ag—O(Ac), C—N and N—C—N, bond lengths and N—C_{NHC}—N bond angles were comparable to those of compound **2**.

Synthesis and crystallization

A 20 ml scintillation vial with a stir bar was charged with 33 mg (0.1 mmol) of 1–1-(2,4,6-trimethylphenyl)-3-(benzyl)imidazolium chloride (Samantaray *et al.*, 2011), compound (**1**), $NaN(SiCH_3)_2$ (20 mg, 0.11 mmol) and 5 ml of dry toluene. The resulting mixture was stirred at 298 K for 1 h, which resulted in a yellow solution and a suspended white precipitate. The heterogeneous mixture was filtered through a plug of Celite into a clean 20 ml scintillation vial containing AgOAc (17 mg, 0.1 mmol) in 5 ml of THF. The resulting mixture was stirred at 298 K for 12 h in the dark. The resulting dark-yellow solution was filtered through a plug of Celite and the volatiles were removed under vacuum. The obtained yellow residue was dissolved in a minimum amount of dichloromethane (1 ml) and triturated with 25 ml of hexanes, resulting in a colorless precipitate. The supernatant liquid was decanted and the precipitate was washed with 5 ml of hexane and dried under vacuum for 24 h to yield the title compound, 30.6 mg, 69% yield, IR, 1562 cm^{-1}.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.39–7.30 (*m*, 5H), 7.08 (*s*, 1H), 6.95 (*s*, 2H), 6.93 (*s*, 1H), 5.43 (*s*, 2H), 2.32 (*s*, 3H), 1.99 (*s*, 9H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 178.45, 139.43, 135.70, 135.42, 134.73, 129.37, 129.11, 128.58, 127.73, 123.12, 120.89, 55.88, 23.16, 21.04, 17.67. X-ray diffraction quality single crystals were obtained by diffusing diethyl ether into a saturated solution of **2** in CH_2Cl_2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ag_2(C_2H_3O_2)_2(C_{19}H_{20}N_2)_2]$
M_r	886.57
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	183
a, *b*, *c* (Å)	9.078 (2), 10.473 (2), 12.236 (3)
α, β, γ (°)	65.065 (6), 77.420 (7), 65.229 (7)
V (Å^3)	956.7 (4)
Z	1
Radiation type	Mo *K*α
μ (mm^{-1})	1.07
Crystal size (mm)	0.64 × 0.26 × 0.2
Data collection	
Diffractometer	Bruker SMART X2S benchtop
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.783, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15885, 3354, 2837
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.035, 0.080, 1.05
No. of reflections	3354
No. of parameters	239
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.78, −0.43

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), OLEX2 (Dolomanov *et al.*, 2009), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2006).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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The authors thank Wright State University for instrument infrastructure and Dr David Grossie (Wright State University) for valuable crystallographic discussions.

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full crystallographic data

IUCrData (2019). **4**, x191003 [https://doi.org/10.1107/S2414314619010034]

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Crystal data

$[Ag_2(C_2H_3O_2)_2(C_{19}H_{20}N_2)_2]$
M_r = 886.57
Triclinic, $P\overline{1}$
a = 9.078 (2) Å
b = 10.473 (2) Å
c = 12.236 (3) Å
α = 65.065 (6)°
β = 77.420 (7)°
γ = 65.229 (7)°
V = 956.7 (4) Å^3
Z = 1
$F(000)$ = 452
D_x = 1.539 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3884 reflections
θ = 2.5–22.8°
μ = 1.07 mm^{-1}
T = 183 K
Needle, colorless
0.64 × 0.26 × 0.2 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*; Krause *et al.*, 2015)
T_{min} = 0.783, T_{max} = 1.000
15885 measured reflections
3354 independent reflections
2837 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −10→10
k = −12→12
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.080
S = 1.05
3354 reflections
239 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 0.9398P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 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)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.67227 (4)	0.80738 (3)	0.56178 (3)	0.03206 (12)
O1	0.3866 (3)	0.9810 (3)	0.5928 (2)	0.0339 (6)
O2	0.1564 (3)	1.0757 (3)	0.6868 (3)	0.0416 (7)
N1	0.8628 (3)	0.4584 (3)	0.6776 (3)	0.0238 (6)
N2	0.8626 (3)	0.5700 (3)	0.7896 (3)	0.0240 (7)
C1	0.8045 (4)	0.5972 (4)	0.6853 (3)	0.0236 (8)
C4	0.8287 (4)	0.4281 (4)	0.5811 (3)	0.0288 (8)
H4A	0.9266	0.3556	0.5593	0.035*
H4B	0.7985	0.5212	0.5105	0.035*
C5	0.6935 (4)	0.3665 (4)	0.6172 (3)	0.0256 (8)
C6	0.7160 (5)	0.2350 (4)	0.6026 (3)	0.0324 (9)
H6	0.8166	0.1818	0.5741	0.039*
C7	0.5909 (5)	0.1818 (4)	0.6298 (4)	0.0376 (10)
H7	0.6080	0.0943	0.6182	0.045*
C8	0.4421 (5)	0.2568 (4)	0.6736 (3)	0.0354 (9)
H8	0.3585	0.2205	0.6925	0.042*
C9	0.4189 (5)	0.3870 (4)	0.6892 (4)	0.0358 (9)
H9	0.3186	0.4383	0.7194	0.043*
C10	0.5421 (4)	0.4429 (4)	0.6607 (3)	0.0320 (9)
H10	0.5234	0.5318	0.6707	0.038*
C2	0.9553 (4)	0.3484 (4)	0.7744 (3)	0.0308 (9)
H2	1.0077	0.2458	0.7880	0.037*
C3	0.9553 (4)	0.4173 (4)	0.8454 (3)	0.0317 (9)
H3	1.0071	0.3719	0.9175	0.038*
C11	0.8354 (4)	0.6847 (4)	0.8361 (3)	0.0239 (8)
C12	0.9159 (4)	0.7872 (4)	0.7781 (3)	0.0253 (8)
C17	1.0252 (5)	0.7852 (5)	0.6671 (4)	0.0416 (10)
H17A	0.9612	0.8202	0.6000	0.062*
H17B	1.1011	0.6837	0.6802	0.062*
H17C	1.0833	0.8503	0.6502	0.062*
C13	0.8878 (4)	0.8938 (4)	0.8275 (3)	0.0290 (8)
H13	0.9419	0.9610	0.7924	0.035*
C14	0.7822 (4)	0.9036 (4)	0.9272 (3)	0.0277 (8)
C15	0.7065 (4)	0.7999 (4)	0.9809 (3)	0.0292 (8)
H15	0.6363	0.8050	1.0481	0.035*
C16	0.7312 (4)	0.6879 (4)	0.9383 (3)	0.0265 (8)
C19	0.6529 (5)	0.5716 (5)	1.0031 (4)	0.0409 (10)
H19A	0.7295	0.4801	1.0545	0.061*
H19B	0.6200	0.5507	0.9450	0.061*

H19C	0.5596	0.6103	1.0510	0.061*
C18	0.7545 (5)	1.0233 (5)	0.9749 (4)	0.0432 (11)
H18A	0.8551	1.0086	1.0004	0.065*
H18B	0.6768	1.0159	1.0423	0.065*
H18C	0.7138	1.1216	0.9125	0.065*
C20	0.2867 (4)	0.9732 (4)	0.6823 (3)	0.0239 (8)
C21	0.3356 (5)	0.8255 (4)	0.7907 (4)	0.0387 (10)
H21A	0.4238	0.8174	0.8277	0.058*
H21B	0.3692	0.7421	0.7651	0.058*
H21C	0.2447	0.8237	0.8479	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0419 (2)	0.01798 (16)	0.03125 (18)	−0.00692 (13)	−0.01203 (13)	−0.00377 (12)
O1	0.0329 (15)	0.0224 (13)	0.0305 (15)	−0.0037 (12)	−0.0004 (13)	−0.0024 (11)
O2	0.0340 (17)	0.0239 (15)	0.0545 (19)	−0.0078 (13)	0.0107 (14)	−0.0124 (14)
N1	0.0225 (16)	0.0170 (15)	0.0297 (17)	−0.0057 (12)	−0.0006 (13)	−0.0088 (13)
N2	0.0244 (16)	0.0179 (15)	0.0290 (17)	−0.0068 (13)	−0.0062 (13)	−0.0067 (13)
C1	0.0231 (19)	0.0199 (18)	0.0257 (19)	−0.0100 (15)	−0.0027 (15)	−0.0040 (15)
C4	0.032 (2)	0.027 (2)	0.031 (2)	−0.0120 (17)	0.0036 (17)	−0.0157 (17)
C5	0.031 (2)	0.0229 (19)	0.0235 (19)	−0.0097 (16)	−0.0057 (16)	−0.0069 (16)
C6	0.041 (2)	0.025 (2)	0.030 (2)	−0.0099 (18)	−0.0005 (18)	−0.0113 (17)
C7	0.049 (3)	0.028 (2)	0.042 (2)	−0.016 (2)	−0.012 (2)	−0.0131 (19)
C8	0.040 (3)	0.036 (2)	0.032 (2)	−0.020 (2)	−0.0085 (19)	−0.0066 (19)
C9	0.028 (2)	0.037 (2)	0.039 (2)	−0.0090 (18)	−0.0012 (18)	−0.0144 (19)
C10	0.031 (2)	0.027 (2)	0.040 (2)	−0.0072 (18)	−0.0014 (18)	−0.0188 (18)
C2	0.026 (2)	0.0164 (18)	0.043 (2)	−0.0017 (16)	−0.0081 (17)	−0.0081 (17)
C3	0.031 (2)	0.0168 (18)	0.039 (2)	−0.0038 (16)	−0.0178 (18)	−0.0008 (17)
C11	0.0218 (19)	0.0195 (18)	0.029 (2)	−0.0038 (15)	−0.0111 (16)	−0.0071 (15)
C12	0.0222 (19)	0.0215 (18)	0.030 (2)	−0.0077 (15)	−0.0031 (16)	−0.0071 (16)
C17	0.045 (3)	0.041 (2)	0.048 (3)	−0.026 (2)	0.012 (2)	−0.022 (2)
C13	0.030 (2)	0.0222 (19)	0.037 (2)	−0.0132 (16)	−0.0048 (17)	−0.0079 (17)
C14	0.023 (2)	0.0252 (19)	0.032 (2)	−0.0050 (16)	−0.0059 (16)	−0.0093 (17)
C15	0.030 (2)	0.034 (2)	0.0240 (19)	−0.0141 (17)	−0.0051 (16)	−0.0074 (17)
C16	0.026 (2)	0.0251 (19)	0.026 (2)	−0.0101 (16)	−0.0092 (16)	−0.0019 (16)
C19	0.051 (3)	0.042 (2)	0.037 (2)	−0.031 (2)	0.000 (2)	−0.008 (2)
C18	0.044 (3)	0.044 (3)	0.052 (3)	−0.018 (2)	−0.002 (2)	−0.026 (2)
C20	0.029 (2)	0.0200 (19)	0.028 (2)	−0.0118 (17)	0.0016 (17)	−0.0122 (16)
C21	0.045 (3)	0.029 (2)	0.033 (2)	−0.0116 (19)	0.0011 (19)	−0.0067 (18)

Geometric parameters (Å, º)

Ag1—O1^{i}	2.165 (2)	C2—C3	1.343 (5)
Ag1—O1	2.525 (3)	C3—H3	0.9300
Ag1—C1	2.084 (3)	C11—C12	1.407 (5)
O1—Ag1^{i}	2.165 (2)	C11—C16	1.398 (5)
O1—C20	1.258 (4)	C12—C17	1.500 (5)

O2—C20	1.230 (4)	C12—C13	1.392 (5)
N1—C1	1.360 (4)	C17—H17A	0.9600
N1—C4	1.467 (4)	C17—H17B	0.9600
N1—C2	1.381 (4)	C17—H17C	0.9600
N2—C1	1.360 (4)	C13—H13	0.9300
N2—C3	1.390 (4)	C13—C14	1.390 (5)
N2—C11	1.446 (4)	C14—C15	1.382 (5)
C4—H4A	0.9700	C14—C18	1.505 (5)
C4—H4B	0.9700	C15—H15	0.9300
C4—C5	1.518 (5)	C15—C16	1.393 (5)
C5—C6	1.387 (5)	C16—C19	1.511 (5)
C5—C10	1.390 (5)	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C6—C7	1.386 (5)	C19—H19C	0.9600
C7—H7	0.9300	C18—H18A	0.9600
C7—C8	1.371 (6)	C18—H18B	0.9600
C8—H8	0.9300	C18—H18C	0.9600
C8—C9	1.379 (5)	C20—C21	1.516 (5)
C9—H9	0.9300	C21—H21A	0.9600
C9—C10	1.387 (5)	C21—H21B	0.9600
C10—H10	0.9300	C21—H21C	0.9600
C2—H2	0.9300		
Ag1···C1	2.084 (3)	C20···O2	1.230 (4)
Ag1···O1	2.165 (2)	C1···N1	1.360 (4)
O1···C20	1.258 (4)	C2···C3	1.343 (5)
O1^{i}—Ag1—O1	70.65 (11)	C12—C11—N2	119.1 (3)
C1—Ag1—O1	127.22 (11)	C16—C11—N2	118.4 (3)
C1—Ag1—O1^{i}	161.35 (12)	C16—C11—C12	122.5 (3)
Ag1^{i}—O1—Ag1	109.35 (11)	C11—C12—C17	122.3 (3)
C20—O1—Ag1^{i}	117.5 (2)	C13—C12—C11	116.9 (3)
C20—O1—Ag1	132.6 (2)	C13—C12—C17	120.8 (3)
C1—N1—C4	124.6 (3)	C12—C17—H17A	109.5
C1—N1—C2	111.2 (3)	C12—C17—H17B	109.5
C2—N1—C4	124.1 (3)	C12—C17—H17C	109.5
C1—N2—C3	111.3 (3)	H17A—C17—H17B	109.5
C1—N2—C11	124.8 (3)	H17A—C17—H17C	109.5
C3—N2—C11	123.9 (3)	H17B—C17—H17C	109.5
N1—C1—Ag1	129.0 (2)	C12—C13—H13	118.7
N2—C1—Ag1	126.9 (2)	C14—C13—C12	122.6 (3)
N2—C1—N1	104.0 (3)	C14—C13—H13	118.7
N1—C4—H4A	109.0	C13—C14—C18	120.1 (3)
N1—C4—H4B	109.0	C15—C14—C13	118.1 (3)
N1—C4—C5	112.7 (3)	C15—C14—C18	121.8 (4)
H4A—C4—H4B	107.8	C14—C15—H15	118.7
C5—C4—H4A	109.0	C14—C15—C16	122.6 (4)
C5—C4—H4B	109.0	C16—C15—H15	118.7

C6—C5—C4	120.6 (3)	C11—C16—C19	121.7 (3)
C6—C5—C10	118.1 (3)	C15—C16—C11	117.3 (3)
C10—C5—C4	121.2 (3)	C15—C16—C19	121.0 (3)
C5—C6—H6	119.5	C16—C19—H19A	109.5
C7—C6—C5	121.0 (4)	C16—C19—H19B	109.5
C7—C6—H6	119.5	C16—C19—H19C	109.5
C6—C7—H7	119.6	H19A—C19—H19B	109.5
C8—C7—C6	120.7 (3)	H19A—C19—H19C	109.5
C8—C7—H7	119.6	H19B—C19—H19C	109.5
C7—C8—H8	120.7	C14—C18—H18A	109.5
C7—C8—C9	118.7 (4)	C14—C18—H18B	109.5
C9—C8—H8	120.7	C14—C18—H18C	109.5
C8—C9—H9	119.4	H18A—C18—H18B	109.5
C8—C9—C10	121.3 (4)	H18A—C18—H18C	109.5
C10—C9—H9	119.4	H18B—C18—H18C	109.5
C5—C10—H10	119.9	O1—C20—C21	115.9 (3)
C9—C10—C5	120.2 (3)	O2—C20—O1	124.6 (3)
C9—C10—H10	119.9	O2—C20—C21	119.5 (3)
N1—C2—H2	126.4	C20—C21—H21A	109.5
C3—C2—N1	107.2 (3)	C20—C21—H21B	109.5
C3—C2—H2	126.4	C20—C21—H21C	109.5
N2—C3—H3	126.8	H21A—C21—H21B	109.5
C2—C3—N2	106.4 (3)	H21A—C21—H21C	109.5
C2—C3—H3	126.8	H21B—C21—H21C	109.5

Symmetry code: (i) $-x+1, -y+2, -z+1$.