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Bis(μ-2-hydroxybenzoato-κ^2O:O')bis-[(2,2′-bipyridine-κ^2N,N')bis(2-hydroxybenzoato-κ^2O,O')bismuth(III)]

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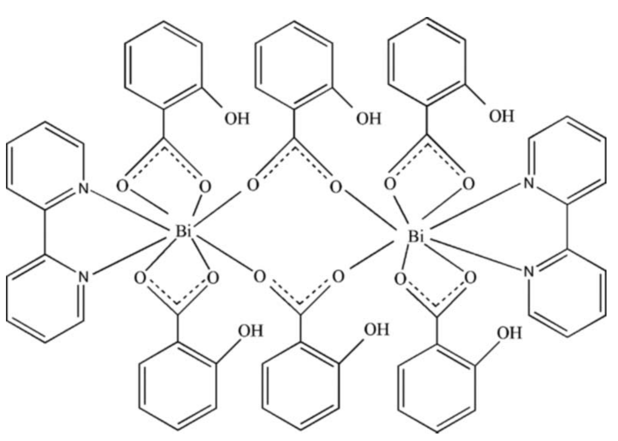
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.025; wR factor = 0.063; data-to-parameter ratio = 13.7.

The structure of the title compound, $[Bi_2(C_7H_5O_3)_6(C_{10}H_8N_2)_2]$, consists of centrosymmetric dimeric units in which salicylate ligands bridge two metal centres. The Bi atom is eight-coordinated, with Bi—O and Bi—N bond lengths in the ranges 2.377 (3)–3.044 (3) and 2.387 (3)–2.511 (3) Å, respectively. Each of the salicylate ligands shows an intramolecular hydrogen bond.

Related literature

For related literature, see: Briand & Burford (1999); Guo & Sadler (1999); Sadler *et al.* (1999); Suerbaum & Michetti (2003); Thompson & Orvig (2003); Thurston *et al.* (2002).



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Experimental

Crystal data

$[Bi_2(C_7H_5O_3)_6(C_{10}H_8N_2)_2]$
M_r = 1552.98
Monoclinic, $C2/c$
a = 21.4583 (3) Å
b = 13.6698 (2) Å
c = 21.6097 (1) Å
β = 117.72 (1)°
V = 5624.00 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.33 mm^{-1}
T = 293 (2) K
0.2 × 0.1 × 0.1 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.486, T_{max} = 1.000 (expected range = 0.258–0.531)
14948 measured reflections
5322 independent reflections
4590 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.063
S = 1.07
5322 reflections
388 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Bi1—O7	2.377 (3)	C2—O3	1.325 (8)
Bi1—N2	2.387 (3)	O4—C14	1.269 (5)
Bi1—O5	2.392 (3)	O2—C7	1.253 (5)
Bi1—N1	2.511 (3)	O6—C9	1.342 (6)
Bi1—O2	2.520 (3)	O7—C21	1.283 (5)
Bi1—O1	2.568 (3)	C8—C14	1.473 (6)
Bi1—O4	2.705 (3)	O8—C21	1.262 (5)
Bi1—O8^i	2.801 (3)	O5—C14	1.277 (5)
O1—C7	1.278 (5)		
O7—Bi1—N2	81.88 (11)	O7—Bi1—O1	76.31 (10)
O7—Bi1—O5	76.88 (11)	N2—Bi1—O1	72.50 (11)
N2—Bi1—O5	78.22 (11)	O2—Bi1—O1	51.16 (10)
N2—Bi1—N1	67.01 (11)	O5—Bi1—O4	51.00 (9)
O5—Bi1—N1	73.19 (11)	N1—Bi1—O4	75.21 (11)
N2—Bi1—O2	77.66 (11)	N1—Bi1—O8^i	79.84 (10)
N1—Bi1—O2	70.90 (11)	O4—Bi1—O8^i	65.86 (9)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2330).

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supplementary materials

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Bis(μ-2-hydroxybenzoato-κ^2O:O')bis[(2,2'-bipyridine-κ^2N,N')bis(2-hydroxybenzoato-κ^2O,O')bismuth(III)]

Y.-J. Wang, J. Zhao, Z.-H. Dang and L. Xu

Comment

Bismuth compounds have long been associated with medicine and healthcare for the treatment of various diseases (Thompson & Orvig, 2003; Suerbaum & Michetti, 2003; Briand & Burford, 1999). Bismuth subsalicylate is used to treat some digestive tract disorders such as gastric ulcers and is effective against Helicobacter pylori infection (Guo & Sadler, 1999; Sadler *et al.*, 1999). In the present study, we have synthesized and characterized an isomer of the previously reported compound bis[[(μ_2-salicylato-O,*O*')(2,2'- bipyridine)bis(salicylate)bismuth(III)]toluene] (Thurston *et al.*, 2002).

The asymmetric unit of the title compound is composed of one Bi atom, one 2,2'-bipyridine ligand and three salicylate ligands (Fig. 1). The Bi atoms have

two terminal salicylate ligands that chelate the metal through their carboxylate functionality. A third salicylate ion bridges two Bi atoms to form a dimer (Fig.2). The Bi—*O*(carboxylate) bond lengths range from 2.377 (3) to 2.801 (3) Å. The two N atoms of the 2,2'-bipyridine ligand coordinate to the Bi atom with bond lengths of 2.387 (3) and 2.511 (3) Å.

Each of the salicylate ligands shows an intramolecular H bond.

Experimental

A methanolic solution of $[Bi(Hsal)_3]_n$ (Hsal = $O_2CC_6H_4$-2-OH) was carefully layered with a methanolic solution of 2,2'-bipyridine. The colourless solution was allowed to stand undisturbed at room temperature for one week, during which time large colourless crystals of the title compound deposited on the wall of the tube.

Refinement

All H atoms were included in calculated positions, with C—H = 0.93 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*O*).

Figures

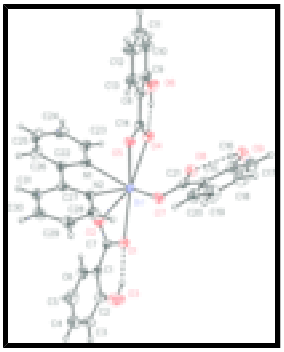


Fig. 1. A view of the asymmetric unit of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

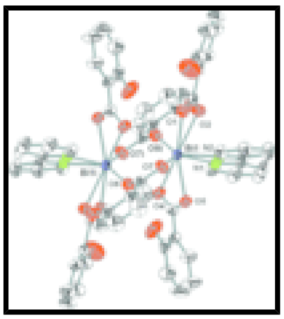


Fig. 2. Dimeric units of the title compound. [Symmetry code: (i) 1 − *x*, −*y*, −*z*.]

Bis(μ-2-hydroxybenzoato-κ^2*O*:*O*')bis[(2,2'-bipyridine-κ^2*N*,*N*')bis(2- hydroxybenzoato-κ^2*O*,*O*')bismuth(III)]

Crystal data

$[Bi_2(C_7H_5O_3)_6(C_{10}H_8N_2)_2]$	F_{000} = 3024
M_r = 1552.98	D_x = 1.834 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 21.4583 (3) Å	Cell parameters from 14948 reflections
b = 13.6698 (2) Å	θ = 1.8–25.6°
c = 21.60970 (10) Å	μ = 6.33 mm^{-1}
β = 117.4720 (10)°	*T* = 293 (2) K
V = 5624.00 (12) Å^3	Block, colourless
Z = 4	0.2 × 0.1 × 0.1 mm

Data collection

Bruker SMART CCD area-detector diffractometer	5322 independent reflections
Radiation source: fine-focus sealed tube	4590 reflections with *I* > 2σ(*I*)
Monochromator: graphite	R_{int} = 0.028
T = 293(2) K	$θ_{max}$ = 25.6°
φ and ω scans	$θ_{min}$ = 1.8°
Absorption correction: empirical (using intensity measurements)	*h* = −26→18

(SADABS; Sheldrick, 1996)	
T_{min} = 0.486, T_{max} = 1.000	k = −14→16
14948 measured reflections	l = −24→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.025	H-atom parameters constrained
$wR(F^2)$ = 0.063	$w = 1/[\sigma^2(F_o^2) + (0.0258P)^2 + 23.4426P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.003
5322 reflections	$\Delta\rho_{max}$ = 0.81 e Å^{-3}
388 parameters	$\Delta\rho_{min}$ = −1.26 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.557548 (7)	−0.053031 (12)	−0.039024 (7)	0.02992 (6)
C1	0.5214 (2)	−0.3657 (3)	−0.0917 (3)	0.0446 (12)
N1	0.68538 (18)	−0.0770 (3)	0.04387 (18)	0.0349 (8)
O1	0.50042 (16)	−0.1969 (2)	−0.12275 (17)	0.0445 (8)
C2	0.4803 (3)	−0.3989 (5)	−0.1598 (4)	0.0662 (16)
O4	0.58818 (17)	0.0884 (3)	0.05826 (16)	0.0428 (7)
N2	0.62695 (18)	−0.0854 (3)	−0.09692 (17)	0.0318 (8)
O2	0.58232 (17)	−0.2334 (2)	−0.01744 (16)	0.0444 (8)
C3	0.4740 (4)	−0.4984 (6)	−0.1734 (5)	0.104 (3)
H3A	0.4470	−0.5199	−0.2189	0.125*
C4	0.5059 (5)	−0.5651 (5)	−0.1225 (7)	0.108 (3)
H4A	0.5025	−0.6314	−0.1333	0.130*
O3	0.4454 (3)	−0.3395 (4)	−0.2132 (3)	0.1076 (19)
H3B	0.4530	−0.2826	−0.1998	0.161*
C5	0.5443 (4)	−0.5338 (5)	−0.0534 (6)	0.095 (3)

H5A	0.5638	−0.5798	−0.0178	0.113*
C6	0.5535 (3)	−0.4343 (4)	−0.0374 (4)	0.0620 (17)
H6A	0.5804	−0.4136	0.0084	0.074*
O6	0.6500 (2)	0.2041 (4)	0.16486 (18)	0.0753 (13)
H6B	0.6269	0.1566	0.1431	0.113*
C7	0.5352 (2)	−0.2600 (3)	−0.0758 (2)	0.0357 (10)
O7	0.48413 (17)	0.0242 (2)	−0.14704 (16)	0.0454 (8)
C8	0.6552 (2)	0.2260 (3)	0.0570 (2)	0.0364 (10)
O8	0.45182 (16)	0.1136 (2)	−0.08025 (16)	0.0422 (7)
C9	0.6689 (2)	0.2569 (4)	0.1239 (3)	0.0491 (12)
O5	0.61390 (16)	0.1012 (2)	−0.02946 (15)	0.0393 (7)
C10	0.7060 (3)	0.3428 (5)	0.1511 (3)	0.0734 (19)
H10A	0.7147	0.3640	0.1952	0.088*
O9	0.36991 (19)	0.2678 (3)	−0.13324 (18)	0.0556 (9)
H10B	0.3921	0.2278	−0.1027	0.083*
C11	0.7299 (4)	0.3963 (5)	0.1127 (4)	0.083 (2)
H11A	0.7540	0.4543	0.1310	0.099*
C12	0.7190 (4)	0.3663 (5)	0.0476 (4)	0.0771 (19)
H12A	0.7368	0.4024	0.0229	0.093*
C13	0.6815 (3)	0.2823 (4)	0.0198 (3)	0.0546 (13)
H13A	0.6733	0.2623	−0.0244	0.065*
C14	0.6168 (2)	0.1345 (3)	0.0270 (2)	0.0340 (9)
C15	0.4140 (2)	0.1663 (3)	−0.1969 (2)	0.0383 (10)
C16	0.3771 (2)	0.2473 (4)	−0.1911 (2)	0.0420 (11)
C17	0.3459 (3)	0.3119 (4)	−0.2465 (3)	0.0544 (13)
H17A	0.3210	0.3653	−0.2427	0.065*
C18	0.3513 (3)	0.2983 (5)	−0.3067 (3)	0.0651 (16)
H18A	0.3303	0.3428	−0.3431	0.078*
C19	0.3876 (3)	0.2187 (5)	−0.3139 (3)	0.0677 (17)
H19A	0.3916	0.2097	−0.3545	0.081*
C20	0.4177 (3)	0.1531 (4)	−0.2592 (2)	0.0527 (13)
H20A	0.4411	0.0987	−0.2641	0.063*
C21	0.4519 (2)	0.0972 (3)	−0.1377 (2)	0.0344 (9)
C22	0.7282 (2)	−0.1021 (3)	0.0166 (2)	0.0337 (9)
C23	0.7133 (2)	−0.0643 (4)	0.1133 (2)	0.0441 (11)
H23A	0.6838	−0.0475	0.1324	0.053*
C24	0.7843 (3)	−0.0755 (4)	0.1572 (3)	0.0527 (13)
H24A	0.8023	−0.0658	0.2050	0.063*
C25	0.8278 (3)	−0.1012 (5)	0.1290 (3)	0.0568 (14)
H25A	0.8757	−0.1093	0.1576	0.068*
C26	0.7999 (2)	−0.1150 (4)	0.0581 (3)	0.0487 (12)
H26A	0.8286	−0.1326	0.0383	0.058*
C27	0.6946 (2)	−0.1129 (3)	−0.0610 (2)	0.0327 (9)
C28	0.5949 (3)	−0.0908 (4)	−0.1671 (2)	0.0432 (11)
H28A	0.5481	−0.0719	−0.1916	0.052*
C29	0.6293 (3)	−0.1232 (4)	−0.2037 (3)	0.0484 (12)
H29A	0.6064	−0.1243	−0.2522	0.058*
C30	0.6978 (3)	−0.1540 (4)	−0.1674 (3)	0.0501 (12)
H30A	0.7213	−0.1781	−0.1911	0.060*

C31	0.7314 (2)	−0.1489 (4)	−0.0953 (3)	0.0429 (11)
H31A	0.7779	−0.1692	−0.0700	0.051*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.02658 (9)	0.03395 (10)	0.02873 (9)	−0.00108 (7)	0.01234 (7)	−0.00507 (7)
C1	0.032 (2)	0.034 (3)	0.070 (3)	−0.0048 (19)	0.025 (2)	−0.009 (2)
N1	0.0298 (18)	0.040 (2)	0.0309 (18)	−0.0038 (15)	0.0108 (15)	−0.0025 (15)
O1	0.0339 (16)	0.044 (2)	0.0443 (18)	0.0015 (14)	0.0083 (14)	−0.0036 (15)
C2	0.048 (3)	0.058 (4)	0.079 (4)	−0.006 (3)	0.017 (3)	−0.027 (3)
O4	0.0433 (18)	0.049 (2)	0.0395 (17)	−0.0098 (15)	0.0222 (15)	−0.0006 (15)
N2	0.0301 (18)	0.036 (2)	0.0293 (18)	−0.0007 (15)	0.0134 (15)	−0.0029 (15)
O2	0.0482 (19)	0.0413 (19)	0.0378 (17)	−0.0042 (15)	0.0148 (15)	−0.0065 (14)
C3	0.071 (5)	0.069 (5)	0.151 (8)	−0.024 (4)	0.034 (5)	−0.070 (6)
C4	0.074 (5)	0.042 (4)	0.204 (11)	−0.014 (4)	0.060 (6)	−0.039 (6)
O3	0.101 (4)	0.097 (4)	0.076 (3)	−0.003 (3)	−0.001 (3)	−0.038 (3)
C5	0.068 (4)	0.047 (4)	0.172 (9)	0.003 (3)	0.059 (5)	0.019 (5)
C6	0.051 (3)	0.041 (3)	0.106 (5)	−0.001 (2)	0.047 (4)	0.008 (3)
O6	0.064 (2)	0.128 (4)	0.041 (2)	−0.041 (3)	0.0304 (19)	−0.030 (2)
C7	0.028 (2)	0.040 (3)	0.043 (3)	−0.0014 (19)	0.020 (2)	−0.007 (2)
O7	0.0451 (18)	0.0417 (19)	0.0389 (17)	0.0097 (15)	0.0105 (15)	−0.0041 (14)
C8	0.033 (2)	0.036 (3)	0.037 (2)	−0.0035 (18)	0.0127 (19)	−0.0045 (19)
O8	0.0476 (18)	0.0439 (19)	0.0367 (17)	0.0040 (15)	0.0207 (15)	0.0061 (14)
C9	0.034 (2)	0.065 (4)	0.046 (3)	−0.006 (2)	0.017 (2)	−0.017 (2)
O5	0.0432 (17)	0.0426 (19)	0.0347 (16)	−0.0098 (14)	0.0201 (14)	−0.0088 (14)
C10	0.065 (4)	0.078 (5)	0.072 (4)	−0.023 (3)	0.027 (3)	−0.044 (4)
O9	0.065 (2)	0.051 (2)	0.055 (2)	0.0181 (18)	0.0319 (19)	0.0082 (17)
C11	0.082 (5)	0.043 (4)	0.101 (6)	−0.021 (3)	0.023 (4)	−0.017 (4)
C12	0.091 (5)	0.048 (4)	0.080 (4)	−0.026 (3)	0.029 (4)	0.008 (3)
C13	0.059 (3)	0.044 (3)	0.052 (3)	−0.011 (2)	0.018 (3)	0.004 (2)
C14	0.034 (2)	0.036 (3)	0.031 (2)	−0.0019 (18)	0.0141 (18)	−0.0006 (18)
C15	0.031 (2)	0.042 (3)	0.035 (2)	−0.0033 (19)	0.0092 (18)	0.001 (2)
C16	0.035 (2)	0.044 (3)	0.043 (3)	0.000 (2)	0.014 (2)	0.002 (2)
C17	0.051 (3)	0.045 (3)	0.054 (3)	0.006 (2)	0.014 (3)	0.010 (2)
C18	0.068 (4)	0.065 (4)	0.045 (3)	0.007 (3)	0.011 (3)	0.022 (3)
C19	0.074 (4)	0.087 (5)	0.037 (3)	0.011 (3)	0.021 (3)	0.012 (3)
C20	0.052 (3)	0.061 (4)	0.040 (3)	0.007 (3)	0.017 (2)	0.003 (2)
C21	0.027 (2)	0.033 (2)	0.036 (2)	−0.0046 (18)	0.0083 (18)	−0.0016 (19)
C22	0.028 (2)	0.032 (2)	0.040 (2)	−0.0027 (17)	0.0150 (18)	0.0056 (19)
C23	0.039 (2)	0.057 (3)	0.034 (2)	−0.007 (2)	0.014 (2)	−0.002 (2)
C24	0.042 (3)	0.066 (4)	0.036 (3)	−0.008 (2)	0.007 (2)	0.005 (2)
C25	0.030 (2)	0.080 (4)	0.046 (3)	0.001 (3)	0.006 (2)	0.013 (3)
C26	0.031 (2)	0.066 (4)	0.048 (3)	0.002 (2)	0.017 (2)	0.009 (3)
C27	0.033 (2)	0.030 (2)	0.036 (2)	−0.0010 (17)	0.0165 (18)	0.0031 (18)
C28	0.043 (3)	0.056 (3)	0.030 (2)	−0.001 (2)	0.017 (2)	−0.007 (2)
C29	0.060 (3)	0.054 (3)	0.038 (3)	−0.002 (2)	0.028 (2)	−0.008 (2)
C30	0.058 (3)	0.051 (3)	0.055 (3)	0.000 (2)	0.038 (3)	−0.009 (2)

C31	0.039 (2)	0.043 (3)	0.054 (3)	0.002 (2)	0.028 (2)	−0.001 (2)

Geometric parameters (Å, °)

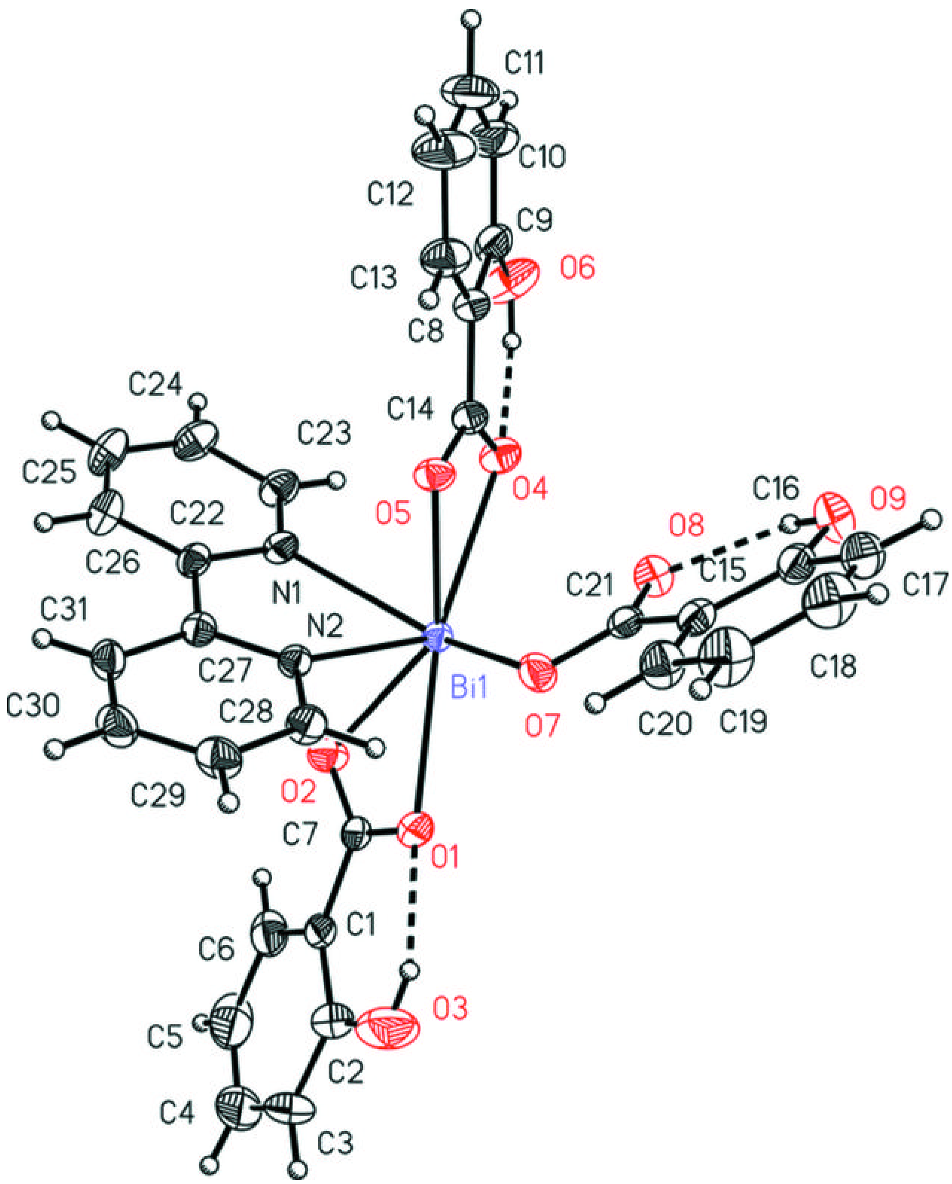
Bi1—O7	2.377 (3)	C10—C11	1.370 (10)
Bi1—N2	2.387 (3)	C10—H10A	0.9300
Bi1—O5	2.392 (3)	O9—C16	1.358 (6)
Bi1—N1	2.511 (3)	O9—H10B	0.8200
Bi1—O2	2.520 (3)	C11—C12	1.377 (10)
Bi1—O1	2.568 (3)	C11—H11A	0.9300
Bi1—O4	2.705 (3)	C12—C13	1.371 (8)
Bi1—O8^{i}	2.801 (3)	C12—H12A	0.9300
C1—C2	1.399 (8)	C13—H13A	0.9300
C1—C6	1.409 (8)	C15—C20	1.397 (7)
C1—C7	1.482 (6)	C15—C16	1.400 (7)
N1—C23	1.345 (6)	C15—C21	1.493 (6)
N1—C22	1.346 (5)	C16—C17	1.386 (7)
O1—C7	1.278 (5)	C17—C18	1.370 (8)
C2—O3	1.325 (8)	C17—H17A	0.9300
C2—C3	1.385 (9)	C18—C19	1.389 (9)
O4—C14	1.269 (5)	C18—H18A	0.9300
N2—C27	1.347 (5)	C19—C20	1.383 (7)
N2—C28	1.347 (5)	C19—H19A	0.9300
O2—C7	1.253 (5)	C20—H20A	0.9300
C3—C4	1.346 (13)	C22—C26	1.389 (6)
C3—H3A	0.9300	C22—C27	1.494 (6)
C4—C5	1.398 (13)	C23—C24	1.383 (7)
C4—H4A	0.9300	C23—H23A	0.9300
O3—H3B	0.8200	C24—C25	1.375 (8)
C5—C6	1.395 (9)	C24—H24A	0.9300
C5—H5A	0.9300	C25—C26	1.377 (7)
C6—H6A	0.9300	C25—H25A	0.9300
O6—C9	1.342 (6)	C26—H26A	0.9300
O6—H6B	0.8200	C27—C31	1.399 (6)
O7—C21	1.283 (5)	C28—C29	1.381 (6)
C8—C9	1.401 (6)	C28—H28A	0.9300
C8—C13	1.405 (7)	C29—C30	1.375 (7)
C8—C14	1.473 (6)	C29—H29A	0.9300
O8—C21	1.262 (5)	C30—C31	1.384 (7)
O8—Bi1^{i}	2.801 (3)	C30—H30A	0.9300
C9—C10	1.388 (8)	C31—H31A	0.9300
O5—C14	1.277 (5)		
O7—Bi1—N2	81.88 (11)	C14—O5—Bi1	101.3 (3)
O7—Bi1—O5	76.88 (11)	C11—C10—C9	119.8 (6)
N2—Bi1—O5	78.22 (11)	C11—C10—H10A	120.1
O7—Bi1—N1	140.29 (12)	C9—C10—H10A	120.1
N2—Bi1—N1	67.01 (11)	C16—O9—H10B	109.5
O5—Bi1—N1	73.19 (11)	C10—C11—C12	121.6 (6)

O7—Bi1—O2	127.14 (11)	C10—C11—H11A	119.2
N2—Bi1—O2	77.66 (11)	C12—C11—H11A	119.2
O5—Bi1—O2	142.33 (11)	C13—C12—C11	119.1 (6)
N1—Bi1—O2	70.90 (11)	C13—C12—H12A	120.5
O7—Bi1—O1	76.31 (10)	C11—C12—H12A	120.5
N2—Bi1—O1	72.50 (11)	C12—C13—C8	121.2 (5)
O5—Bi1—O1	142.54 (10)	C12—C13—H13A	119.4
N1—Bi1—O1	114.34 (11)	C8—C13—H13A	119.4
O2—Bi1—O1	51.16 (10)	O4—C14—O5	120.6 (4)
O7—Bi1—O4	105.02 (10)	O4—C14—C8	119.8 (4)
N2—Bi1—O4	123.59 (10)	O5—C14—C8	119.6 (4)
O5—Bi1—O4	51.00 (9)	C20—C15—C16	118.3 (4)
N1—Bi1—O4	75.21 (11)	C20—C15—C21	119.6 (4)
O2—Bi1—O4	126.92 (10)	C16—C15—C21	122.0 (4)
O1—Bi1—O4	163.90 (10)	O9—C16—C17	116.7 (5)
O7—Bi1—O8^{i}	137.59 (10)	O9—C16—C15	123.7 (4)
N2—Bi1—O8^{i}	138.97 (11)	C17—C16—C15	119.6 (5)
O5—Bi1—O8^{i}	115.41 (10)	C18—C17—C16	121.0 (5)
N1—Bi1—O8^{i}	79.84 (10)	C18—C17—H17A	119.5
O2—Bi1—O8^{i}	68.84 (10)	C16—C17—H17A	119.5
O1—Bi1—O8^{i}	102.03 (10)	C17—C18—C19	120.7 (5)
O4—Bi1—O8^{i}	65.86 (9)	C17—C18—H18A	119.7
C2—C1—C6	119.3 (5)	C19—C18—H18A	119.7
C2—C1—C7	121.4 (5)	C20—C19—C18	118.6 (5)
C6—C1—C7	119.2 (5)	C20—C19—H19A	120.7
C23—N1—C22	118.6 (4)	C18—C19—H19A	120.7
C23—N1—Bi1	123.8 (3)	C19—C20—C15	121.8 (5)
C22—N1—Bi1	117.5 (3)	C19—C20—H20A	119.1
C7—O1—Bi1	92.5 (3)	C15—C20—H20A	119.1
O3—C2—C3	117.2 (7)	O8—C21—O7	122.6 (4)
O3—C2—C1	123.1 (6)	O8—C21—C15	118.9 (4)
C3—C2—C1	119.6 (7)	O7—C21—C15	118.5 (4)
C14—O4—Bi1	86.9 (2)	N1—C22—C26	121.7 (4)
C27—N2—C28	119.3 (4)	N1—C22—C27	116.3 (4)
C27—N2—Bi1	121.1 (3)	C26—C22—C27	122.0 (4)
C28—N2—Bi1	118.8 (3)	N1—C23—C24	122.3 (5)
C7—O2—Bi1	95.5 (3)	N1—C23—H23A	118.9
C4—C3—C2	121.9 (8)	C24—C23—H23A	118.9
C4—C3—H3A	119.0	C25—C24—C23	118.8 (5)
C2—C3—H3A	119.0	C25—C24—H24A	120.6
C3—C4—C5	119.5 (7)	C23—C24—H24A	120.6
C3—C4—H4A	120.3	C24—C25—C26	119.5 (5)
C5—C4—H4A	120.3	C24—C25—H25A	120.2
C2—O3—H3B	109.5	C26—C25—H25A	120.2
C6—C5—C4	120.6 (8)	C25—C26—C22	119.0 (5)
C6—C5—H5A	119.7	C25—C26—H26A	120.5
C4—C5—H5A	119.7	C22—C26—H26A	120.5

C5—C6—C1	118.9 (7)	N2—C27—C31	121.0 (4)
C5—C6—H6A	120.6	N2—C27—C22	116.9 (4)
C1—C6—H6A	120.6	C31—C27—C22	122.1 (4)
C9—O6—H6B	109.5	N2—C28—C29	122.2 (5)
O2—C7—O1	120.5 (4)	N2—C28—H28A	118.9
O2—C7—C1	119.9 (4)	C29—C28—H28A	118.9
O1—C7—C1	119.6 (4)	C30—C29—C28	118.9 (5)
C21—O7—Bi1	110.6 (3)	C30—C29—H29A	120.5
C9—C8—C13	118.4 (4)	C28—C29—H29A	120.5
C9—C8—C14	121.2 (4)	C29—C30—C31	119.5 (4)
C13—C8—C14	120.3 (4)	C29—C30—H30A	120.2
C21—O8—Bi1^{i}	152.4 (3)	C31—C30—H30A	120.2
O6—C9—C10	117.8 (5)	C30—C31—C27	119.0 (4)
O6—C9—C8	122.3 (5)	C30—C31—H31A	120.5
C10—C9—C8	119.9 (5)	C27—C31—H31A	120.5

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

Fig. 1


C11
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O7
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C19
C29
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C7
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C6
O3
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C2
C4
C3

Fig. 2