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Poly[piperazinediium [[aquabismuthate(III)]-di-μ-pyridine-2,6-dicarboxylato-bismuthate(III)-di-μ-pyridine-2,6-dicarboxylato] monohydrate]

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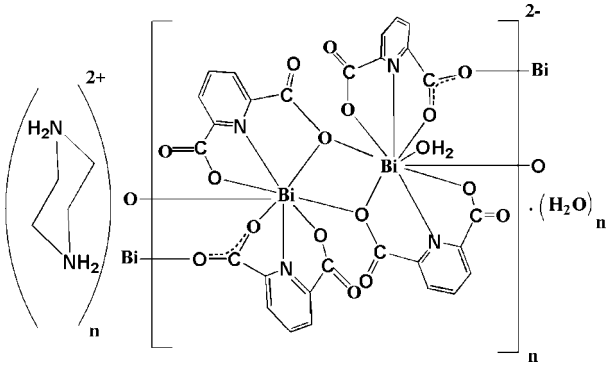
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.022; wR factor = 0.048; data-to-parameter ratio = 15.3.

The title compound, $\{(C_4H_{12}N_2)[Bi_2(C_7H_3NO_4)_4(H_2O)]\cdot H_2O\}_n$ or $\{(pipzH_2)[Bi_2(pydc)_4(H_2O)]\cdot H_2O\}_n$, where $pydcH_2$ is pyridine-2,6-dicarboxylic acid and pipz is piperazine, was obtained by reaction of $Bi(NO_3)_3\cdot 5H_2O$ with $(pipzH_2)(pydcH)_2\cdot 3H_2O$ in a 1:2 molar ratio in aqueous solution. There are two independent Bi^{III} atoms in the structure, one of which is eight-coordinate with a distorted bicapped trigonal-prismatic geometry, and another which is nine-coordinate with a distorted tricapped trigonal-prismatic geometry. The carboxylate groups of the $(pydc)^{2-}$ ligands link dinuclear $[Bi_2(C_7H_3NO_4)_4(H_2O)]^{2-}$ units into one-dimensional coordination polymers. The $pipzH_2^{2+}$ cations (site symmetry $\overline{1}$) and non-coordinated water molecules lie between these polymers, forming N—H···O and O—H···O hydrogen bonds to the O atoms of the carboxylate groups.

Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki, Ghadermazi *et al.* (2007); Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.* (2007); Aghabozorg, Motyeian *et al.* (2007); Aghabozorg, Daneshvar *et al.* (2007); Sharif *et al.* (2007); Sheshmani *et al.* (2006).



Experimental

Crystal data

$(C_4H_{12}N_2)[Bi_2(C_7H_3NO_4)_4(H_2O)]\cdot H_2O$
M_r = 1202.56
Triclinic, $P\overline{1}$
a = 10.8111 (4) Å
b = 12.1660 (5) Å
c = 14.0402 (5) Å
α = 96.094 (1)°
β = 93.169 (1)°
γ = 113.848 (1)°
V = 1669.65 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 10.62 mm^{-1}
T = 100 (2) K
0.15 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.204, T_{max} = 0.346
22723 measured reflections
8005 independent reflections
6952 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.048
S = 1.03
8005 reflections
523 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5N1···O2W^{i}	0.90	2.00	2.761 (4)	141
N5—H5N2···O6	0.90	1.86	2.722 (4)	160
N6—H6N1···O16^{ii}	0.90	1.78	2.676 (4)	176
N6—H6N2···O12	0.90	1.95	2.762 (4)	149
O1W—H1W1···O7	0.85	2.08	2.891 (3)	160
O1W—H1W2···O9^{iii}	0.85	2.53	3.337 (4)	158
O2W—H2W1···O14	0.85	2.04	2.887 (4)	176
O2W—H2W2···O5	0.85	2.35	3.162 (4)	159

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $-x-1, -y, -z$; (iii) $-x, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2264).

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supporting information

Acta Cryst. (2008). E**64**, m374 [doi:10.1107/S160053680800161X]

Poly[piperazinediium [[aquabismuthate(III)]-di-μ-pyridine-2,6-dicarboxylato-bismuthate(III)-di-μ-pyridine-2,6-dicarboxylato] monohydrate]

Hossein Aghabozorg, Andya Nemati, Zohreh Derikvand and Mohammad Ghadermazi

S1. Comment

The preparation and characterization of self-assembling systems have been considered by chemists in recent years. A literature review shows that the $(pydc)^{2-}$ ligand can form complexes with transition metals (Aghabozorg, Attar Gharamaleki, Ghadermazi *et al.*, 2007; Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.*, 2007; Aghabozorg, Motyeian *et al.*, 2007; Aghabozorg, Daneshvar *et al.*, 2007; Sharif *et al.*, 2007). In this work, $(pydc)^{2-}$ acts as tridentate ligand with one N atom of pyridine and two O atoms of carboxylates acting as donors and also has a bridging role between the binuclear units containing Bi1 and Bi2. The binuclear units consist of two Bi^{III} atoms, four $(pydc)^{2-}$ ligands, and one coordinated water molecule, while one $(pipzH_2)^{2+}$ cation and one uncoordinated water molecule are also present in the asymmetric unit (Fig. 1).

Two Bi1—O7—C14—O8—Bi2 bridging bonds between neighboring binuclear units link them together and form several rings with four Bi^{III} atoms, six O atoms and two C atoms (Fig. 2). Atom Bi1 is eight coordinated by two tridentate $(pydc)^{2-}$ ligands, one O atom from the Bi1—O9—Bi2 bridge and one O atom from the neighbouring carboxylate group ($Bi1—O14^{i}$ = 2.971 (3) Å, symmetry code: (i) -*x*, 1 - *y*, 1 - *z*). Atom Bi2 is nine coordinated by two tridentate $(pydc)^{2-}$ ligands, one O atom from the Bi1—O1—Bi2 bridge, one O atom from a coordinated water molecule (Bi2—O1W = 2.960 (3) Å) and one O atom from a neighbouring carboxylate group ($Bi2—O8^{ii}$ = 2.883 (2) Å, symmetry code: (ii) -*x*, 1 - *y*, -*z*). The sum of the van der Waals radii for Bi and O is 3.86 Å, which is significantly longer than the bond distances for $Bi1—O14^{i}$ and $Bi2—O8^{ii}$. The coordination polyhedron around Bi1 is a distorted bicapped trigonal prism which is nearly eclipsed, in which O1, O7, O9 and O3, O5, O14 form two triangles and N1 and N2 form two caps of the prism. The sum of the bond angles N3—Bi2—O1W (113.37 (8)°), O1W—Bi2—N4 (125.24 (8)°) and N4—Bi2—N3 (121.00 (9)°) is equal to 359.61°, indicating that Bi2 is located in the center of the O1W/N3/N4 plane. Atoms O8, O11, O15 and O1, O9, O13 build two triangles. So, a prism consisting of six O atoms and three caps (N3, N4 and O1W) on its faces is formed around Bi2, that is the coordination polyhedron may be described as a distorted tricapped trigonal prism.

N—H···O hydrogen bonds are formed between $(pipzH_2)^{2+}$ and the carboxylate groups (Table1) and also O—H···O hydrogen bonds are formed between uncoordinated water molecules and the carboxylate groups. In addition, C—H···O contacts with C···O distances ranging from 2.887 (4)Å to 3.656 (4) Å are observed between $(pipzH_2)^{2+}$ cations and carboxylate groups. There are C29—H29B···*Cg*1 interactions (3.638 (5) Å; *x*, *y* + 1, *z*), where *Cg*1 is the centroid of the N4/C23—C27 ring and also C32—H32B···*Cg*2 interactions (3.656 (5) Å; *x* - 1,*y*, *z*), where *Cg*2 is the centroid of the N2/C9—C13 ring (Fig. 3).

S2. Experimental

The proton transfer compound $(pipzH_2)(pydcH)_2.3H_2O$ was prepared by reaction of pyridine-2,6-dicarboxylic acid ($pydcH_2$) with piperazine (pipz) (Sheshmani *et al.*, 2006). A solution of $Bi(NO_3)_3.5H_2O$ (242 mg, 0.5 mmol) in water (25 ml) was added to $(pipzH_2)(pydcH)_2.3H_2O$ (253 mg, 1.0 mmol) in 25 ml water and colorless crystals were obtained by slow evaporation of the solvent at room temperature.

S3. Refinement

H atoms attached to O and N atoms were found in difference Fourier maps, then their distances were normalized to O—H = 0.85, N—H = 0.90 Å along the observed O/N—H vector. H atoms bound to C atoms were placed in calculated positions. All H atoms were then refined as riding with $U_{iso}(H) = 1.2U_{eq}(C/N)$ or $1.5U_{eq}(O)$.

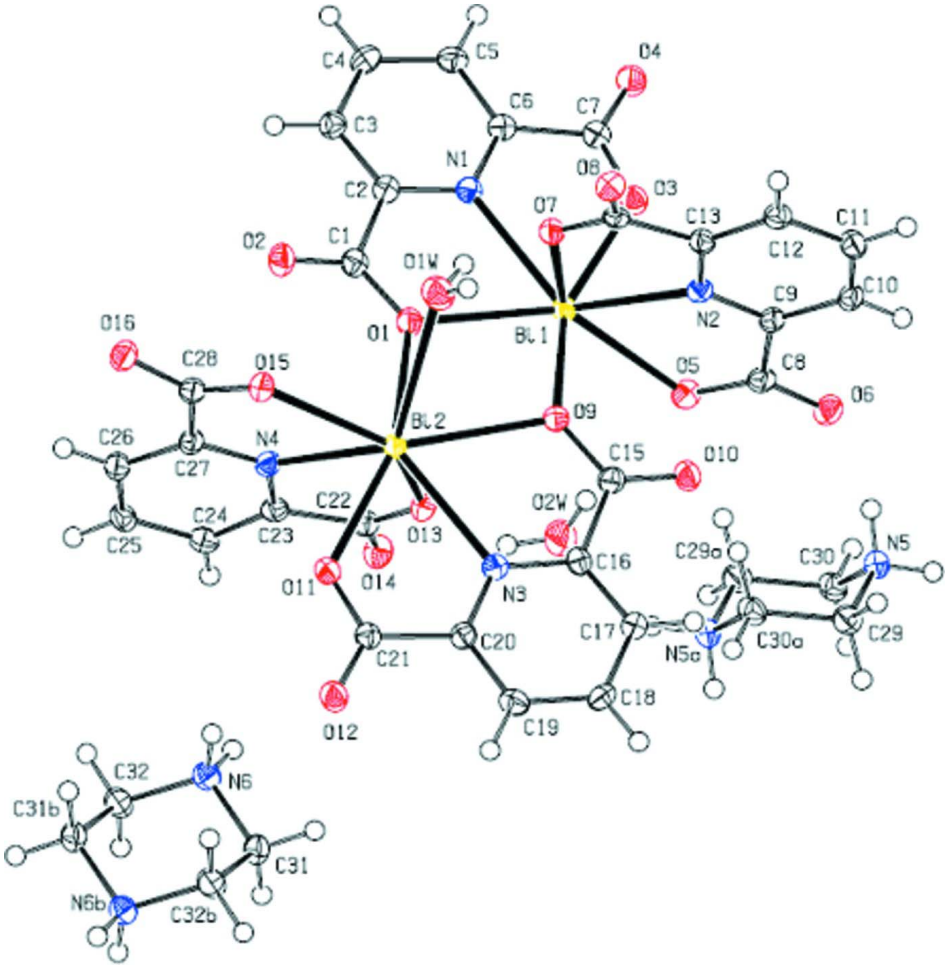

Figure 1

The asymmetric unit of the title compound with displacement ellipsoids drawn at 50% probability for non-H atoms.

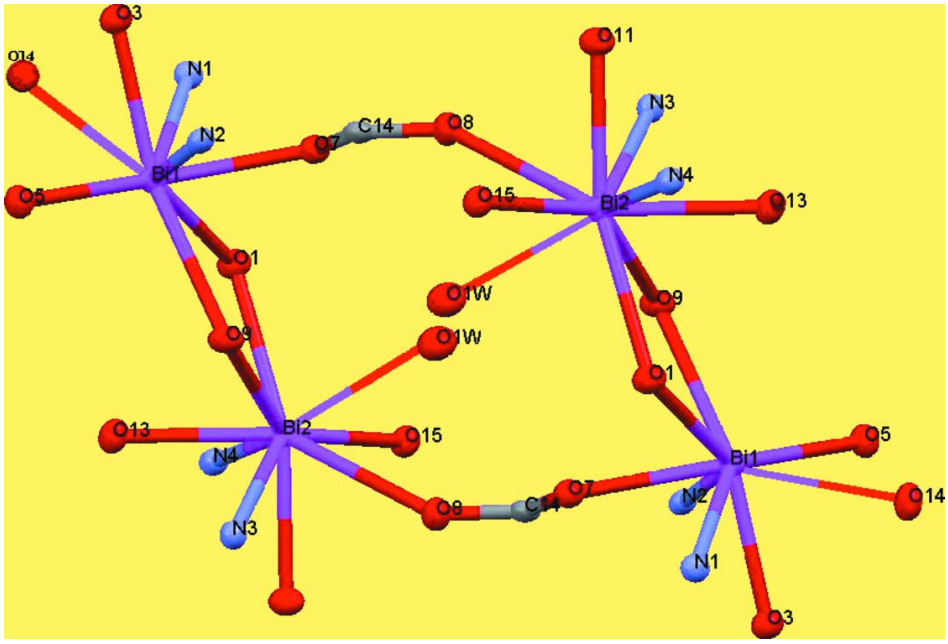

Figure 2

Rings of four Bi^{III} atoms within the 1-D coordination polymers.

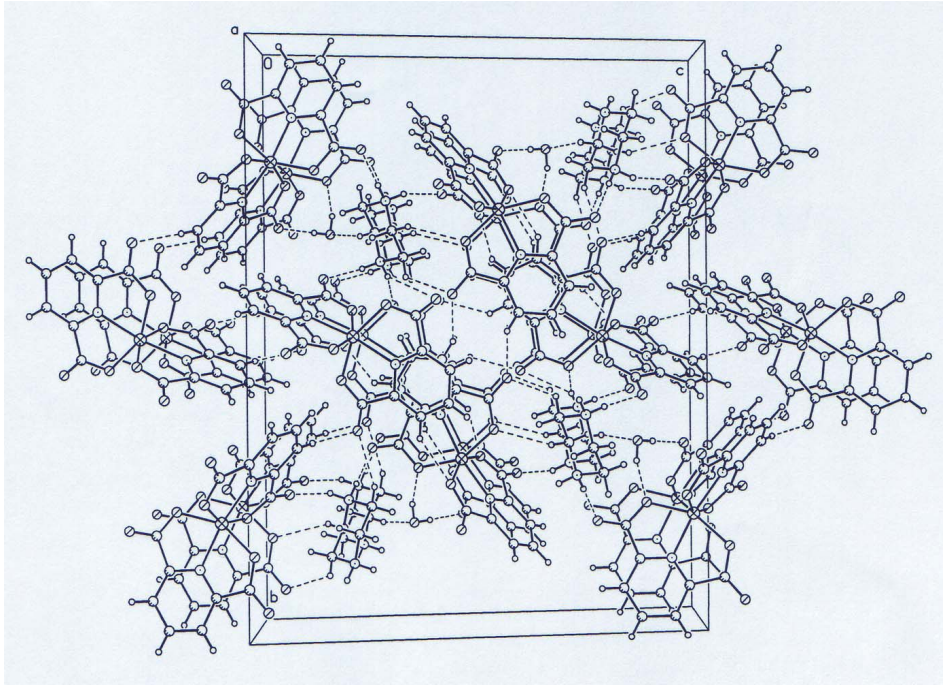

Figure 3

Crystal packing with hydrogen bonds shown as dashed lines.

Poly[piperazinediium [[aquabismuthate(III)]-di-μ-pyridine-2,6-dicarboxylato- bismuthate(III)-di-μ-pyridine-2,6-dicarboxylato] monohydrate]

Crystal data

$(C_4H_{12}N_2)[Bi_2(C_7H_3NO_4)_4(H_2O)]\cdot H_2O$
M_r = 1202.56
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 10.8111 (4) Å
b = 12.1660 (5) Å
c = 14.0402 (5) Å
α = 96.094 (1)°
β = 93.169 (1)°
γ = 113.848 (1)°
V = 1669.65 (11) Å^3
Z = 2
$F(000)$ = 1144
D_x = 2.392 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5207 reflections
θ = 2.6–29.4°
μ = 10.62 mm^{-1}
T = 100 K
Prism, colourless
0.15 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.204, T_{max} = 0.346
22723 measured reflections
8005 independent reflections
6952 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 28.0°, θ_{min} = 1.5°
h = −14→14
k = −16→16
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.048
S = 1.03
8005 reflections
523 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.019P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Bi1	0.187854 (12)	0.622892 (10)	0.307230 (9)	0.01470 (4)
Bi2	−0.184337 (12)	0.356548 (10)	0.178059 (9)	0.01477 (4)

O1	0.0427 (2)	0.3934 (2)	0.26028 (18)	0.0193 (5)
O2	0.0375 (3)	0.2059 (2)	0.23943 (18)	0.0225 (5)
O3	0.4159 (2)	0.7303 (2)	0.35552 (17)	0.0195 (5)
O4	0.6152 (3)	0.7375 (2)	0.41582 (19)	0.0246 (6)
O5	0.1821 (3)	0.8179 (2)	0.39201 (17)	0.0202 (5)
O6	0.2563 (3)	1.0190 (2)	0.39225 (18)	0.0228 (5)
O7	0.2296 (2)	0.5669 (2)	0.15750 (17)	0.0175 (5)
O8	0.2740 (3)	0.6124 (2)	0.01038 (17)	0.0207 (5)
O9	−0.0239 (2)	0.5885 (2)	0.20041 (18)	0.0196 (5)
O10	−0.0098 (2)	0.7798 (2)	0.21948 (19)	0.0225 (5)
O11	−0.4218 (2)	0.2606 (2)	0.15982 (18)	0.0203 (5)
O12	−0.6215 (2)	0.2613 (2)	0.11226 (19)	0.0234 (5)
O13	−0.1855 (3)	0.4370 (2)	0.33567 (17)	0.0193 (5)
O14	−0.2198 (3)	0.4114 (2)	0.48793 (18)	0.0228 (5)
O15	−0.2214 (2)	0.1481 (2)	0.10123 (17)	0.0183 (5)
O16	−0.2602 (3)	−0.0419 (2)	0.12412 (18)	0.0226 (5)
N1	0.3057 (3)	0.4903 (3)	0.3281 (2)	0.0165 (6)
N2	0.2716 (3)	0.7927 (2)	0.2211 (2)	0.0152 (6)
N3	−0.2965 (3)	0.4993 (2)	0.1700 (2)	0.0161 (6)
N4	−0.2525 (3)	0.2036 (2)	0.2842 (2)	0.0164 (6)
C1	0.0944 (4)	0.3157 (3)	0.2662 (2)	0.0180 (7)
C2	0.2423 (4)	0.3687 (3)	0.3098 (2)	0.0171 (7)
C3	0.3090 (4)	0.2964 (3)	0.3301 (2)	0.0191 (7)
H3A	0.2627	0.2105	0.3175	0.023*
C4	0.4432 (4)	0.3505 (3)	0.3688 (3)	0.0221 (7)
H4A	0.4899	0.3021	0.3841	0.026*
C5	0.5101 (4)	0.4771 (3)	0.3854 (3)	0.0204 (7)
H5A	0.6033	0.5165	0.4104	0.025*
C6	0.4356 (3)	0.5435 (3)	0.3640 (2)	0.0173 (7)
C7	0.4970 (3)	0.6814 (3)	0.3806 (2)	0.0174 (7)
C8	0.2402 (3)	0.9155 (3)	0.3569 (3)	0.0183 (7)
C9	0.2945 (3)	0.9050 (3)	0.2603 (2)	0.0160 (7)
C10	0.3618 (3)	1.0040 (3)	0.2131 (3)	0.0186 (7)
H10A	0.3786	1.0838	0.2414	0.022*
C11	0.4038 (4)	0.9842 (3)	0.1244 (3)	0.0213 (7)
H11A	0.4521	1.0509	0.0918	0.026*
C12	0.3756 (3)	0.8668 (3)	0.0827 (3)	0.0184 (7)
H12A	0.4016	0.8513	0.0209	0.022*
C13	0.3087 (3)	0.7735 (3)	0.1339 (2)	0.0169 (7)
C14	0.2686 (3)	0.6421 (3)	0.0956 (2)	0.0164 (7)
C15	−0.0753 (4)	0.6690 (3)	0.2024 (2)	0.0181 (7)
C16	−0.2269 (3)	0.6196 (3)	0.1788 (2)	0.0167 (7)
C17	−0.2899 (4)	0.6960 (3)	0.1640 (3)	0.0200 (7)
H17A	−0.2392	0.7816	0.1732	0.024*
C18	−0.4288 (4)	0.6453 (3)	0.1355 (3)	0.0213 (7)
H18A	−0.4743	0.6955	0.1229	0.026*
C19	−0.5008 (4)	0.5192 (3)	0.1255 (3)	0.0216 (7)
H19A	−0.5959	0.4819	0.1062	0.026*

C20	−0.4299 (3)	0.4504 (3)	0.1445 (2)	0.0173 (7)
C21	−0.4988 (3)	0.3139 (3)	0.1373 (2)	0.0169 (7)
C22	−0.2236 (3)	0.3715 (3)	0.4019 (3)	0.0181 (7)
C23	−0.2778 (3)	0.2360 (3)	0.3722 (2)	0.0169 (7)
C24	−0.3469 (3)	0.1508 (3)	0.4298 (2)	0.0182 (7)
H24A	−0.3693	0.1749	0.4907	0.022*
C25	−0.3832 (3)	0.0283 (3)	0.3965 (3)	0.0191 (7)
H25A	−0.4301	−0.0325	0.4348	0.023*
C26	−0.3498 (3)	−0.0034 (3)	0.3066 (3)	0.0183 (7)
H26A	−0.3702	−0.0858	0.2834	0.022*
C27	−0.2863 (3)	0.0871 (3)	0.2518 (2)	0.0167 (7)
C28	−0.2530 (3)	0.0622 (3)	0.1510 (3)	0.0184 (7)
N5	0.1037 (3)	1.1154 (3)	0.4887 (2)	0.0199 (6)
H5N1	0.1350	1.1969	0.4971	0.024*
H5N2	0.1704	1.0994	0.4636	0.024*
C29	−0.0256 (4)	1.0593 (3)	0.4221 (3)	0.0216 (7)
H29A	−0.0078	1.0848	0.3577	0.026*
H29B	−0.0931	1.0876	0.4471	0.026*
C30	0.0819 (4)	1.0776 (3)	0.5865 (3)	0.0210 (7)
H30A	0.0173	1.1065	0.6159	0.025*
H30B	0.1692	1.1143	0.6286	0.025*
N6	−0.8584 (3)	0.0656 (3)	0.0345 (2)	0.0192 (6)
H6N1	−0.8147	0.0590	−0.0171	0.023*
H6N2	−0.7844	0.1111	0.0761	0.023*
C31	−0.9440 (4)	0.1308 (3)	0.0061 (3)	0.0216 (7)
H31A	−0.8868	0.2061	−0.0189	0.026*
H31B	−0.9830	0.1534	0.0632	0.026*
C32	−0.9431 (4)	−0.0495 (3)	0.0703 (3)	0.0231 (8)
H32A	−0.9823	−0.0312	0.1287	0.028*
H32B	−0.8854	−0.0917	0.0878	0.028*
O1W	0.0082 (3)	0.3774 (2)	0.0319 (2)	0.0287 (6)
H1W1	0.0826	0.4211	0.0666	0.043*
H1W2	0.0135	0.4062	−0.0211	0.043*
O2W	−0.0696 (3)	0.6708 (2)	0.5000 (2)	0.0348 (7)
H2W1	−0.1177	0.5951	0.4969	0.052*
H2W2	−0.0142	0.6958	0.4583	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.01464 (7)	0.01425 (6)	0.01526 (7)	0.00582 (5)	0.00170 (5)	0.00288 (5)
Bi2	0.01454 (7)	0.01311 (6)	0.01629 (7)	0.00520 (5)	0.00116 (5)	0.00279 (5)
O1	0.0178 (12)	0.0164 (11)	0.0229 (13)	0.0061 (10)	0.0002 (10)	0.0041 (10)
O2	0.0236 (14)	0.0161 (11)	0.0245 (13)	0.0058 (10)	−0.0020 (11)	0.0011 (10)
O3	0.0184 (12)	0.0182 (11)	0.0207 (13)	0.0064 (10)	0.0001 (10)	0.0037 (10)
O4	0.0189 (13)	0.0227 (13)	0.0304 (15)	0.0072 (11)	−0.0034 (11)	0.0043 (11)
O5	0.0240 (13)	0.0219 (12)	0.0168 (12)	0.0112 (11)	0.0038 (10)	0.0043 (10)
O6	0.0265 (14)	0.0198 (12)	0.0238 (13)	0.0114 (11)	0.0052 (11)	0.0010 (10)

O7	0.0166 (12)	0.0164 (11)	0.0193 (12)	0.0065 (10)	0.0015 (10)	0.0035 (9)
O8	0.0232 (13)	0.0215 (12)	0.0180 (12)	0.0102 (11)	0.0017 (10)	0.0016 (10)
O9	0.0154 (12)	0.0173 (11)	0.0265 (13)	0.0069 (10)	0.0014 (10)	0.0049 (10)
O10	0.0180 (13)	0.0172 (12)	0.0287 (14)	0.0043 (10)	−0.0010 (11)	0.0033 (10)
O11	0.0161 (12)	0.0177 (11)	0.0258 (13)	0.0053 (10)	0.0019 (10)	0.0048 (10)
O12	0.0181 (13)	0.0197 (12)	0.0299 (14)	0.0052 (10)	−0.0018 (11)	0.0051 (10)
O13	0.0245 (13)	0.0161 (11)	0.0178 (12)	0.0091 (10)	−0.0005 (10)	0.0025 (9)
O14	0.0295 (14)	0.0201 (12)	0.0177 (13)	0.0100 (11)	0.0021 (11)	0.0000 (10)
O15	0.0207 (13)	0.0157 (11)	0.0182 (12)	0.0074 (10)	0.0007 (10)	0.0027 (9)
O16	0.0294 (14)	0.0185 (12)	0.0233 (13)	0.0122 (11)	0.0086 (11)	0.0048 (10)
N1	0.0167 (14)	0.0187 (13)	0.0154 (14)	0.0078 (12)	0.0025 (11)	0.0057 (11)
N2	0.0144 (14)	0.0173 (13)	0.0147 (14)	0.0077 (11)	−0.0016 (11)	0.0020 (11)
N3	0.0174 (14)	0.0177 (13)	0.0143 (14)	0.0079 (11)	0.0020 (11)	0.0032 (11)
N4	0.0157 (14)	0.0158 (13)	0.0181 (14)	0.0074 (11)	0.0000 (11)	0.0014 (11)
C1	0.0195 (18)	0.0192 (16)	0.0161 (17)	0.0080 (14)	0.0023 (14)	0.0050 (13)
C2	0.0215 (18)	0.0185 (16)	0.0123 (15)	0.0089 (14)	0.0039 (13)	0.0030 (12)
C3	0.0212 (18)	0.0184 (16)	0.0193 (17)	0.0092 (14)	0.0047 (14)	0.0034 (13)
C4	0.0236 (19)	0.0238 (17)	0.0235 (19)	0.0145 (15)	0.0005 (15)	0.0049 (14)
C5	0.0173 (17)	0.0251 (17)	0.0204 (18)	0.0100 (14)	0.0018 (14)	0.0042 (14)
C6	0.0185 (17)	0.0208 (16)	0.0136 (16)	0.0090 (14)	0.0022 (13)	0.0040 (13)
C7	0.0188 (17)	0.0200 (16)	0.0135 (16)	0.0078 (14)	0.0013 (13)	0.0034 (13)
C8	0.0159 (17)	0.0205 (16)	0.0200 (17)	0.0092 (14)	−0.0008 (14)	0.0031 (14)
C9	0.0149 (16)	0.0167 (15)	0.0175 (17)	0.0076 (13)	−0.0004 (13)	0.0029 (13)
C10	0.0162 (17)	0.0150 (15)	0.0240 (18)	0.0069 (13)	−0.0034 (14)	0.0014 (13)
C11	0.0173 (17)	0.0181 (16)	0.0267 (19)	0.0050 (14)	0.0015 (15)	0.0054 (14)
C12	0.0182 (17)	0.0208 (16)	0.0182 (17)	0.0095 (14)	0.0028 (14)	0.0050 (13)
C13	0.0143 (16)	0.0173 (15)	0.0187 (17)	0.0061 (13)	0.0007 (13)	0.0029 (13)
C14	0.0107 (15)	0.0185 (15)	0.0203 (17)	0.0065 (13)	0.0005 (13)	0.0020 (13)
C15	0.0188 (18)	0.0201 (16)	0.0178 (17)	0.0095 (14)	0.0026 (14)	0.0058 (13)
C16	0.0182 (17)	0.0163 (15)	0.0140 (16)	0.0054 (13)	0.0025 (13)	0.0028 (12)
C17	0.0189 (17)	0.0171 (16)	0.0244 (18)	0.0077 (14)	0.0031 (14)	0.0031 (14)
C18	0.0211 (18)	0.0194 (16)	0.0275 (19)	0.0126 (14)	0.0022 (15)	0.0027 (14)
C19	0.0163 (17)	0.0231 (17)	0.0237 (18)	0.0067 (14)	0.0018 (14)	0.0027 (14)
C20	0.0186 (17)	0.0165 (15)	0.0162 (16)	0.0071 (14)	0.0023 (13)	0.0006 (13)
C21	0.0179 (17)	0.0171 (15)	0.0154 (16)	0.0068 (13)	0.0027 (13)	0.0028 (13)
C22	0.0164 (17)	0.0182 (16)	0.0201 (17)	0.0076 (13)	0.0009 (13)	0.0023 (13)
C23	0.0146 (16)	0.0191 (16)	0.0171 (17)	0.0076 (13)	−0.0007 (13)	0.0015 (13)
C24	0.0152 (16)	0.0231 (17)	0.0150 (16)	0.0071 (14)	0.0000 (13)	0.0009 (13)
C25	0.0171 (17)	0.0194 (16)	0.0203 (18)	0.0059 (14)	0.0021 (14)	0.0074 (13)
C26	0.0175 (17)	0.0161 (15)	0.0203 (17)	0.0064 (13)	−0.0003 (14)	0.0029 (13)
C27	0.0153 (16)	0.0145 (15)	0.0199 (17)	0.0063 (13)	−0.0021 (13)	0.0015 (13)
C28	0.0140 (16)	0.0170 (15)	0.0237 (18)	0.0065 (13)	−0.0017 (14)	0.0024 (13)
N5	0.0190 (15)	0.0161 (13)	0.0242 (16)	0.0061 (12)	0.0037 (12)	0.0046 (12)
C29	0.0200 (18)	0.0232 (17)	0.0218 (18)	0.0087 (15)	0.0016 (14)	0.0054 (14)
C30	0.0167 (17)	0.0198 (16)	0.0216 (18)	0.0039 (14)	−0.0002 (14)	−0.0009 (14)
N6	0.0178 (15)	0.0197 (14)	0.0181 (15)	0.0060 (12)	0.0002 (12)	0.0025 (11)
C31	0.0225 (18)	0.0157 (16)	0.0247 (19)	0.0063 (14)	0.0034 (15)	0.0015 (14)
C32	0.0187 (18)	0.0221 (17)	0.0271 (19)	0.0059 (14)	0.0016 (15)	0.0079 (15)

O1W	0.0237 (14)	0.0264 (14)	0.0319 (15)	0.0067 (11)	0.0002 (12)	0.0035 (12)
O2W	0.0361 (17)	0.0240 (14)	0.0426 (18)	0.0106 (13)	0.0117 (14)	0.0016 (12)

Geometric parameters (Å, º)

Bi1—O7	2.266 (2)	C8—C9	1.521 (5)
Bi1—O3	2.295 (2)	C9—C10	1.390 (5)
Bi1—N2	2.385 (3)	C10—C11	1.379 (5)
Bi1—N1	2.456 (3)	C10—H10A	0.950
Bi1—O9	2.526 (2)	C11—C12	1.388 (5)
Bi1—O5	2.565 (2)	C11—H11A	0.950
Bi1—O1	2.578 (2)	C12—C13	1.376 (5)
Bi1—O14^{i}	2.971 (3)	C12—H12A	0.950
Bi2—O13	2.326 (2)	C13—C14	1.505 (4)
Bi2—O11	2.337 (2)	C15—C16	1.503 (5)
Bi2—N4	2.414 (3)	C16—C17	1.382 (5)
Bi2—N3	2.496 (3)	C17—C18	1.388 (5)
Bi2—O1	2.499 (2)	C17—H17A	0.950
Bi2—O15	2.512 (2)	C18—C19	1.398 (5)
Bi2—O9	2.620 (2)	C18—H18A	0.950
Bi2—O8^{ii}	2.883 (2)	C19—C20	1.379 (5)
Bi2—O1W	2.960 (3)	C19—H19A	0.950
O1—C1	1.285 (4)	C20—C21	1.510 (5)
O2—C1	1.227 (4)	C22—C23	1.511 (5)
O3—C7	1.295 (4)	C23—C24	1.380 (5)
O4—C7	1.223 (4)	C24—C25	1.397 (5)
O5—C8	1.266 (4)	C24—H24A	0.950
O6—C8	1.242 (4)	C25—C26	1.391 (5)
O7—C14	1.292 (4)	C25—H25A	0.950
O8—C14	1.224 (4)	C26—C27	1.380 (5)
O8—Bi2^{ii}	2.883 (2)	C26—H26A	0.950
O9—C15	1.306 (4)	C27—C28	1.509 (5)
O10—C15	1.231 (4)	N5—C30	1.496 (5)
O11—C21	1.290 (4)	N5—C29	1.497 (4)
O12—C21	1.228 (4)	N5—H5N1	0.900
O13—C22	1.267 (4)	N5—H5N2	0.900
O14—C22	1.244 (4)	C29—C30^{iii}	1.513 (5)
O14—Bi1^{i}	2.971 (3)	C29—H29A	0.990
O15—C28	1.260 (4)	C29—H29B	0.990
O16—C28	1.252 (4)	C30—C29^{iii}	1.513 (5)
N1—C6	1.328 (4)	C30—H30A	0.990
N1—C2	1.343 (4)	C30—H30B	0.990
N2—C13	1.336 (4)	N6—C32	1.488 (4)
N2—C9	1.336 (4)	N6—C31	1.505 (4)
N3—C20	1.328 (4)	N6—H6N1	0.900
N3—C16	1.335 (4)	N6—H6N2	0.900
N4—C27	1.333 (4)	C31—C32^{iv}	1.507 (5)
N4—C23	1.333 (4)	C31—H31A	0.990

C1—C2	1.523 (5)	C31—H31B	0.990
C2—C3	1.384 (5)	C32—C31^{iv}	1.507 (5)
C3—C4	1.378 (5)	C32—H32A	0.990
C3—H3A	0.950	C32—H32B	0.990
C4—C5	1.397 (5)	O1W—H1W1	0.850
C4—H4A	0.950	O1W—H1W2	0.850
C5—C6	1.394 (5)	O2W—H2W1	0.850
C5—H5A	0.950	O2W—H2W2	0.850
C6—C7	1.520 (5)		

O7—Bi1—O3	91.67 (8)	C5—C6—C7	122.4 (3)
O7—Bi1—N2	69.13 (9)	O4—C7—O3	125.1 (3)
O3—Bi1—N2	71.64 (9)	O4—C7—C6	119.6 (3)
O7—Bi1—N1	74.33 (9)	O3—C7—C6	115.3 (3)
O3—Bi1—N1	67.54 (9)	O6—C8—O5	127.0 (3)
N2—Bi1—N1	123.21 (9)	O6—C8—C9	116.3 (3)
O7—Bi1—O9	75.63 (8)	O5—C8—C9	116.7 (3)
O3—Bi1—O9	150.67 (8)	N2—C9—C10	120.8 (3)
N2—Bi1—O9	79.11 (8)	N2—C9—C8	115.7 (3)
N1—Bi1—O9	130.88 (8)	C10—C9—C8	123.5 (3)
O7—Bi1—O5	133.72 (8)	C11—C10—C9	118.9 (3)
O3—Bi1—O5	80.95 (8)	C11—C10—H10A	120.6
N2—Bi1—O5	65.17 (8)	C9—C10—H10A	120.6
N1—Bi1—O5	139.27 (8)	C10—C11—C12	120.0 (3)
O9—Bi1—O5	88.88 (8)	C10—C11—H11A	120.0
O7—Bi1—O1	71.85 (8)	C12—C11—H11A	120.0
O3—Bi1—O1	131.37 (8)	C13—C12—C11	117.7 (3)
N2—Bi1—O1	134.97 (8)	C13—C12—H12A	121.1
N1—Bi1—O1	64.02 (8)	C11—C12—H12A	121.1
O9—Bi1—O1	70.14 (8)	N2—C13—C12	122.4 (3)
O5—Bi1—O1	142.67 (8)	N2—C13—C14	114.6 (3)
O7—Bi1—O14^{i}	142.66 (8)	C12—C13—C14	122.9 (3)
O3—Bi1—O14^{i}	75.43 (8)	O8—C14—O7	124.1 (3)
N2—Bi1—O14^{i}	134.51 (8)	O8—C14—C13	120.0 (3)
N1—Bi1—O14^{i}	68.34 (8)	O7—C14—C13	115.8 (3)
O9—Bi1—O14^{i}	129.79 (8)	O10—C15—O9	125.5 (3)
O5—Bi1—O14^{i}	79.51 (7)	O10—C15—C16	118.7 (3)
O1—Bi1—O14^{i}	90.47 (7)	O9—C15—C16	115.8 (3)
O13—Bi2—O11	90.55 (9)	N3—C16—C17	121.9 (3)
O13—Bi2—N4	67.58 (9)	N3—C16—C15	117.2 (3)
O11—Bi2—N4	72.05 (9)	C17—C16—C15	120.8 (3)
O13—Bi2—N3	72.91 (9)	C16—C17—C18	118.6 (3)
O11—Bi2—N3	66.29 (9)	C16—C17—H17A	120.7
N4—Bi2—N3	121.00 (9)	C18—C17—H17A	120.7
O13—Bi2—O1	75.37 (8)	C17—C18—C19	119.1 (3)
O11—Bi2—O1	151.73 (8)	C17—C18—H18A	120.5
N4—Bi2—O1	79.89 (9)	C19—C18—H18A	120.5
N3—Bi2—O1	129.27 (8)	C20—C19—C18	118.1 (3)

O13—Bi2—O15	132.74 (8)	C20—C19—H19A	120.9
O11—Bi2—O15	79.38 (8)	C18—C19—H19A	120.9
N4—Bi2—O15	65.37 (8)	N3—C20—C19	122.5 (3)
N3—Bi2—O15	138.11 (8)	N3—C20—C21	115.3 (3)
O1—Bi2—O15	92.19 (7)	C19—C20—C21	122.1 (3)
O13—Bi2—O9	72.26 (8)	O12—C21—O11	124.5 (3)
O11—Bi2—O9	129.51 (8)	O12—C21—C20	119.4 (3)
N4—Bi2—O9	134.46 (8)	O11—C21—C20	116.1 (3)
N3—Bi2—O9	63.32 (8)	O14—C22—O13	124.5 (3)
O1—Bi2—O9	69.86 (8)	O14—C22—C23	119.0 (3)
O15—Bi2—O9	145.72 (8)	O13—C22—C23	116.4 (3)
O13—Bi2—O8^{ii}	135.52 (7)	N4—C23—C24	121.6 (3)
O11—Bi2—O8^{ii}	73.14 (8)	N4—C23—C22	114.2 (3)
N4—Bi2—O8^{ii}	137.85 (8)	C24—C23—C22	124.1 (3)
N3—Bi2—O8^{ii}	62.62 (8)	C23—C24—C25	118.5 (3)
O1—Bi2—O8^{ii}	133.56 (8)	C23—C24—H24A	120.8
O15—Bi2—O8^{ii}	85.53 (7)	C25—C24—H24A	120.8
O9—Bi2—O8^{ii}	86.61 (7)	C26—C25—C24	119.0 (3)
O13—Bi2—O1W	139.60 (8)	C26—C25—H25A	120.5
O11—Bi2—O1W	129.27 (8)	C24—C25—H25A	120.5
N4—Bi2—O1W	125.24 (8)	C27—C26—C25	118.7 (3)
N3—Bi2—O1W	113.37 (8)	C27—C26—H26A	120.7
O1—Bi2—O1W	70.76 (8)	C25—C26—H26A	120.7
O15—Bi2—O1W	70.62 (7)	N4—C27—C26	121.7 (3)
O9—Bi2—O1W	75.85 (7)	N4—C27—C28	115.2 (3)
O8^{ii}—Bi2—O1W	64.79 (7)	C26—C27—C28	123.1 (3)
C1—O1—Bi2	127.3 (2)	O16—C28—O15	125.9 (3)
C1—O1—Bi1	121.4 (2)	O16—C28—C27	117.2 (3)
Bi2—O1—Bi1	110.39 (9)	O15—C28—C27	116.9 (3)
C7—O3—Bi1	124.1 (2)	C30—N5—C29	111.4 (3)
C8—O5—Bi1	118.5 (2)	C30—N5—H5N1	106.3
C14—O7—Bi1	122.1 (2)	C29—N5—H5N1	110.5
C14—O8—Bi2^{ii}	140.2 (2)	C30—N5—H5N2	111.7
C15—O9—Bi1	122.0 (2)	C29—N5—H5N2	111.4
C15—O9—Bi2	120.3 (2)	H5N1—N5—H5N2	105.1
Bi1—O9—Bi2	108.23 (9)	N5—C29—C30^{iii}	110.0 (3)
C21—O11—Bi2	123.5 (2)	N5—C29—H29A	109.7
C22—O13—Bi2	122.5 (2)	C30^{iii}—C29—H29A	109.7
C22—O14—Bi1^{i}	147.0 (2)	N5—C29—H29B	109.7
C28—O15—Bi2	119.9 (2)	C30^{iii}—C29—H29B	109.7
C6—N1—C2	120.1 (3)	H29A—C29—H29B	108.2
C6—N1—Bi1	117.1 (2)	N5—C30—C29^{iii}	109.5 (3)
C2—N1—Bi1	122.8 (2)	N5—C30—H30A	109.8
C13—N2—C9	120.1 (3)	C29^{iii}—C30—H30A	109.8
C13—N2—Bi1	116.9 (2)	N5—C30—H30B	109.8
C9—N2—Bi1	122.7 (2)	C29^{iii}—C30—H30B	109.8
C20—N3—C16	119.7 (3)	H30A—C30—H30B	108.2
C20—N3—Bi2	116.9 (2)	C32—N6—C31	110.7 (3)

C16—N3—Bi2	122.9 (2)	C32—N6—H6N1	116.6
C27—N4—C23	120.3 (3)	C31—N6—H6N1	105.6
C27—N4—Bi2	121.4 (2)	C32—N6—H6N2	111.5
C23—N4—Bi2	117.3 (2)	C31—N6—H6N2	114.5
O2—C1—O1	126.6 (3)	H6N1—N6—H6N2	97.4
O2—C1—C2	118.3 (3)	N6—C31—C32^{iv}	109.6 (3)
O1—C1—C2	115.1 (3)	N6—C31—H31A	109.7
N1—C2—C3	121.2 (3)	C32^{iv}—C31—H31A	109.8
N1—C2—C1	116.5 (3)	N6—C31—H31B	109.7
C3—C2—C1	122.3 (3)	C32^{iv}—C31—H31B	109.7
C4—C3—C2	119.3 (3)	H31A—C31—H31B	108.2
C4—C3—H3A	120.4	N6—C32—C31^{iv}	110.3 (3)
C2—C3—H3A	120.4	N6—C32—H32A	109.6
C3—C4—C5	119.5 (3)	C31^{iv}—C32—H32A	109.6
C3—C4—H4A	120.3	N6—C32—H32B	109.6
C5—C4—H4A	120.3	C31^{iv}—C32—H32B	109.6
C6—C5—C4	117.8 (3)	H32A—C32—H32B	108.1
C6—C5—H5A	121.1	Bi2—O1W—H1W1	99.6
C4—C5—H5A	121.1	Bi2—O1W—H1W2	130.1
N1—C6—C5	122.2 (3)	H1W1—O1W—H1W2	106.1
N1—C6—C7	115.4 (3)	H2W1—O2W—H2W2	119.0

O13—Bi2—O1—C1	124.0 (3)	O13—Bi2—N3—C16	79.3 (3)
O11—Bi2—O1—C1	61.7 (3)	O11—Bi2—N3—C16	177.7 (3)
N4—Bi2—O1—C1	54.7 (3)	N4—Bi2—N3—C16	128.7 (2)
N3—Bi2—O1—C1	176.7 (3)	O1—Bi2—N3—C16	25.6 (3)
O15—Bi2—O1—C1	−9.8 (3)	O15—Bi2—N3—C16	−144.6 (2)
O9—Bi2—O1—C1	−159.9 (3)	O9—Bi2—N3—C16	1.0 (2)
O8^{ii}—Bi2—O1—C1	−95.7 (3)	O8^{ii}—Bi2—N3—C16	−99.7 (3)
O1W—Bi2—O1—C1	−78.4 (3)	O1W—Bi2—N3—C16	−58.0 (3)
O13—Bi2—O1—Bi1	−67.02 (10)	O13—Bi2—N4—C27	179.2 (3)
O11—Bi2—O1—Bi1	−129.36 (14)	O11—Bi2—N4—C27	80.9 (3)
N4—Bi2—O1—Bi1	−136.30 (11)	N3—Bi2—N4—C27	127.4 (2)
N3—Bi2—O1—Bi1	−14.30 (15)	O1—Bi2—N4—C27	−102.5 (3)
O15—Bi2—O1—Bi1	159.20 (10)	O15—Bi2—N4—C27	−5.4 (2)
O9—Bi2—O1—Bi1	9.11 (8)	O9—Bi2—N4—C27	−150.8 (2)
O8^{ii}—Bi2—O1—Bi1	73.28 (12)	O8^{ii}—Bi2—N4—C27	45.2 (3)
O1W—Bi2—O1—Bi1	90.61 (10)	O1W—Bi2—N4—C27	−44.9 (3)
O7—Bi1—O1—C1	79.5 (3)	O13—Bi2—N4—C23	10.5 (2)
O3—Bi1—O1—C1	3.8 (3)	O11—Bi2—N4—C23	−87.8 (2)
N2—Bi1—O1—C1	110.5 (3)	N3—Bi2—N4—C23	−41.3 (3)
N1—Bi1—O1—C1	−1.5 (2)	O1—Bi2—N4—C23	88.7 (2)
O9—Bi1—O1—C1	160.3 (3)	O15—Bi2—N4—C23	−174.1 (3)
O5—Bi1—O1—C1	−140.2 (2)	O9—Bi2—N4—C23	40.4 (3)
O14^{i}—Bi1—O1—C1	−67.0 (3)	O8^{ii}—Bi2—N4—C23	−123.5 (2)
O7—Bi1—O1—Bi2	−90.28 (10)	O1W—Bi2—N4—C23	146.3 (2)
O3—Bi1—O1—Bi2	−165.93 (9)	Bi2—O1—C1—O2	−6.5 (5)
N2—Bi1—O1—Bi2	−59.29 (15)	Bi1—O1—C1—O2	−174.4 (3)

N1—Bi1—O1—Bi2	−171.27 (13)	Bi2—O1—C1—C2	172.4 (2)
O9—Bi1—O1—Bi2	−9.44 (9)	Bi1—O1—C1—C2	4.5 (4)
O5—Bi1—O1—Bi2	50.04 (16)	C6—N1—C2—C3	1.8 (5)
O14^{i}—Bi1—O1—Bi2	123.22 (9)	Bi1—N1—C2—C3	−174.4 (2)
O7—Bi1—O3—C7	−79.5 (3)	C6—N1—C2—C1	−178.4 (3)
N2—Bi1—O3—C7	−146.9 (3)	Bi1—N1—C2—C1	5.3 (4)
N1—Bi1—O3—C7	−7.2 (2)	O2—C1—C2—N1	172.7 (3)
O9—Bi1—O3—C7	−142.5 (2)	O1—C1—C2—N1	−6.3 (5)
O5—Bi1—O3—C7	146.4 (3)	O2—C1—C2—C3	−7.6 (5)
O1—Bi1—O3—C7	−12.4 (3)	O1—C1—C2—C3	173.5 (3)
O14^{i}—Bi1—O3—C7	65.0 (3)	N1—C2—C3—C4	−0.7 (5)
O7—Bi1—O5—C8	−18.4 (3)	C1—C2—C3—C4	179.5 (3)
O3—Bi1—O5—C8	65.2 (2)	C2—C3—C4—C5	−1.0 (5)
N2—Bi1—O5—C8	−8.7 (2)	C3—C4—C5—C6	1.7 (5)
N1—Bi1—O5—C8	104.1 (3)	C2—N1—C6—C5	−1.1 (5)
O9—Bi1—O5—C8	−87.2 (2)	Bi1—N1—C6—C5	175.4 (3)
O1—Bi1—O5—C8	−141.3 (2)	C2—N1—C6—C7	179.3 (3)
O14^{i}—Bi1—O5—C8	141.9 (3)	Bi1—N1—C6—C7	−4.3 (4)
O3—Bi1—O7—C14	−73.4 (2)	C4—C5—C6—N1	−0.7 (5)
N2—Bi1—O7—C14	−3.8 (2)	C4—C5—C6—C7	178.9 (3)
N1—Bi1—O7—C14	−139.5 (3)	Bi1—O3—C7—O4	−172.1 (3)
O9—Bi1—O7—C14	79.8 (2)	Bi1—O3—C7—C6	7.7 (4)
O5—Bi1—O7—C14	5.6 (3)	N1—C6—C7—O4	178.1 (3)
O1—Bi1—O7—C14	153.2 (3)	C5—C6—C7—O4	−1.5 (5)
O14^{i}—Bi1—O7—C14	−141.3 (2)	N1—C6—C7—O3	−1.6 (4)
O7—Bi1—O9—C15	−129.3 (3)	C5—C6—C7—O3	178.7 (3)
O3—Bi1—O9—C15	−62.6 (3)	Bi1—O5—C8—O6	−174.0 (3)
N2—Bi1—O9—C15	−58.3 (3)	Bi1—O5—C8—C9	6.9 (4)
N1—Bi1—O9—C15	176.9 (2)	C13—N2—C9—C10	−2.6 (5)
O5—Bi1—O9—C15	6.6 (3)	Bi1—N2—C9—C10	170.4 (2)
O1—Bi1—O9—C15	155.1 (3)	C13—N2—C9—C8	176.3 (3)
O14^{i}—Bi1—O9—C15	81.9 (3)	Bi1—N2—C9—C8	−10.7 (4)
O7—Bi1—O9—Bi2	84.45 (9)	O6—C8—C9—N2	−177.4 (3)
O3—Bi1—O9—Bi2	151.22 (13)	O5—C8—C9—N2	1.8 (4)
N2—Bi1—O9—Bi2	155.47 (11)	O6—C8—C9—C10	1.5 (5)
N1—Bi1—O9—Bi2	30.64 (15)	O5—C8—C9—C10	−179.3 (3)
O5—Bi1—O9—Bi2	−139.62 (9)	N2—C9—C10—C11	0.5 (5)
O1—Bi1—O9—Bi2	8.88 (8)	C8—C9—C10—C11	−178.2 (3)
O14^{i}—Bi1—O9—Bi2	−64.28 (12)	C9—C10—C11—C12	1.6 (5)
O13—Bi2—O9—C15	−75.6 (2)	C10—C11—C12—C13	−1.7 (5)
O11—Bi2—O9—C15	−0.1 (3)	C9—N2—C13—C12	2.5 (5)
N4—Bi2—O9—C15	−104.6 (3)	Bi1—N2—C13—C12	−170.9 (3)
N3—Bi2—O9—C15	3.8 (2)	C9—N2—C13—C14	−176.1 (3)
O1—Bi2—O9—C15	−156.1 (3)	Bi1—N2—C13—C14	10.5 (4)
O15—Bi2—O9—C15	141.7 (2)	C11—C12—C13—N2	−0.3 (5)
O8^{ii}—Bi2—O9—C15	64.7 (2)	C11—C12—C13—C14	178.2 (3)
O1W—Bi2—O9—C15	129.5 (3)	Bi2^{ii}—O8—C14—O7	128.7 (3)
O13—Bi2—O9—Bi1	71.32 (10)	Bi2^{ii}—O8—C14—C13	−51.2 (5)

O11—Bi2—O9—Bi1	146.80 (9)	Bi1—O7—C14—O8	−169.4 (2)
N4—Bi2—O9—Bi1	42.35 (15)	Bi1—O7—C14—C13	10.5 (4)
N3—Bi2—O9—Bi1	150.68 (12)	N2—C13—C14—O8	166.2 (3)
O1—Bi2—O9—Bi1	−9.18 (8)	C12—C13—C14—O8	−12.4 (5)
O15—Bi2—O9—Bi1	−71.42 (16)	N2—C13—C14—O7	−13.7 (4)
O8^{ii}—Bi2—O9—Bi1	−148.38 (9)	C12—C13—C14—O7	167.7 (3)
O1W—Bi2—O9—Bi1	−83.55 (9)	Bi1—O9—C15—O10	32.0 (5)
O13—Bi2—O11—C21	83.7 (3)	Bi2—O9—C15—O10	174.4 (3)
N4—Bi2—O11—C21	149.8 (3)	Bi1—O9—C15—C16	−149.7 (2)
N3—Bi2—O11—C21	12.7 (2)	Bi2—O9—C15—C16	−7.4 (4)
O1—Bi2—O11—C21	142.7 (2)	C20—N3—C16—C17	1.3 (5)
O15—Bi2—O11—C21	−142.8 (3)	Bi2—N3—C16—C17	173.0 (3)
O9—Bi2—O11—C21	16.4 (3)	C20—N3—C16—C15	−176.7 (3)
O8^{ii}—Bi2—O11—C21	−54.3 (2)	Bi2—N3—C16—C15	−4.9 (4)
O1W—Bi2—O11—C21	−88.9 (3)	O10—C15—C16—N3	−173.6 (3)
O11—Bi2—O13—C22	67.3 (3)	O9—C15—C16—N3	8.1 (5)
N4—Bi2—O13—C22	−3.0 (2)	O10—C15—C16—C17	8.5 (5)
N3—Bi2—O13—C22	132.2 (3)	O9—C15—C16—C17	−169.9 (3)
O1—Bi2—O13—C22	−87.9 (3)	N3—C16—C17—C18	−2.6 (5)
O15—Bi2—O13—C22	−8.7 (3)	C15—C16—C17—C18	175.3 (3)
O9—Bi2—O13—C22	−161.0 (3)	C16—C17—C18—C19	1.9 (5)
O8^{ii}—Bi2—O13—C22	133.4 (2)	C17—C18—C19—C20	−0.1 (5)
O1W—Bi2—O13—C22	−121.6 (3)	C16—N3—C20—C19	0.7 (5)
O13—Bi2—O15—C28	3.6 (3)	Bi2—N3—C20—C19	−171.5 (3)
O11—Bi2—O15—C28	−77.2 (2)	C16—N3—C20—C21	−179.6 (3)
N4—Bi2—O15—C28	−2.2 (2)	Bi2—N3—C20—C21	8.1 (4)
N3—Bi2—O15—C28	−111.9 (3)	C18—C19—C20—N3	−1.3 (5)
O1—Bi2—O15—C28	75.6 (2)	C18—C19—C20—C21	179.1 (3)
O9—Bi2—O15—C28	131.8 (2)	Bi2—O11—C21—O12	167.7 (3)
O8^{ii}—Bi2—O15—C28	−150.9 (2)	Bi2—O11—C21—C20	−13.3 (4)
O1W—Bi2—O15—C28	144.3 (3)	N3—C20—C21—O12	−178.5 (3)
O7—Bi1—N1—C6	104.3 (3)	C19—C20—C21—O12	1.1 (5)
O3—Bi1—N1—C6	5.7 (2)	N3—C20—C21—O11	2.4 (4)
N2—Bi1—N1—C6	53.0 (3)	C19—C20—C21—O11	−177.9 (3)
O9—Bi1—N1—C6	158.5 (2)	Bi1^{i}—O14—C22—O13	−149.2 (3)
O5—Bi1—N1—C6	−36.5 (3)	Bi1^{i}—O14—C22—C23	31.2 (6)
O1—Bi1—N1—C6	−178.6 (3)	Bi2—O13—C22—O14	176.5 (3)
O14^{i}—Bi1—N1—C6	−76.9 (2)	Bi2—O13—C22—C23	−3.9 (4)
O7—Bi1—N1—C2	−79.4 (3)	C27—N4—C23—C24	−4.3 (5)
O3—Bi1—N1—C2	−178.0 (3)	Bi2—N4—C23—C24	164.6 (3)
N2—Bi1—N1—C2	−130.7 (2)	C27—N4—C23—C22	175.3 (3)
O9—Bi1—N1—C2	−25.1 (3)	Bi2—N4—C23—C22	−15.9 (4)
O5—Bi1—N1—C2	139.9 (2)	O14—C22—C23—N4	−167.1 (3)
O1—Bi1—N1—C2	−2.3 (2)	O13—C22—C23—N4	13.3 (4)
O14^{i}—Bi1—N1—C2	99.4 (3)	O14—C22—C23—C24	12.5 (5)
O7—Bi1—N2—C13	−4.3 (2)	O13—C22—C23—C24	−167.2 (3)
O3—Bi1—N2—C13	94.9 (2)	N4—C23—C24—C25	4.0 (5)
N1—Bi1—N2—C13	49.2 (3)	C22—C23—C24—C25	−175.5 (3)

O9—Bi1—N2—C13	−82.9 (2)	C23—C24—C25—C26	−0.6 (5)
O5—Bi1—N2—C13	−176.8 (3)	C24—C25—C26—C27	−2.4 (5)
O1—Bi1—N2—C13	−35.8 (3)	C23—N4—C27—C26	1.1 (5)
O14^{i}—Bi1—N2—C13	140.6 (2)	Bi2—N4—C27—C26	−167.3 (3)
O7—Bi1—N2—C9	−177.5 (3)	C23—N4—C27—C28	179.7 (3)
O3—Bi1—N2—C9	−78.3 (2)	Bi2—N4—C27—C28	11.3 (4)
N1—Bi1—N2—C9	−124.0 (2)	C25—C26—C27—N4	2.3 (5)
O9—Bi1—N2—C9	103.9 (3)	C25—C26—C27—C28	−176.2 (3)
O5—Bi1—N2—C9	10.0 (2)	Bi2—O15—C28—O16	−172.0 (3)
O1—Bi1—N2—C9	150.9 (2)	Bi2—O15—C28—C27	8.5 (4)
O14^{i}—Bi1—N2—C9	−32.6 (3)	N4—C27—C28—O16	167.6 (3)
O13—Bi2—N3—C20	−108.7 (3)	C26—C27—C28—O16	−13.8 (5)
O11—Bi2—N3—C20	−10.3 (2)	N4—C27—C28—O15	−12.9 (4)
N4—Bi2—N3—C20	−59.3 (3)	C26—C27—C28—O15	165.7 (3)
O1—Bi2—N3—C20	−162.4 (2)	C30—N5—C29—C30^{iii}	−58.4 (4)
O15—Bi2—N3—C20	27.4 (3)	C29—N5—C30—C29^{iii}	58.0 (4)
O9—Bi2—N3—C20	172.9 (3)	C32—N6—C31—C32^{iv}	−58.1 (4)
O8^{ii}—Bi2—N3—C20	72.2 (2)	C31—N6—C32—C31^{iv}	58.5 (4)
O1W—Bi2—N3—C20	114.0 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*N*1···O2*W*^{iii}	0.90	2.00	2.761 (4)	141
N5—H5*N*2···O6	0.90	1.86	2.722 (4)	160
N6—H6*N*1···O16^{v}	0.90	1.78	2.676 (4)	176
N6—H6*N*2···O12	0.90	1.95	2.762 (4)	149
O1*W*—H1*W*1···O7	0.85	2.08	2.891 (3)	160
O1*W*—H1*W*2···O9^{ii}	0.85	2.53	3.337 (4)	158
O2*W*—H2*W*1···O14	0.85	2.04	2.887 (4)	176
O2*W*—H2*W*2···O5	0.85	2.35	3.162 (4)	159

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