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catena-Poly[[bis[μ-2-(3-pyridyl)-1*H*-benzimidazole]-$\kappa^2N^2:N^3;\kappa^2N^3:N^2$-disilver(I)]-$\mu$-2,5-dicarboxybenzene-1,4-dicarboxylato-$\kappa^2O^2:O^5$]

Jie Chen‡

Department of Civil Engineering, Fujian University of Technology, Fuzhou, Fujian 350002, People's Republic of China
Correspondence e-mail: yq014@163.com

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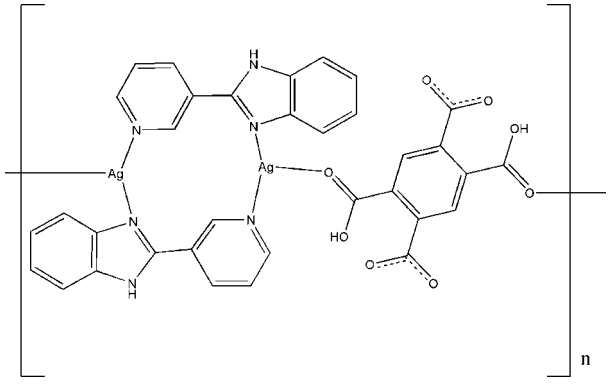
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.075; data-to-parameter ratio = 14.8.

The title coordination polymer, $[Ag_2(C_{10}H_4O_8)(C_{12}H_9N_3)_2]_n$, was prepared by a hydrothermal method. The Ag^I atom exists in a strongly distorted trigonal coordination environment. Two Ag^I ions related by an inversion centre are coordinated by two 2-(3-pyridyl)benzimidazole ligands, forming a centrosymmetric cyclic dimer. The bridging bidentate 2,5-dicarboxybenzene-1,4-dicarboxylate ligand is also located on an inversion centre and connects the binuclear units, generating a one-dimensional polymer. The almost-planar conformation of this ligand allows it to form a strong intramolecular O—H···O hydrogen bond. Finally, intermolecular N—H···O hydrogen bonds aggregate the chains into a three-dimensional framework.

Related literature

For related literature, see: Alcalde *et al.* (1992); Cao *et al.* (2002); Hu *et al.* (2004); Li *et al.* (2003); Xia *et al.* (2007).



Experimental

Crystal data

$[Ag_2(C_{10}H_4O_8)(C_{12}H_9N_3)_2]$
M_r = 858.32
Monoclinic, $P2_1/n$
a = 4.8940 (11) Å
b = 16.011 (4) Å
c = 19.077 (4) Å
β = 92.393 (3)°
V = 1493.6 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.38 mm^{-1}
T = 293 (2) K
0.48 × 0.13 × 0.13 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.806, T_{max} = 0.842
11420 measured reflections
3405 independent reflections
3079 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.075
S = 1.07
3405 reflections
230 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N2	2.1663 (18)	Ag1—O1	2.3889 (18)
Ag1—N1^{i}	2.207 (2)		
N2—Ag1—N1^{i}	150.61 (7)	N1^{i}—Ag1—O1	93.66 (7)
N2—Ag1—O1	115.06 (7)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···O4	0.846 (19)	1.56 (2)	2.399 (3)	171 (4)
N3—H3A···O3^{ii}	0.86	1.92	2.742 (3)	159

Symmetry code: (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2158).

‡ Alternative address: Fuzhou University, Fuzhou, Fujian 350002 People's Republic of China.

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supporting information

Acta Cryst. (2008). E**64**, m498–m499 [doi:10.1107/S1600536808004984]

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S1. Comment

1,2,4,5-Benzenetetracarboxylic acid (H_4BTEC) has been regarded as an excellent candidate for the construction of multi-dimensional coordination polymers for its versatile coordination modes and rich hydrogen bonding (Cao *et al.*, 2002; Hu *et al.*, 2004; Li *et al.*, 2003). The coordination supramolecular architectures are controlled by the extent of the deprotonation of H_4BTEC, nature of the auxiliary ligands, and metal coordination centers.

In the title coordination polymer, (I), the Ag^I is three coordinated (Fig. 1). Two symmetry related Ag^I ions are bonded by four N atoms from two 2-(3-pyridyl)-1*H*-benzimidazole ligands in the head to end mode, forming a centrosymmetric cyclic dimer. The coordination sphere of the cyclic dimer is completed by the 2,5-dicarboxybenzene-1,4-dicarboxylate coordinating in a bis(monodentate) fashion, which is similar to the coordination mode reported by Xia *et al.* (2007). The centrosymmetric bridging 2,5-dicarboxybenzene-1,4-dicarboxylate ligands link the binuclear units into a one-dimensional polymeric chain (Fig. 2). Interestingly, the coordinating O atom is provided by the undeprotonated carboxylic group rather than the deprotonated one. The O2—H group in the undeprotonated carboxylic group forms a strong intramolecular hydrogen bond with the adjacent carboxylate group [O2···O4: 2.399 (3) Å]. This contact allows planarity for the bridging ligand, which may be related to the non-coordinating character of carboxylate functionalities. The uncoordinated carboxylate group also provides another O atom for the formation of intermolecular hydrogen bonds [N3···O3: 2.742 (3) Å], forming a three-dimensional framework (Fig. 3). Despite of the presence of aromatic rings, no apparent $\pi\cdots\pi$ stacking interactions are found in the crystal structure.

S2. Experimental

A solution of Ag_2O (0.07 g, 0.30 mmol), 2-(3-pyridyl)-1*H*-benzimidazole (Alcalde *et al.*, 1992) (0.14 g, 0.61 mmol), 1,2,4,5-benzenetetracarboxylic acid (0.066 g, 0.30 mmol) and H_2O (15 ml) was stirred under ambient conditions. The solution was sealed in a 25 ml Teflon-lined stainless steel vessel, heated at 413 K for 4 days and cooled to room temperature for 3 days. The resulting product was recovered by filtration, washed with distilled water and dried in air (65% yield).

S3. Refinement

Anisotropic thermal parameters were applied to all non-hydrogen atoms. The carboxylic acid H atom H2B was initially located in a difference map, and then refined with a restrained O—H bond length of 0.83 (1) Å. Other H atoms were fixed geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å, N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(carrier atom).

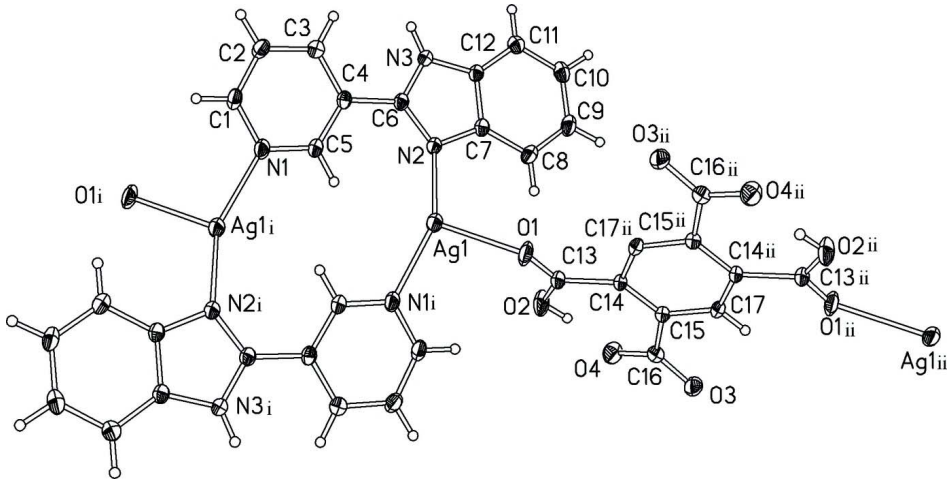

Figure 1

The structure of (I), with the atomic labels and 30% probability displacement ellipsoids for non-H atoms. [Symmetry codes: (*i*) 2 - *x*, -*y*, 2 - *z*; (*ii*) 1 - *x*, 1 - *y*, 2 - *z*].

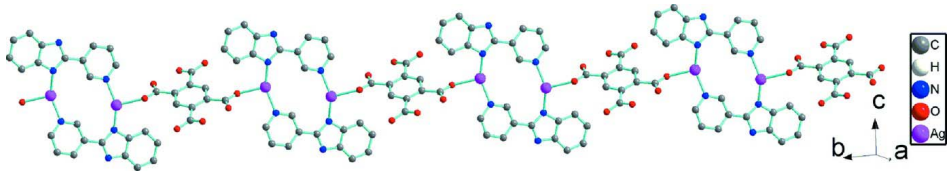

Figure 2

A view of the one-dimensional chain of (I). H atoms are omitted for clarity.

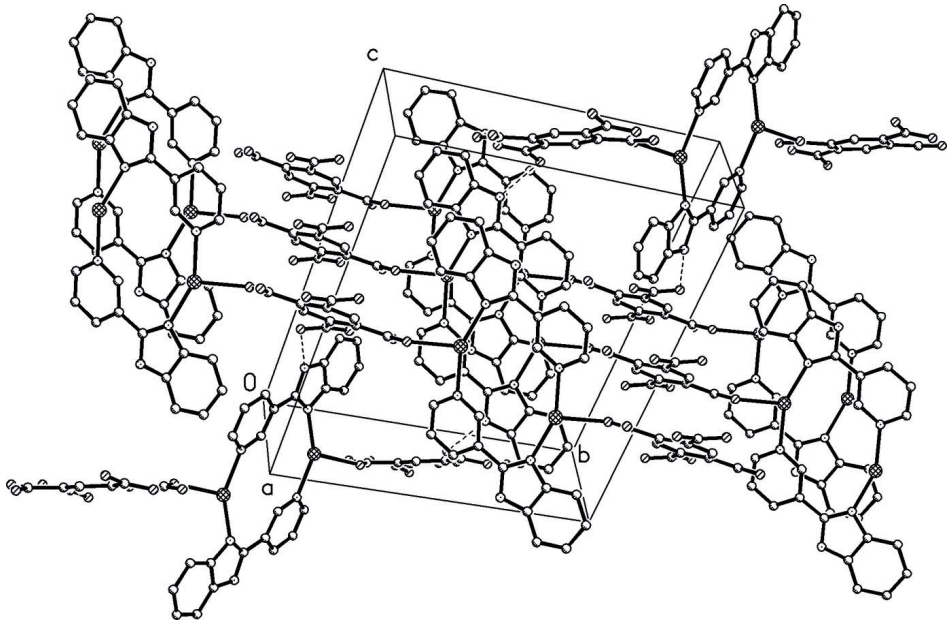

Figure 3

The crystal packing of (I). H atoms are omitted for clarity.

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Hall symbol: -P 2yn
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b = 16.011 (4) Å
c = 19.077 (4) Å
β = 92.393 (3)°
V = 1493.6 (6) Å^3
Z = 2
$F(000)$ = 852
D_x = 1.909 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3641 reflections
θ = 2.5–27.5°
μ = 1.38 mm^{-1}
T = 293 K
Prism, colourless
0.48 × 0.13 × 0.13 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.806, T_{max} = 0.842
11420 measured reflections
3405 independent reflections
3079 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.5°
h = −6→6
k = −20→20
l = −18→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.075
S = 1.07
3405 reflections
230 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.9191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.71244 (4)	0.134099 (11)	1.018347 (10)	0.04125 (9)
C1	1.1680 (5)	−0.15500 (14)	1.13812 (13)	0.0343 (5)
H1A	1.2997	−0.1963	1.1336	0.041*
C2	1.0649 (5)	−0.14053 (14)	1.20320 (14)	0.0359 (5)
H2A	1.1275	−0.1717	1.2418	0.043*
C3	0.8688 (5)	−0.07976 (15)	1.21087 (12)	0.0329 (5)
H3B	0.7980	−0.0695	1.2545	0.039*
C4	0.7781 (4)	−0.03380 (13)	1.15231 (12)	0.0265 (4)
C5	0.8913 (5)	−0.05275 (13)	1.08884 (12)	0.0324 (5)
H5A	0.8300	−0.0232	1.0493	0.039*
C6	0.5728 (4)	0.03242 (13)	1.15806 (11)	0.0264 (4)

C7	0.3021 (5)	0.13812 (13)	1.13776 (12)	0.0269 (4)
C8	0.1575 (5)	0.20687 (14)	1.11051 (13)	0.0347 (5)
H8A	0.1860	0.2269	1.0656	0.042*
C9	−0.0299 (5)	0.24392 (16)	1.15313 (14)	0.0386 (6)
H9A	−0.1287	0.2900	1.1365	0.046*
C10	−0.0745 (5)	0.21380 (16)	1.22058 (14)	0.0383 (6)
H10A	−0.2039	0.2399	1.2474	0.046*
C11	0.0682 (5)	0.14644 (15)	1.24842 (13)	0.0332 (5)
H11A	0.0396	0.1267	1.2934	0.040*
C12	0.2577 (4)	0.10963 (13)	1.20541 (11)	0.0264 (4)
C13	0.5075 (5)	0.32005 (13)	0.96973 (12)	0.0322 (5)
C14	0.4884 (5)	0.41435 (13)	0.98108 (11)	0.0271 (4)
C15	0.3175 (5)	0.47238 (13)	0.94531 (11)	0.0271 (4)
C16	0.1144 (5)	0.45603 (15)	0.88456 (12)	0.0320 (5)
C17	0.3352 (5)	0.55568 (14)	0.96571 (12)	0.0297 (5)
H17A	0.2214	0.5939	0.9422	0.036*
N1	1.0845 (4)	−0.11132 (12)	1.08101 (11)	0.0347 (4)
N2	0.5015 (4)	0.08847 (11)	1.10831 (9)	0.0273 (4)
N3	0.4299 (4)	0.04296 (11)	1.21627 (9)	0.0273 (4)
H3A	0.4443	0.0131	1.2537	0.033*
O1	0.6918 (4)	0.28180 (11)	1.00119 (11)	0.0484 (5)
O2	0.3341 (4)	0.28260 (11)	0.92949 (12)	0.0486 (5)
H2B	0.217 (7)	0.316 (2)	0.912 (2)	0.082 (13)*
O3	0.0298 (4)	0.51666 (11)	0.84962 (9)	0.0440 (4)
O4	0.0356 (4)	0.38153 (11)	0.87095 (10)	0.0456 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.05515 (15)	0.02899 (12)	0.04086 (13)	0.01185 (8)	0.01680 (9)	0.00789 (7)
C1	0.0358 (12)	0.0225 (10)	0.0449 (14)	0.0059 (9)	0.0042 (10)	0.0043 (9)
C2	0.0383 (13)	0.0301 (12)	0.0393 (13)	0.0058 (10)	0.0011 (10)	0.0093 (9)
C3	0.0362 (12)	0.0305 (12)	0.0320 (12)	0.0041 (10)	0.0018 (9)	0.0010 (9)
C4	0.0274 (11)	0.0187 (9)	0.0333 (11)	−0.0010 (8)	0.0010 (8)	−0.0001 (8)
C5	0.0411 (13)	0.0216 (10)	0.0347 (12)	0.0054 (9)	0.0037 (10)	0.0026 (8)
C6	0.0283 (11)	0.0205 (10)	0.0303 (11)	−0.0005 (8)	−0.0007 (8)	−0.0007 (8)
C7	0.0263 (11)	0.0219 (10)	0.0323 (11)	−0.0002 (8)	−0.0002 (8)	−0.0008 (8)
C8	0.0368 (13)	0.0280 (11)	0.0386 (13)	0.0034 (10)	−0.0037 (10)	0.0050 (9)
C9	0.0372 (13)	0.0284 (12)	0.0492 (15)	0.0097 (10)	−0.0073 (11)	−0.0006 (10)
C10	0.0324 (12)	0.0360 (13)	0.0463 (14)	0.0081 (10)	0.0001 (10)	−0.0107 (10)
C11	0.0319 (12)	0.0337 (12)	0.0339 (12)	0.0015 (9)	0.0014 (9)	−0.0027 (9)
C12	0.0259 (11)	0.0223 (10)	0.0307 (11)	0.0005 (8)	−0.0023 (8)	−0.0012 (8)
C13	0.0455 (14)	0.0189 (10)	0.0327 (12)	0.0017 (9)	0.0057 (10)	−0.0001 (8)
C14	0.0379 (12)	0.0173 (9)	0.0261 (10)	0.0030 (8)	0.0037 (9)	0.0002 (7)
C15	0.0347 (12)	0.0219 (10)	0.0249 (10)	0.0022 (9)	0.0035 (8)	0.0003 (8)
C16	0.0380 (13)	0.0309 (11)	0.0269 (11)	0.0029 (9)	0.0012 (9)	−0.0016 (9)
C17	0.0400 (13)	0.0207 (10)	0.0282 (11)	0.0055 (9)	−0.0013 (9)	0.0031 (8)
N1	0.0428 (12)	0.0208 (9)	0.0410 (11)	0.0040 (8)	0.0082 (9)	0.0028 (8)

N2	0.0303 (10)	0.0220 (9)	0.0297 (9)	0.0025 (7)	0.0020 (7)	0.0016 (7)
N3	0.0304 (10)	0.0244 (9)	0.0272 (9)	0.0038 (7)	0.0014 (7)	0.0023 (7)
O1	0.0691 (13)	0.0194 (8)	0.0554 (11)	0.0126 (8)	−0.0126 (10)	0.0003 (7)
O2	0.0545 (12)	0.0220 (8)	0.0680 (13)	0.0009 (8)	−0.0133 (10)	−0.0091 (8)
O3	0.0638 (12)	0.0335 (9)	0.0334 (9)	0.0062 (9)	−0.0137 (8)	−0.0009 (7)
O4	0.0538 (12)	0.0345 (9)	0.0471 (11)	−0.0065 (8)	−0.0147 (9)	−0.0035 (8)

Geometric parameters (Å, º)

Ag1—N2	2.1663 (18)	C9—H9A	0.9300
Ag1—N1^{i}	2.207 (2)	C10—C11	1.379 (3)
Ag1—O1	2.3889 (18)	C10—H10A	0.9300
C1—N1	1.344 (3)	C11—C12	1.394 (3)
C1—C2	1.379 (4)	C11—H11A	0.9300
C1—H1A	0.9300	C12—N3	1.370 (3)
C2—C3	1.379 (3)	C13—O1	1.226 (3)
C2—H2A	0.9300	C13—O2	1.271 (3)
C3—C4	1.395 (3)	C13—C14	1.529 (3)
C3—H3B	0.9300	C14—C17^{ii}	1.390 (3)
C4—C5	1.386 (3)	C14—C15	1.407 (3)
C4—C6	1.468 (3)	C15—C17	1.391 (3)
C5—N1	1.344 (3)	C15—C16	1.518 (3)
C5—H5A	0.9300	C16—O3	1.239 (3)
C6—N3	1.347 (3)	C16—O4	1.277 (3)
C6—N2	1.342 (3)	C16—O4	1.277 (3)
C7—C8	1.397 (3)	C17—H17A	0.9300
C7—N2	1.395 (3)	N3—O3^{iii}	2.742 (3)
C7—C12	1.394 (3)	N3—H3A	0.8600
C8—C9	1.384 (4)	O2—O4	2.399 (3)
C8—H8A	0.9300	O2—H2B	0.846 (19)
C9—C10	1.400 (4)		
N2—Ag1—N1^{i}	150.61 (7)	C12—C11—H11A	121.9
N2—Ag1—O1	115.06 (7)	N3—C12—C11	131.3 (2)
N1^{i}—Ag1—O1	93.66 (7)	N3—C12—C7	106.02 (18)
N1—C1—C2	122.1 (2)	C11—C12—C7	122.7 (2)
N1—C1—H1A	118.9	O1—C13—O2	121.3 (2)
C2—C1—H1A	118.9	O1—C13—C14	118.2 (2)
C3—C2—C1	119.8 (2)	O2—C13—C14	120.5 (2)
C3—C2—H2A	120.1	C17^{ii}—C14—C15	117.68 (19)
C1—C2—H2A	120.1	C17^{ii}—C14—C13	113.86 (19)
C2—C3—C4	119.1 (2)	C15—C14—C13	128.5 (2)
C2—C3—H3B	120.4	C17—C15—C14	117.9 (2)
C4—C3—H3B	120.4	C17—C15—C16	114.22 (19)
C5—C4—C3	117.3 (2)	C14—C15—C16	127.83 (19)
C5—C4—C6	121.6 (2)	O3—C16—O4	122.1 (2)
C3—C4—C6	121.1 (2)	O3—C16—O4	122.1 (2)
N1—C5—C4	124.0 (2)	O3—C16—C15	118.0 (2)

N1—C5—H5A	118.0	O4—C16—C15	119.9 (2)
C4—C5—H5A	118.0	O4—C16—C15	119.9 (2)
N3—C6—N2	111.75 (19)	C15—C17—C14^{ii}	124.4 (2)
N3—C6—C4	122.18 (19)	C15—C17—H17A	117.8
N2—C6—C4	126.1 (2)	C14^{ii}—C17—H17A	117.8
C8—C7—N2	130.6 (2)	C5—N1—C1	117.7 (2)
C8—C7—C12	120.4 (2)	C5—N1—Ag1^{i}	123.69 (16)
N2—C7—C12	108.97 (19)	C1—N1—Ag1^{i}	118.53 (16)
C9—C8—C7	117.2 (2)	C6—N2—C7	105.18 (18)
C9—C8—H8A	121.4	C6—N2—Ag1	131.88 (15)
C7—C8—H8A	121.4	C7—N2—Ag1	119.44 (14)
C8—C9—C10	121.7 (2)	C6—N3—C12	108.07 (18)
C8—C9—H9A	119.2	C6—N3—O3^{iii}	129.98 (14)
C10—C9—H9A	119.2	C12—N3—O3^{iii}	119.74 (14)
C11—C10—C9	121.9 (2)	C6—N3—H3A	126.0
C11—C10—H10A	119.1	C12—N3—H3A	126.0
C9—C10—H10A	119.1	C13—O1—Ag1	125.98 (17)
C10—C11—C12	116.3 (2)	C13—O2—O4	110.37 (15)
C10—C11—H11A	121.9	C13—O2—H2B	111 (3)

N1—C1—C2—C3	0.3 (4)	C14—C15—C17—C14^{ii}	0.3 (4)
C1—C2—C3—C4	0.0 (4)	C16—C15—C17—C14^{ii}	−178.4 (2)
C2—C3—C4—C5	0.4 (3)	C4—C5—N1—C1	1.3 (4)
C2—C3—C4—C6	−179.0 (2)	C4—C5—N1—Ag1^{i}	−174.85 (17)
C3—C4—C5—N1	−1.1 (4)	C2—C1—N1—C5	−0.9 (4)
C6—C4—C5—N1	178.3 (2)	C2—C1—N1—Ag1^{i}	175.50 (19)
C5—C4—C6—N3	169.4 (2)	N3—C6—N2—C7	0.7 (2)
C3—C4—C6—N3	−11.2 (3)	C4—C6—N2—C7	−179.8 (2)
C5—C4—C6—N2	−10.2 (3)	N3—C6—N2—Ag1	158.67 (15)
C3—C4—C6—N2	169.2 (2)	C4—C6—N2—Ag1	−21.7 (3)
N2—C7—C8—C9	−179.8 (2)	C8—C7—N2—C6	179.0 (2)
C12—C7—C8—C9	−0.6 (3)	C12—C7—N2—C6	−0.3 (2)
C7—C8—C9—C10	−0.3 (4)	C8—C7—N2—Ag1	17.7 (3)
C8—C9—C10—C11	0.9 (4)	C12—C7—N2—Ag1	−161.64 (14)
C9—C10—C11—C12	−0.5 (4)	N1^{i}—Ag1—N2—C6	57.2 (3)
C10—C11—C12—N3	−179.8 (2)	O1—Ag1—N2—C6	−135.92 (19)
C10—C11—C12—C7	−0.4 (4)	N1^{i}—Ag1—N2—C7	−147.28 (17)
C8—C7—C12—N3	−179.5 (2)	O1—Ag1—N2—C7	19.57 (18)
N2—C7—C12—N3	−0.1 (2)	N2—C6—N3—C12	−0.8 (2)
C8—C7—C12—C11	0.9 (4)	C4—C6—N3—C12	179.6 (2)
N2—C7—C12—C11	−179.7 (2)	N2—C6—N3—O3^{iii}	−163.40 (15)
O1—C13—C14—C17^{ii}	−8.4 (3)	C4—C6—N3—O3^{iii}	17.0 (3)
O2—C13—C14—C17^{ii}	170.6 (2)	C11—C12—N3—C6	−180.0 (2)
O1—C13—C14—C15	172.0 (2)	C7—C12—N3—C6	0.5 (2)
O2—C13—C14—C15	−9.0 (4)	C11—C12—N3—O3^{iii}	−15.2 (3)
C17^{ii}—C14—C15—C17	−0.3 (4)	C7—C12—N3—O3^{iii}	165.26 (14)
C13—C14—C15—C17	179.3 (2)	O2—C13—O1—Ag1	−15.7 (4)
C17^{ii}—C14—C15—C16	178.2 (2)	C14—C13—O1—Ag1	163.34 (15)

C13—C14—C15—C16	−2.1 (4)	N2—Ag1—O1—C13	−85.5 (2)
C17—C15—C16—O3	15.1 (3)	N1^{i}—Ag1—O1—C13	88.1 (2)
C14—C15—C16—O3	−163.5 (2)	O1—C13—O2—O4	−175.0 (2)
C17—C15—C16—O4	−164.8 (2)	C14—C13—O2—O4	6.0 (3)
C14—C15—C16—O4	16.6 (4)	O3—C16—O4—O4	0.0 (4)
C17—C15—C16—O4	−164.8 (2)	C15—C16—O4—O4	0.0 (3)
C14—C15—C16—O4	16.6 (4)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) *x*+1/2, −*y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···O4	0.85 (2)	1.56 (2)	2.399 (3)	171 (4)
N3—H3*A*···O3^{iii}	0.86	1.92	2.742 (3)	159

Symmetry code: (iii) *x*+1/2, −*y*+1/2, *z*+1/2.