Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chloridobis((*E*)-2-{(*Z*)-[(4-hydroxyphenyl)(oxido)methylene]hydrazono}propanoato)bismuth(III) pentahydrate

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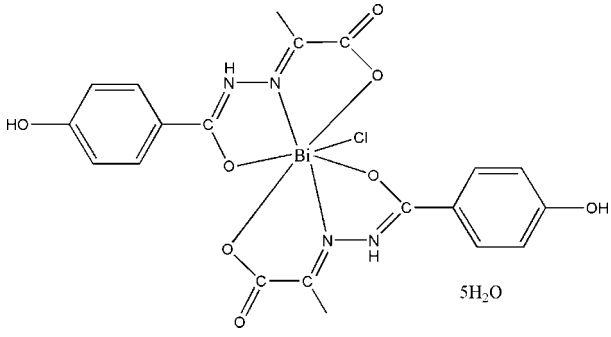
Received 9 November 2007; accepted 15 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; disorder in solvent or counterion; R factor = 0.041; wR factor = 0.106; data-to-parameter ratio = 13.1.

The asymmetric unit of the title complex, $[Bi(C_{10}H_9N_2O_4)_2Cl]\cdot5H_2O$, contains the Bi^{III} complex and five solvent water molecules. The Bi atom is chelated by four O atoms and two N atoms of two (*E*)-2-{(*Z*)-[(4-hydroxyphenyl)oxidomethylene]hydrazono}propanoate ligands. A chloride anion completes the coordination environment, with the seven-coordinate Bi atom adopting a distorted capped octahedral geometry. The molecules are connected by extensive O—H···O hydrogen-bonding interactions involving the solvent water molecules into a two-dimensional supramolecular network. One water molecule is disordered over two sites with almost equal occupancy factors.

Related literature

For a related structure, see: Hong *et al.* (2005)



Experimental

Crystal data

$[Bi(C_{10}H_9N_2O_4)_2Cl]\cdot5H_2O$
M_r = 776.89
Monoclinic, $P2_1/c$
a = 10.2622 (10) Å
b = 29.432 (3) Å
c = 9.6869 (11) Å
β = 114.331 (2)°
V = 2665.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.79 mm^{-1}
T = 298 (2) K
0.59 × 0.18 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.108, T_{max} = 0.550
(expected range = 0.100–0.507)
12001 measured reflections
4682 independent reflections
3743 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
S = 1.01
4682 reflections
358 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.01 e Å^{-3}
$\Delta\rho_{min}$ = −2.68 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O13′—H13G···O12^{i}	0.85	2.21	3.052 (18)	170
O13′—H13F···Cl1^{ii}	0.85	2.15	2.991 (16)	172
O13—H13D···O7^{ii}	0.85	2.40	3.24 (2)	169
O12—H12B···O12^{iii}	0.85	2.17	3.01 (3)	173
O12—H12A···O11	0.85	1.81	2.656 (15)	176
O11—H11B···Cl1^{iv}	0.85	2.40	3.241 (9)	173
O11—H11A···O9	0.85	1.94	2.785 (12)	172
O10—H10B···Cl1^{v}	0.85	2.74	3.505 (6)	150
O10—H10A···O2^{v}	0.85	2.53	3.326 (8)	156
O10—H10A···O1^{v}	0.85	2.00	2.749 (7)	147
O9—H9B···O2^{v}	0.85	2.19	3.013 (9)	163
O9—H9A···O6	0.85	2.15	2.979 (10)	163
O8—H8···O12^{vi}	0.82	1.88	2.688 (14)	170
O4—H4A···O10^{vii}	0.82	1.84	2.651 (8)	172
N4—H4···O13′^{i}	0.86	2.54	3.39 (2)	173
N2—H2···O5^{viii}	0.86	2.29	3.029 (8)	145

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1, y, z$; (iii) $-x+1, -y, -z+2$; (iv) $x+1, y, z+1$; (v) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (vi) $-x, -y, -z+2$; (vii) $x, y, z+1$; (viii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

We acknowledge the financial support of the Shandong Province Science Foundation and the State Key Laboratory of Crystalline Materials, Shandong University, People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2427).

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  doi:10.1107/S1600536807059740

supplementary materials

Acta Cryst. (2007). E**63**, m3066 [**doi:10.1107/S1600536807059740**]

Chloridobis((*E*)-2-{(*Z*)-[(4-hydroxyphenyl)(oxido)methylene]hydrazono}propanoato)bismuth(III) pentahydrate

J. Zhai, H. Yin, F. Li and D. Wang

Comment

In the title complex, (I), the Bi(III) atom exists in a distorted capped octahedral coordination environment in which two tridentate pyruvic acid 4-hydroxybenzoylhydrazone ligands and a chloride anion coordinate to each Bi(III) center. Atoms O1, O7 lie in axial positions, with the axial angleO1—Bi1—O7 147.87 (19)°, deviating substantially from the linear value of 180° and atoms N1, N3, O3, Cl1 in the equatorial plane. The remaining O5 atom caps the N1/N3/O3 face of this octahedron, giving a highly distorted capped octahedral coordination geometry.

The water molecules play a significant role in the crystal packing linking the complex molecules by O—H···O hydrogen bonds to form a two-dimensional supramolecular network.

Experimental

Pyruvic acid 4-hydroxybenzoylhydrazone (1 mmol) were added to acetone(20 ml) and then bismuth trichloride (0.5 mmol) was added. The reaction mixture was stirred for 6 h at room temperature and then filtered. Orange crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol/dichloromethane (1:1 *v*/*v*) solution over a period of two weeks (yield 90%. m.p. 450k). Anal. Calcd (%) for $C_{20}H_{28}N_4O_{13}ClBi$ (Mr = 776.89): C, 30.92; H, 3.63; N, 7.21. Found (%): C, 31.06; H, 3.52; N, 7.34.

Refinement

One of the water molecules is disordered over two positions with occupancies that refined to 0.486 (11) for O13, H13D and H13E, and 0.514 (11) for O13', H13F and H13G. All H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å, O—H = 0.82–0.85 Å, and treated as riding on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C, O) or 1.5 U_{eq}(C) for the methyl group.

Figures

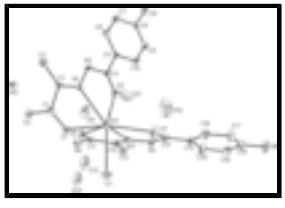

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

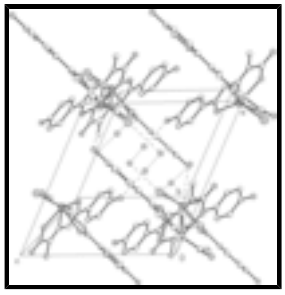

Fig. 2. Crystal packing of (I),showing a two-dimensional supramolecular network, linked by O—H···O hydrogen bonds (dashed lines). H atoms have been omitted for clarity.

Chloridobis((*E*)-2-{(*Z*)-[(4- hydroxyphenyl)(oxido)methylene]hydrazono}propanoato)bismuth(III) pentahydrate

Crystal data

$[Bi(C_{10}H_9N_2O_4)_2Cl]\cdot 5H_2O$	F_{000} = 1520
M_r = 776.89	D_x = 1.936 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5343 reflections
a = 10.2622 (10) Å	θ = 2.3–28.1º
b = 29.432 (3) Å	μ = 6.79 mm^{-1}
c = 9.6869 (11) Å	T = 298 (2) K
β = 114.331 (2)º	Block, orange
V = 2665.9 (5) Å^3	0.59 × 0.18 × 0.10 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	4682 independent reflections
Radiation source: fine-focus sealed tube	3743 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→8
T_{min} = 0.108, T_{max} = 0.550	k = −35→32
12001 measured reflections	l = −11→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H-atom parameters constrained
$wR(F^2)$ = 0.106	$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 4.9896P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001

4682 reflections	$\Delta\rho_{max}$ = 2.01 e Å^{-3}
358 parameters	$\Delta\rho_{min}$ = −2.67 e Å^{-3}
7 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Bi1	−0.04673 (3)	0.168890 (9)	0.47561 (3)	0.02567 (12)	
Cl1	−0.1881 (2)	0.11864 (8)	0.2294 (3)	0.0477 (6)	
N1	0.0589 (6)	0.2481 (2)	0.5622 (6)	0.0223 (13)	
N2	0.1561 (6)	0.25210 (19)	0.7095 (6)	0.0243 (14)	
H2	0.1803	0.2780	0.7539	0.029*	
N3	0.1003 (7)	0.0968 (2)	0.5409 (7)	0.0272 (14)	
N4	0.0703 (7)	0.0622 (2)	0.6195 (8)	0.0343 (16)	
H4	0.1233	0.0384	0.6481	0.041*	
O1	−0.1202 (5)	0.22702 (16)	0.2883 (6)	0.0286 (12)	
O2	−0.1310 (6)	0.29888 (17)	0.2168 (6)	0.0358 (13)	
O3	0.1708 (6)	0.17552 (16)	0.7129 (6)	0.0356 (14)	
O4	0.6275 (6)	0.20384 (18)	1.3799 (6)	0.0372 (13)	
H4A	0.6593	0.2290	1.4137	0.056*	
O5	0.1261 (6)	0.16861 (17)	0.3936 (6)	0.0315 (12)	
O6	0.3224 (6)	0.1396 (2)	0.3877 (7)	0.0466 (16)	
O7	−0.1204 (7)	0.10203 (19)	0.6070 (8)	0.0528 (18)	
O8	−0.2118 (8)	−0.0677 (2)	0.9533 (8)	0.065 (2)	
H8	−0.2786	−0.0587	0.9717	0.098*	
O9	0.6106 (8)	0.1415 (2)	0.6445 (10)	0.078 (2)	
H9A	0.5349	0.1456	0.5645	0.093*	
H9B	0.6725	0.1611	0.6473	0.093*	
O10	0.7055 (6)	0.2870 (2)	0.4876 (6)	0.0465 (15)	
H10A	0.7551	0.2719	0.5668	0.056*	
H10B	0.7108	0.3148	0.5128	0.056*	
O11	0.5671 (10)	0.1060 (3)	0.8888 (10)	0.111 (3)	
H11A	0.5883	0.1176	0.8203	0.133*	
H11B	0.6360	0.1107	0.9743	0.133*	
O12	0.4145 (15)	0.0433 (5)	0.9531 (14)	0.177 (6)	
H12A	0.4649	0.0638	0.9372	0.212*	
H12B	0.4665	0.0199	0.9872	0.212*	
O13	0.569 (2)	0.0642 (7)	0.378 (2)	0.118 (5)	0.486 (11)
H13D	0.6457	0.0747	0.4468	0.141*	0.486 (11)
H13E	0.5854	0.0381	0.3506	0.141*	0.486 (11)
O13'	0.7088 (18)	0.0292 (6)	0.2920 (19)	0.118 (5)	0.514 (11)
H13F	0.7368	0.0536	0.2657	0.141*	0.514 (11)
H13G	0.6791	0.0111	0.2172	0.141*	0.514 (11)
C1	−0.0913 (8)	0.2690 (2)	0.3151 (8)	0.0265 (17)	
C2	0.0044 (8)	0.2826 (3)	0.4759 (8)	0.0238 (16)	
C3	0.0291 (9)	0.3312 (2)	0.5176 (9)	0.037 (2)	

H3A	−0.0345	0.3408	0.5621	0.056*
H3B	0.0114	0.3490	0.4285	0.056*
H3C	0.1263	0.3355	0.5891	0.056*
C4	0.2126 (8)	0.2119 (2)	0.7816 (8)	0.0252 (16)
C5	0.3226 (8)	0.2133 (2)	0.9364 (8)	0.0255 (16)
C6	0.3894 (8)	0.2529 (3)	1.0144 (9)	0.0294 (18)
H6	0.3659	0.2810	0.9670	0.035*
C7	0.4894 (8)	0.2496 (3)	1.1610 (9)	0.0352 (19)
H7	0.5327	0.2760	1.2126	0.042*
C8	0.5277 (8)	0.2082 (3)	1.2344 (8)	0.0289 (17)
C9	0.4633 (9)	0.1687 (2)	1.1568 (9)	0.0337 (19)
H9	0.4886	0.1406	1.2047	0.040*
C10	0.3635 (8)	0.1710 (2)	1.0110 (9)	0.0331 (19)
H10	0.3218	0.1445	0.9600	0.040*
C11	0.2214 (8)	0.1369 (3)	0.4249 (8)	0.0314 (18)
C12	0.2063 (8)	0.0953 (3)	0.5075 (9)	0.0295 (17)
C13	0.3157 (10)	0.0584 (3)	0.5435 (12)	0.049 (2)
H13A	0.4053	0.0690	0.6189	0.074*
H13B	0.3275	0.0502	0.4534	0.074*
H13C	0.2846	0.0324	0.5814	0.074*
C14	−0.0469 (9)	0.0674 (3)	0.6499 (9)	0.0328 (19)
C15	−0.0870 (9)	0.0308 (2)	0.7282 (9)	0.0331 (19)
C16	−0.2006 (10)	0.0389 (3)	0.7675 (11)	0.044 (2)
H16	−0.2487	0.0665	0.7424	0.053*
C17	−0.2436 (10)	0.0065 (3)	0.8435 (11)	0.048 (2)
H17	−0.3186	0.0124	0.8710	0.057*
C18	−0.1741 (10)	−0.0347 (3)	0.8779 (10)	0.042 (2)
C19	−0.0620 (10)	−0.0439 (3)	0.8380 (11)	0.046 (2)
H19	−0.0164	−0.0720	0.8601	0.055*
C20	−0.0187 (9)	−0.0110 (3)	0.7651 (11)	0.044 (2)
H20	0.0579	−0.0168	0.7400	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.02656 (17)	0.02425 (17)	0.02060 (17)	−0.00148 (13)	0.00408 (12)	0.00184 (12)
Cl1	0.0423 (12)	0.0460 (13)	0.0384 (13)	−0.0040 (10)	0.0002 (10)	−0.0123 (10)
N1	0.021 (3)	0.022 (3)	0.015 (3)	−0.003 (3)	−0.001 (2)	0.002 (2)
N2	0.028 (3)	0.016 (3)	0.018 (3)	−0.004 (3)	−0.002 (3)	−0.003 (2)
N3	0.033 (3)	0.022 (3)	0.019 (3)	−0.002 (3)	0.003 (3)	0.002 (3)
N4	0.041 (4)	0.022 (3)	0.041 (4)	0.003 (3)	0.018 (3)	0.009 (3)
O1	0.035 (3)	0.015 (3)	0.024 (3)	0.001 (2)	0.000 (2)	0.005 (2)
O2	0.043 (3)	0.029 (3)	0.024 (3)	0.000 (3)	0.002 (3)	0.007 (2)
O3	0.034 (3)	0.023 (3)	0.030 (3)	0.004 (2)	−0.007 (2)	−0.002 (2)
O4	0.040 (3)	0.038 (3)	0.018 (3)	−0.002 (3)	−0.003 (2)	−0.001 (2)
O5	0.031 (3)	0.039 (3)	0.020 (3)	−0.004 (3)	0.006 (2)	0.004 (2)
O6	0.037 (3)	0.052 (4)	0.058 (4)	0.000 (3)	0.027 (3)	0.005 (3)
O7	0.059 (4)	0.035 (4)	0.083 (5)	0.008 (3)	0.048 (4)	0.020 (3)

O8	0.088 (5)	0.039 (4)	0.082 (6)	−0.003 (4)	0.050 (5)	0.022 (4)
O9	0.054 (4)	0.058 (5)	0.112 (7)	0.004 (4)	0.025 (5)	0.029 (5)
O10	0.048 (4)	0.047 (4)	0.029 (3)	−0.007 (3)	0.000 (3)	−0.003 (3)
O11	0.107 (7)	0.160 (10)	0.070 (6)	−0.027 (7)	0.041 (6)	−0.032 (6)
O12	0.219 (10)	0.168 (9)	0.208 (10)	0.014 (7)	0.153 (8)	0.041 (7)
O13	0.104 (10)	0.105 (10)	0.127 (13)	−0.032 (9)	0.031 (9)	0.044 (9)
O13'	0.104 (10)	0.105 (10)	0.127 (13)	−0.032 (9)	0.031 (9)	0.044 (9)
C1	0.022 (4)	0.029 (4)	0.024 (4)	0.007 (3)	0.004 (3)	0.008 (3)
C2	0.022 (3)	0.029 (4)	0.019 (4)	−0.004 (3)	0.007 (3)	−0.001 (3)
C3	0.040 (5)	0.029 (4)	0.035 (5)	0.002 (4)	0.008 (4)	0.000 (4)
C4	0.029 (4)	0.015 (4)	0.028 (4)	0.001 (3)	0.007 (3)	0.002 (3)
C5	0.024 (4)	0.029 (4)	0.017 (4)	0.002 (3)	0.003 (3)	0.000 (3)
C6	0.025 (4)	0.027 (4)	0.028 (4)	0.001 (3)	0.003 (3)	0.000 (3)
C7	0.034 (4)	0.034 (5)	0.029 (5)	−0.006 (4)	0.004 (4)	−0.003 (4)
C8	0.029 (4)	0.036 (4)	0.020 (4)	0.004 (4)	0.008 (3)	0.002 (3)
C9	0.036 (4)	0.024 (4)	0.028 (4)	0.006 (4)	0.000 (4)	0.009 (3)
C10	0.028 (4)	0.025 (4)	0.034 (5)	−0.001 (3)	0.001 (4)	−0.002 (3)
C11	0.029 (4)	0.040 (5)	0.017 (4)	−0.004 (4)	0.001 (3)	−0.007 (3)
C12	0.027 (4)	0.026 (4)	0.032 (5)	−0.004 (3)	0.009 (3)	−0.001 (3)
C13	0.053 (6)	0.033 (5)	0.064 (7)	0.011 (4)	0.026 (5)	0.007 (4)
C14	0.038 (5)	0.022 (4)	0.033 (5)	0.004 (4)	0.010 (4)	0.003 (3)
C15	0.043 (5)	0.016 (4)	0.039 (5)	−0.002 (4)	0.015 (4)	0.002 (3)
C16	0.055 (6)	0.026 (4)	0.053 (6)	0.007 (4)	0.025 (5)	0.010 (4)
C17	0.057 (5)	0.034 (5)	0.068 (7)	0.003 (5)	0.042 (5)	0.010 (5)
C18	0.054 (5)	0.035 (5)	0.036 (5)	−0.003 (4)	0.018 (4)	0.007 (4)
C19	0.061 (6)	0.023 (4)	0.054 (6)	0.005 (4)	0.024 (5)	0.008 (4)
C20	0.046 (5)	0.025 (4)	0.062 (6)	0.004 (4)	0.023 (5)	0.011 (4)

Geometric parameters (Å, °)

Bi1—O5	2.222 (5)	O13'—H13F	0.8501
Bi1—O1	2.379 (5)	O13'—H13G	0.8499
Bi1—O3	2.465 (5)	C1—C2	1.514 (10)
Bi1—N3	2.529 (6)	C2—C3	1.481 (10)
Bi1—N1	2.562 (6)	C3—H3A	0.9600
Bi1—O7	2.619 (5)	C3—H3B	0.9600
Bi1—Cl1	2.670 (2)	C3—H3C	0.9600
N1—C2	1.287 (9)	C4—C5	1.460 (10)
N1—N2	1.368 (8)	C5—C6	1.404 (10)
N2—C4	1.376 (8)	C5—C10	1.411 (10)
N2—H2	0.8600	C6—C7	1.370 (11)
N3—C12	1.257 (9)	C6—H6	0.9300
N3—N4	1.380 (9)	C7—C8	1.384 (11)
N4—C14	1.358 (10)	C7—H7	0.9300
N4—H4	0.8600	C8—C9	1.395 (10)
O1—C1	1.272 (9)	C9—C10	1.362 (11)
O2—C1	1.236 (8)	C9—H9	0.9300
O3—C4	1.239 (8)	C10—H10	0.9300
O4—C8	1.365 (9)	C11—C12	1.505 (11)

O4—H4A	0.8200	C12—C13	1.497 (11)
O5—C11	1.294 (9)	C13—H13A	0.9600
O6—C11	1.232 (9)	C13—H13B	0.9600
O7—C14	1.234 (9)	C13—H13C	0.9600
O8—C18	1.364 (10)	C14—C15	1.470 (11)
O8—H8	0.8200	C15—C20	1.388 (11)
O9—H9A	0.8500	C15—C16	1.389 (12)
O9—H9B	0.8501	C16—C17	1.383 (12)
O10—H10A	0.8500	C16—H16	0.9300
O10—H10B	0.8502	C17—C18	1.376 (12)
O11—H11A	0.8501	C17—H17	0.9300
O11—H11B	0.8500	C18—C19	1.383 (13)
O12—H12A	0.8500	C19—C20	1.377 (12)
O12—H12B	0.8498	C19—H19	0.9300
O13—H13D	0.8501	C20—H20	0.9300
O13—H13E	0.8501		
O5—Bi1—O1	77.22 (18)	H3B—C3—H3C	109.5
O5—Bi1—O3	77.6 (2)	O3—C4—N2	119.3 (7)
O1—Bi1—O3	122.34 (17)	O3—C4—C5	121.7 (6)
O5—Bi1—N3	66.70 (19)	N2—C4—C5	118.9 (6)
O1—Bi1—N3	139.76 (19)	C6—C5—C10	118.6 (7)
O3—Bi1—N3	67.38 (17)	C6—C5—C4	125.1 (7)
O5—Bi1—N1	80.10 (19)	C10—C5—C4	116.3 (6)
O1—Bi1—N1	63.50 (17)	C7—C6—C5	119.4 (7)
O3—Bi1—N1	61.59 (16)	C7—C6—H6	120.3
N3—Bi1—N1	123.59 (19)	C5—C6—H6	120.3
O5—Bi1—O7	127.15 (18)	C6—C7—C8	121.7 (7)
O1—Bi1—O7	147.87 (19)	C6—C7—H7	119.1
O3—Bi1—O7	86.4 (2)	C8—C7—H7	119.1
N3—Bi1—O7	60.64 (19)	O4—C8—C7	123.2 (7)
N1—Bi1—O7	133.8 (2)	O4—C8—C9	117.7 (7)
O5—Bi1—Cl1	84.18 (14)	C7—C8—C9	119.1 (7)
O1—Bi1—Cl1	80.34 (13)	C10—C9—C8	120.2 (7)
O3—Bi1—Cl1	145.78 (13)	C10—C9—H9	119.9
N3—Bi1—Cl1	78.89 (14)	C8—C9—H9	119.9
N1—Bi1—Cl1	142.88 (14)	C9—C10—C5	120.9 (7)
O7—Bi1—Cl1	81.87 (17)	C9—C10—H10	119.5
C2—N1—N2	123.0 (6)	C5—C10—H10	119.5
C2—N1—Bi1	119.5 (5)	O6—C11—O5	122.1 (8)
N2—N1—Bi1	116.6 (4)	O6—C11—C12	119.4 (7)
N1—N2—C4	115.4 (6)	O5—C11—C12	118.5 (7)
N1—N2—H2	122.3	N3—C12—C13	127.6 (7)
C4—N2—H2	122.3	N3—C12—C11	113.5 (7)
C12—N3—N4	122.1 (7)	C13—C12—C11	118.9 (7)
C12—N3—Bi1	117.0 (5)	C12—C13—H13A	109.5
N4—N3—Bi1	120.8 (5)	C12—C13—H13B	109.5
C14—N4—N3	117.0 (6)	H13A—C13—H13B	109.5
C14—N4—H4	121.5	C12—C13—H13C	109.5
N3—N4—H4	121.5	H13A—C13—H13C	109.5

C1—O1—Bi1	124.7 (5)	H13B—C13—H13C	109.5
C4—O3—Bi1	123.3 (4)	O7—C14—N4	119.6 (7)
C8—O4—H4A	109.5	O7—C14—C15	121.0 (7)
C11—O5—Bi1	123.8 (5)	N4—C14—C15	119.3 (7)
C14—O7—Bi1	121.7 (5)	C20—C15—C16	118.2 (7)
C18—O8—H8	109.5	C20—C15—C14	124.3 (7)
H9A—O9—H9B	108.8	C16—C15—C14	117.6 (7)
H10A—O10—H10B	107.6	C17—C16—C15	121.1 (8)
H11A—O11—H11B	108.6	C17—C16—H16	119.5
H12A—O12—H12B	108.3	C15—C16—H16	119.5
H13D—O13—H13E	110.0	C18—C17—C16	119.3 (8)
H13F—O13'—H13G	108.7	C18—C17—H17	120.3
O2—C1—O1	124.0 (7)	C16—C17—H17	120.3
O2—C1—C2	118.2 (7)	O8—C18—C17	121.6 (8)
O1—C1—C2	117.7 (6)	O8—C18—C19	117.5 (8)
N1—C2—C3	127.3 (7)	C17—C18—C19	120.8 (8)
N1—C2—C1	112.6 (6)	C20—C19—C18	119.1 (8)
C3—C2—C1	120.1 (6)	C20—C19—H19	120.5
C2—C3—H3A	109.5	C18—C19—H19	120.5
C2—C3—H3B	109.5	C19—C20—C15	121.5 (8)
H3A—C3—H3B	109.5	C19—C20—H20	119.3
C2—C3—H3C	109.5	C15—C20—H20	119.3
H3A—C3—H3C	109.5		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O13'—H13G···O12^{i}	0.85	2.21	3.052 (18)	170
O13'—H13F···Cl1^{ii}	0.85	2.15	2.991 (16)	172
O13—H13D···O7^{ii}	0.85	2.40	3.24 (2)	169
O12—H12B···O12^{iii}	0.85	2.17	3.01 (3)	173
O12—H12A···O11	0.85	1.81	2.656 (15)	176
O11—H11B···Cl1^{iv}	0.85	2.40	3.241 (9)	173
O11—H11A···O9	0.85	1.94	2.785 (12)	172
O10—H10B···Cl1^{v}	0.85	2.74	3.505 (6)	150
O10—H10A···O2^{v}	0.85	2.53	3.326 (8)	156
O10—H10A···O1^{v}	0.85	2.00	2.749 (7)	147
O9—H9B···O2^{v}	0.85	2.19	3.013 (9)	163
O9—H9A···O6	0.85	2.15	2.979 (10)	163
O8—H8···O12^{vi}	0.82	1.88	2.688 (14)	170
O4—H4A···O10^{vii}	0.82	1.84	2.651 (8)	172
N4—H4···O13'^{i}	0.86	2.54	3.39 (2)	173
N2—H2···O5^{viii}	0.86	2.29	3.029 (8)	145

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

Fig. 1

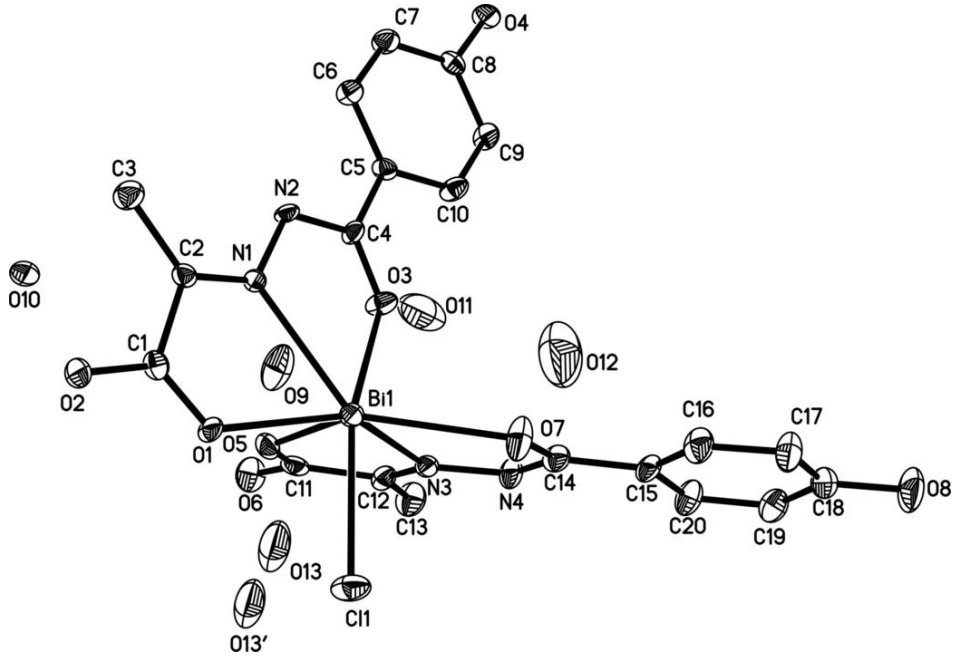
C7
O4
C6
C8
C9
C5
C3
N2
C10
C4
C2
N1
O3
O10
O11
C1
O12
O9
O2
Bi1
C16
C17
O7
O1
O5
C11
N3
C14
O8
O6
C12
N4
C15
C18
C13
C20
C19
O13
Cl1
O13'

Fig. 2