

Bis(5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium) (5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium- κ O)-di- μ -chlorido-heptachlorido-dibismuth(III) monohydrate

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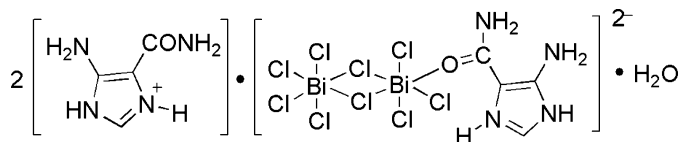
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Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.019$ Å; R factor = 0.075; wR factor = 0.223; data-to-parameter ratio = 15.9.

The title compound, $(\text{C}_4\text{H}_7\text{N}_4\text{O})_2[\text{Bi}_2\text{Cl}_9(\text{C}_4\text{H}_7\text{N}_4\text{O})]\cdot\text{H}_2\text{O}$, was prepared by the reaction of bismuth trichloride and 5-amino-1*H*-imidazole-4-carboxamide in a dilute HCl medium. The asymmetric unit contains two 5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium cations, one edge-shared non-centrosymmetric bioctahedral $[\text{Bi}_2\text{Cl}_9(\text{C}_4\text{H}_7\text{N}_4\text{O})]^{2-}$ dianion and a water molecule. In the dianion, the planar 5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium ligand occupies an equatorial site and is inclined at an angle of $75.7(2)^\circ$ to the $\text{Bi}_2(\mu\text{-Cl})_2$ plane. The salt forms a three-dimensional network arising from hydrogen bonds between cations, anions and water molecules.

Related literature

For general background, see: Turel *et al.* (1998); Goforth *et al.* (2004). For related structures, see: Fu *et al.* (2005); Wu *et al.* (2005); Kyriakidis *et al.*, (1990). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$(\text{C}_4\text{H}_7\text{N}_4\text{O})_2[\text{Bi}_2\text{Cl}_9(\text{C}_4\text{H}_7\text{N}_4\text{O})]\cdot\text{H}_2\text{O}$
 $M_r = 1136.43$

Triclinic, $P\bar{1}$
 $a = 11.3365(5)$ Å
 $b = 12.2486(6)$ Å

$c = 12.7919(6)$ Å
 $\alpha = 74.433(3)^\circ$
 $\beta = 65.939(3)^\circ$
 $\gamma = 75.397(3)^\circ$
 $V = 1541.71(12)$ Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 12.22$ mm⁻¹
 $T = 123(2)$ K
 $0.25 \times 0.22 \times 0.20$ mm

Data collection

Rigaku Mercury diffractometer
 Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\min} = 0.150$, $T_{\max} = 0.194$
 (expected range = 0.067–0.087)

18217 measured reflections
 5695 independent reflections
 4988 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.074$
 $wR(F^2) = 0.223$
 $S = 1.10$
 5695 reflections
 359 parameters
 2 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 5.85$ e Å⁻³
 $\Delta\rho_{\text{min}} = -4.41$ e Å⁻³

Table 1
 Selected bond lengths (Å).

Bi1—O1	2.464 (10)	Bi2—Cl7	2.535 (3)
Bi1—Cl1	2.543 (3)	Bi2—Cl8	2.606 (4)
Bi1—Cl2	2.589 (4)	Bi2—Cl6	2.676 (4)
Bi1—Cl3	2.601 (4)	Bi2—Cl9	2.725 (4)
Bi1—Cl4	2.872 (4)	Bi2—Cl5	2.859 (4)
Bi1—Cl5	2.921 (4)	Bi2—Cl4	2.928 (4)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4C \cdots Cl8 ⁱ	0.82 (12)	2.44 (14)	3.215 (11)	158 (16)
O4—H4D \cdots Cl1	0.83 (12)	2.38 (13)	3.190 (12)	168 (17)
N1—H1 \cdots Cl6 ⁱⁱ	0.88	2.36	3.226 (12)	169
N2—H2 \cdots Cl9 ⁱⁱⁱ	0.88	2.30	3.166 (11)	170
N3—H3A \cdots O1	0.88	2.33	2.869 (17)	120
N3—H3A \cdots Cl1	0.88	2.82	3.649 (15)	157
N3—H3B \cdots Cl8 ^{iv}	0.88	2.71	3.451 (14)	142
N5—H5 \cdots O4 ^v	0.88	1.87	2.725 (16)	163
N6—H6 \cdots Cl3 ^{vi}	0.88	2.40	3.230 (12)	158
N7—H7A \cdots Cl5 ^{vi}	0.88	2.53	3.358 (16)	156
N7—H7B \cdots O2	0.88	2.24	2.802 (18)	121
N8—H8A \cdots O2 ^v	0.88	1.96	2.821 (15)	166
N8—H8B \cdots O4 ^v	0.88	2.04	2.905 (18)	168
N9—H9 \cdots Cl2	0.88	2.63	3.348 (13)	140
N10—H10 \cdots Cl4 ^{vii}	0.88	2.37	3.249 (12)	175
N11—H11A \cdots O3	0.88	2.30	2.850 (18)	120
N11—H11A \cdots Cl5 ^{vi}	0.88	2.83	3.426 (14)	127
N11—H11B \cdots Cl2	0.88	2.70	3.447 (15)	143
N12—H12A \cdots Cl9 ^{viii}	0.88	2.45	3.315 (13)	168
N12—H12B \cdots Cl4 ^{vii}	0.88	2.65	3.529 (15)	177

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

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSO, 2004); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2573).

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supplementary materials

Acta Cryst. (2008). E64, m643-m644 [doi:10.1107/S1600536808009367]

Bis(5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium) (5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium- κ O)-di- μ -chlorido-heptachlorido-dibismuth(III) monohydrate

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Comment

Bismuth trihalides have an extensive coordination chemistry as a result of the Lewis acidity of the group 15 element centre. Recently, there is increasing interest in halobismuthate(III) compounds, due to their anti-ulcer activity (Turel *et al.*, 1998) and their unique optical and electronic properties, including nonlinear optical activity, luminescence and semiconductivity (Goforth *et al.*, 2004). We report here the crystal structure of the title organic-inorganic hybrid complex.

The asymmetric unit of the title compound contains two 5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium ($C_4H_7N_4O^+$) cations, an edge-shared bi-octahedral dianion $\{[Bi_2Cl_9(C_4H_7N_4O)]^{2-}\}$ and a water molecule. The dianion of the title compound is non-centrosymmetric compared to large number of centrosymmetric decachlorobismuthates that have been crystallographically verified, as exemplified by $(C_5H_{14}N_2)_2[Bi_2Cl_{10}].2H_2O$ (Fu *et al.*, 2005) and $(C_4H_{12}N_2)_2[Bi_2Cl_{10}].3H_2O$ (Wu *et al.*, 2005). A search of the Cambridge Structural Database (Version 5.29, January 2008; Allen, 2002) yielded no hits for noncentrosymmetric octachlorobismuthates.

In the noncentrosymmetric edge-shared bi-octahedral dianion, the planar 5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium ligand occupied a octahedral terminal site, inclined at angle of 75.7 (2)° to the $Bi_2(\mu-C1)_2$ plane. Atoms C11, C12, C14, C15, C17, C18, Bi1 and Bi2 are coplaner, with an r.m.s. deviation of 0.120 Å. The Bi—O distance of 2.464 (10) Å is slightly longer compared to the reported value of 2.424 (10) Å (Kyriakidis *et al.*, 1990). The Bi—Cl distances (Table 1) lie in the range 2.535 (3) Å–2.928 (4) Å, with the Bi—C1 distances involving the bridging C1 atoms being longer (2.859 (4) Å–2.928 (4) Å). None of the interbond angles deviate significantly (>10°) from idealized octahedral angles.

The N—H \cdots O, N—H \cdots Cl and O—H \cdots Cl hydrogen bonds (Table 2) link the constituent ions and water molecules into a three-dimensional network (Fig.2).

Experimental

The title compound was prepared by the reaction of bismuth trichloride (0.500 g, 1.59 mmol) and 5-amino-4-carboxamide-1*H*-imidazole (0.601, 4.9 mmol) in a hydrochloric acid medium. Yellow crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution of the title compound at room temperature.

Refinement

Water H atoms were located in a difference map and their positional parameters were refined with a O-H distance restraint of 0.85 (3) Å. All other H atoms were placed at calculated positions (N-H = 0.88 Å and C-H = 0.95 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C,N,O)$. The highest residual density peak is located 0.89 Å from atom Bi1 and the deepest hole is located 0.77 Å from atom Bi2.

Figures

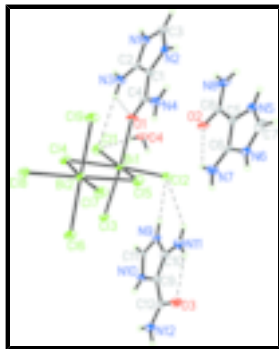


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 40% probability level.

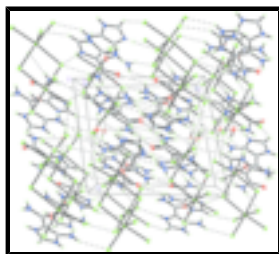


Fig. 2. The crystal packing of the title compound, viewed approximately down the *c* axis. Dashed lines indicate intermolecular hydrogen bonds.

Bis(5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium)(5-amino-4-aminocarbonyl-1*H*-imidazol-3-ium- κ O)-di- μ -chlorido-heptachlorido-dibismuth(III) monohydrate

Crystal data

(C₄H₇N₄O)₂[Bi₂Cl₉(C₄H₇N₄O)]·H₂O

M_r = 1136.43

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

a = 11.3365 (5) Å

b = 12.2486 (6) Å

c = 12.7919 (6) Å

α = 74.433 (3)°

β = 65.939 (3)°

γ = 75.397 (3)°

V = 1541.71 (12) Å³

Z = 2

*F*₀₀₀ = 1060

D_x = 2.448 Mg m⁻³

Mo *K* α radiation

λ = 0.71073 Å

Cell parameters from 5695 reflections

θ = 1.8–25.5°

μ = 12.22 mm⁻¹

T = 123 (2) K

Block, yellow

0.25 × 0.22 × 0.20 mm

Data collection

Rigaku Mercury
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 7.31 pixels mm⁻¹

T = 123(2) K

ω scans

5695 independent reflections

4988 reflections with *I* > 2 σ (*I*)

*R*_{int} = 0.063

θ_{\max} = 25.5°

θ_{\min} = 1.8°

h = -13→13

Absorption correction: multi-scan (Jacobson, 1998) $k = -14 \rightarrow 12$
 $T_{\min} = 0.150$, $T_{\max} = 0.194$ $l = -15 \rightarrow 15$
 18217 measured reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
 Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.075$ H atoms treated by a mixture of independent and constrained refinement
 $wR(F^2) = 0.223$ $w = 1/[\sigma^2(F_o^2) + (0.1568P)^2 + 11.6845P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.10$ $(\Delta/\sigma)_{\max} = 0.001$
 5695 reflections $\Delta\rho_{\max} = 5.85 \text{ e } \text{\AA}^{-3}$
 359 parameters $\Delta\rho_{\min} = -4.41 \text{ e } \text{\AA}^{-3}$
 2 restraints Extinction correction: SHELXL97 (Sheldrick, 2008),
 $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Primary atom site location: structure-invariant direct methods Extinction coefficient: 0.0044 (6)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Bi1	0.88808 (4)	0.20130 (4)	0.77380 (4)	0.0190 (2)
Bi2	1.29373 (4)	0.22332 (4)	0.68713 (4)	0.0197 (2)
Cl1	0.7650 (4)	0.0403 (3)	0.9119 (3)	0.0322 (8)
Cl2	0.6905 (4)	0.3183 (3)	0.7184 (3)	0.0327 (8)
Cl3	0.9668 (4)	0.0975 (3)	0.5986 (3)	0.0260 (8)
Cl4	1.1107 (4)	0.0608 (3)	0.8230 (3)	0.0279 (8)
Cl5	1.0678 (4)	0.3675 (3)	0.6497 (3)	0.0351 (9)
Cl6	1.3711 (4)	0.1462 (3)	0.4887 (3)	0.0303 (8)
Cl7	1.4310 (4)	0.3802 (3)	0.5692 (3)	0.0310 (8)
Cl8	1.4877 (4)	0.0783 (3)	0.7303 (3)	0.0297 (8)
Cl9	1.2315 (4)	0.3140 (3)	0.8792 (3)	0.0332 (9)

supplementary materials

O1	0.8130 (11)	0.2826 (10)	0.9511 (9)	0.032 (2)
O2	0.6215 (10)	0.5277 (8)	0.8614 (8)	0.028 (2)
O3	0.9864 (12)	0.3596 (10)	0.1801 (10)	0.037 (3)
O4	0.4595 (11)	0.1325 (10)	0.9725 (9)	0.036 (2)
H4C	0.448 (17)	0.134 (15)	0.913 (9)	0.043*
H4D	0.535 (6)	0.100 (14)	0.965 (16)	0.043*
N1	0.5550 (11)	0.3189 (10)	1.2864 (10)	0.023 (2)
H1	0.5002	0.2801	1.3472	0.027*
N2	0.6655 (10)	0.4515 (9)	1.1772 (9)	0.021 (2)
H2	0.6968	0.5165	1.1522	0.025*
N3	0.6306 (14)	0.1787 (11)	1.1651 (12)	0.030 (3)
H3A	0.6824	0.1572	1.0986	0.036*
H3B	0.5778	0.1332	1.2196	0.036*
N4	0.8721 (12)	0.4479 (11)	0.9441 (11)	0.032 (3)
H4A	0.9323	0.4469	0.8739	0.038*
H4B	0.8592	0.5043	0.9799	0.038*
N5	0.7091 (11)	0.8051 (10)	0.8213 (10)	0.026 (3)
H5	0.6647	0.8364	0.8836	0.031*
N6	0.8406 (12)	0.7822 (10)	0.6487 (10)	0.026 (3)
H6	0.8993	0.7956	0.5778	0.032*
N7	0.8068 (18)	0.5992 (14)	0.6422 (13)	0.049 (4)
H7A	0.8624	0.6028	0.5697	0.059*
H7B	0.7669	0.5390	0.6781	0.059*
N8	0.5411 (11)	0.6387 (11)	1.0021 (10)	0.029 (3)
H8A	0.4925	0.5889	1.0546	0.035*
H8B	0.5414	0.7033	1.0198	0.035*
N9	0.7241 (11)	0.2073 (10)	0.4935 (10)	0.024 (2)
H9	0.6776	0.2215	0.5642	0.029*
N10	0.8048 (11)	0.1235 (10)	0.3465 (10)	0.023 (2)
H10	0.8222	0.0725	0.3029	0.028*
N11	0.8338 (14)	0.3714 (11)	0.4186 (12)	0.036 (3)
H11A	0.8904	0.4112	0.3607	0.043*
H11B	0.7929	0.3944	0.4859	0.043*
N12	0.9985 (13)	0.2033 (12)	0.1141 (11)	0.030 (3)
H12A	1.0563	0.2282	0.0459	0.037*
H12B	0.9727	0.1373	0.1270	0.037*
C1	0.7034 (12)	0.3655 (11)	1.1141 (11)	0.020 (3)
C2	0.6319 (12)	0.2801 (11)	1.1833 (11)	0.019 (3)
C3	0.5752 (16)	0.4227 (14)	1.2810 (13)	0.030 (3)
H3	0.5331	0.4677	1.3402	0.036*
C4	0.7999 (13)	0.3635 (13)	0.9963 (11)	0.025 (3)
C5	0.7001 (12)	0.7001 (11)	0.8102 (12)	0.021 (3)
C6	0.7828 (13)	0.6855 (13)	0.6981 (12)	0.023 (3)
C7	0.7944 (16)	0.8524 (17)	0.7245 (16)	0.036 (4)
H7	0.8190	0.9250	0.7110	0.043*
C8	0.6157 (13)	0.6159 (12)	0.8940 (11)	0.022 (3)
C9	0.8589 (13)	0.2245 (12)	0.3115 (12)	0.022 (3)
C10	0.8098 (13)	0.2759 (12)	0.4041 (12)	0.023 (3)
C11	0.7240 (12)	0.1182 (10)	0.4551 (11)	0.020 (3)

H11	0.6732	0.0589	0.4993	0.024*
C12	0.9513 (13)	0.2642 (12)	0.1958 (12)	0.022 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.0240 (3)	0.0227 (4)	0.0089 (3)	-0.0076 (2)	-0.0030 (2)	-0.0021 (2)
Bi2	0.0241 (3)	0.0198 (4)	0.0132 (3)	-0.0090 (2)	-0.0041 (2)	0.0009 (2)
Cl1	0.0335 (17)	0.0309 (19)	0.0273 (19)	-0.0177 (15)	-0.0048 (15)	0.0037 (15)
Cl2	0.0371 (18)	0.039 (2)	0.0231 (18)	0.0031 (16)	-0.0130 (15)	-0.0127 (15)
Cl3	0.0366 (17)	0.0275 (18)	0.0119 (16)	-0.0086 (14)	-0.0055 (13)	-0.0029 (13)
Cl4	0.0378 (19)	0.0293 (19)	0.0177 (17)	-0.0132 (15)	-0.0102 (14)	0.0013 (14)
Cl5	0.041 (2)	0.031 (2)	0.0256 (19)	-0.0096 (16)	-0.0075 (16)	0.0039 (16)
Cl6	0.047 (2)	0.0273 (19)	0.0214 (18)	-0.0161 (16)	-0.0126 (16)	-0.0019 (15)
Cl7	0.0423 (19)	0.0284 (19)	0.0200 (18)	-0.0222 (15)	-0.0033 (15)	0.0016 (14)
Cl8	0.0342 (17)	0.0319 (19)	0.0198 (17)	-0.0073 (15)	-0.0083 (14)	-0.0003 (14)
Cl9	0.043 (2)	0.035 (2)	0.0185 (18)	-0.0209 (16)	-0.0029 (15)	-0.0004 (15)
O1	0.050 (6)	0.035 (6)	0.012 (5)	-0.008 (5)	-0.008 (5)	-0.012 (4)
O2	0.042 (5)	0.032 (6)	0.013 (5)	-0.018 (4)	-0.008 (4)	-0.003 (4)
O3	0.049 (6)	0.032 (6)	0.022 (6)	-0.011 (5)	-0.004 (5)	-0.002 (5)
O4	0.039 (6)	0.052 (7)	0.018 (5)	-0.015 (5)	-0.004 (5)	-0.014 (5)
N1	0.035 (6)	0.015 (6)	0.014 (6)	-0.007 (5)	-0.004 (5)	0.001 (5)
N2	0.030 (5)	0.017 (6)	0.018 (6)	-0.010 (5)	-0.011 (5)	0.005 (4)
N3	0.048 (8)	0.020 (7)	0.019 (7)	-0.016 (6)	-0.006 (6)	0.003 (5)
N4	0.042 (7)	0.030 (7)	0.019 (6)	-0.020 (6)	-0.001 (5)	0.000 (5)
N5	0.034 (6)	0.025 (6)	0.021 (6)	-0.011 (5)	-0.008 (5)	-0.003 (5)
N6	0.032 (6)	0.024 (7)	0.015 (6)	-0.008 (5)	-0.004 (5)	0.002 (5)
N7	0.074 (11)	0.032 (8)	0.021 (8)	-0.008 (8)	0.003 (7)	-0.007 (6)
N8	0.034 (6)	0.041 (7)	0.016 (6)	-0.024 (6)	-0.007 (5)	0.003 (5)
N9	0.030 (6)	0.024 (6)	0.014 (6)	-0.004 (5)	-0.006 (5)	0.001 (5)
N10	0.031 (6)	0.026 (6)	0.013 (6)	-0.011 (5)	-0.002 (5)	-0.007 (5)
N11	0.053 (8)	0.024 (7)	0.028 (7)	-0.014 (6)	-0.008 (6)	-0.005 (6)
N12	0.033 (6)	0.029 (7)	0.017 (7)	-0.008 (5)	0.001 (5)	0.001 (5)
C1	0.024 (6)	0.017 (6)	0.012 (6)	0.001 (5)	-0.003 (5)	-0.002 (5)
C2	0.024 (6)	0.021 (7)	0.012 (6)	-0.002 (5)	-0.009 (5)	-0.001 (5)
C3	0.047 (9)	0.027 (8)	0.014 (7)	-0.006 (7)	-0.008 (6)	-0.006 (6)
C4	0.031 (7)	0.037 (8)	0.008 (6)	-0.013 (6)	-0.007 (5)	0.001 (6)
C5	0.023 (6)	0.018 (7)	0.017 (7)	-0.002 (5)	-0.009 (5)	0.003 (5)
C6	0.024 (6)	0.023 (7)	0.013 (7)	0.001 (5)	-0.004 (5)	0.003 (5)
C7	0.029 (8)	0.040 (10)	0.034 (10)	-0.013 (7)	-0.013 (7)	0.009 (8)
C8	0.023 (6)	0.025 (8)	0.011 (6)	0.001 (6)	-0.006 (5)	0.003 (6)
C9	0.027 (6)	0.021 (7)	0.016 (7)	-0.003 (5)	-0.009 (6)	0.001 (6)
C10	0.027 (6)	0.027 (7)	0.016 (7)	-0.010 (6)	-0.010 (6)	0.001 (6)
C11	0.031 (6)	0.007 (6)	0.013 (6)	0.000 (5)	0.000 (5)	-0.001 (5)
C12	0.024 (6)	0.024 (7)	0.015 (7)	-0.009 (5)	-0.007 (5)	0.003 (6)

Geometric parameters (\AA , $^\circ$)

Bi1—O1	2.464 (10)	N5—H5	0.88
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supplementary materials

Bi1—C11	2.543 (3)	N6—C7	1.33 (2)
Bi1—C12	2.589 (4)	N6—C6	1.372 (19)
Bi1—C13	2.601 (4)	N6—H6	0.88
Bi1—C14	2.872 (4)	N7—C6	1.34 (2)
Bi1—C15	2.921 (4)	N7—H7A	0.88
Bi2—C17	2.535 (3)	N7—H7B	0.88
Bi2—C18	2.606 (4)	N8—C8	1.356 (18)
Bi2—C16	2.676 (4)	N8—H8A	0.88
Bi2—C19	2.725 (4)	N8—H8B	0.88
Bi2—C15	2.859 (4)	N9—C11	1.312 (17)
Bi2—C14	2.928 (4)	N9—C10	1.395 (17)
O1—C4	1.226 (18)	N9—H9	0.88
O2—C8	1.237 (17)	N10—C11	1.311 (16)
O3—C12	1.267 (18)	N10—C9	1.403 (18)
O4—H4C	0.82 (12)	N10—H10	0.88
O4—H4D	0.83 (12)	N11—C10	1.340 (19)
N1—C3	1.33 (2)	N11—H11A	0.88
N1—C2	1.383 (18)	N11—H11B	0.88
N1—H1	0.88	N12—C12	1.30 (2)
N2—C3	1.326 (19)	N12—H12A	0.88
N2—C1	1.375 (17)	N12—H12B	0.88
N2—H2	0.88	C1—C2	1.371 (18)
N3—C2	1.328 (19)	C1—C4	1.459 (18)
N3—H3A	0.88	C3—H3	0.95
N3—H3B	0.88	C5—C6	1.39 (2)
N4—C4	1.340 (18)	C5—C8	1.482 (19)
N4—H4A	0.88	C7—H7	0.95
N4—H4B	0.88	C9—C10	1.34 (2)
N5—C7	1.31 (2)	C9—C12	1.459 (19)
N5—C5	1.364 (18)	C11—H11	0.95
O1—Bi1—C11	83.9 (3)	C6—N7—H7B	120.0
O1—Bi1—C12	92.6 (3)	H7A—N7—H7B	120.0
C11—Bi1—C12	94.34 (13)	C8—N8—H8A	120.0
O1—Bi1—C13	174.9 (3)	C8—N8—H8B	120.0
C11—Bi1—C13	91.66 (12)	H8A—N8—H8B	120.0
C12—Bi1—C13	90.18 (12)	C11—N9—C10	108.9 (11)
O1—Bi1—C14	91.6 (3)	C11—N9—H9	125.5
C11—Bi1—C14	84.94 (12)	C10—N9—H9	125.5
C12—Bi1—C14	175.67 (11)	C11—N10—C9	108.3 (11)
C13—Bi1—C14	85.58 (11)	C11—N10—H10	125.9
O1—Bi1—C15	89.9 (3)	C9—N10—H10	125.9
C11—Bi1—C15	166.27 (13)	C10—N11—H11A	120.0
C12—Bi1—C15	98.13 (12)	C10—N11—H11B	120.0
C13—Bi1—C15	94.01 (12)	H11A—N11—H11B	120.0
C14—Bi1—C15	83.05 (11)	C12—N12—H12A	120.0
C17—Bi2—C18	93.94 (13)	C12—N12—H12B	120.0
C17—Bi2—C16	86.98 (12)	H12A—N12—H12B	120.0
C18—Bi2—C16	87.69 (12)	C2—C1—N2	106.6 (11)
C17—Bi2—C19	88.05 (12)	C2—C1—C4	125.7 (12)

C18—Bi2—C19	91.62 (12)	N2—C1—C4	127.6 (12)
C16—Bi2—C19	174.93 (11)	N3—C2—C1	131.4 (13)
C17—Bi2—C15	90.85 (13)	N3—C2—N1	123.2 (12)
C18—Bi2—C15	175.20 (11)	C1—C2—N1	105.4 (12)
C16—Bi2—C15	92.26 (12)	N2—C3—N1	106.9 (13)
C19—Bi2—C15	88.84 (13)	N2—C3—H3	126.6
C17—Bi2—C14	173.86 (12)	N1—C3—H3	126.6
C18—Bi2—C14	92.07 (11)	O1—C4—N4	123.2 (13)
C16—Bi2—C14	94.49 (11)	O1—C4—C1	118.0 (12)
C19—Bi2—C14	90.55 (11)	N4—C4—C1	118.8 (13)
C15—Bi2—C14	83.14 (11)	N5—C5—C6	106.7 (12)
Bi1—C14—Bi2	96.60 (11)	N5—C5—C8	129.6 (13)
Bi2—C15—Bi1	97.04 (12)	C6—C5—C8	123.6 (13)
C4—O1—Bi1	149.3 (9)	N7—C6—N6	123.7 (13)
H4C—O4—H4D	108 (19)	N7—C6—C5	130.7 (14)
C3—N1—C2	110.8 (12)	N6—C6—C5	105.5 (13)
C3—N1—H1	124.6	N5—C7—N6	109.0 (16)
C2—N1—H1	124.6	N5—C7—H7	125.5
C3—N2—C1	110.4 (12)	N6—C7—H7	125.5
C3—N2—H2	124.8	O2—C8—N8	124.5 (13)
C1—N2—H2	124.8	O2—C8—C5	117.4 (12)
C2—N3—H3A	120.0	N8—C8—C5	118.0 (13)
C2—N3—H3B	120.0	C10—C9—N10	106.9 (12)
H3A—N3—H3B	120.0	C10—C9—C12	127.4 (13)
C4—N4—H4A	120.0	N10—C9—C12	125.8 (13)
C4—N4—H4B	120.0	N11—C10—C9	130.9 (13)
H4A—N4—H4B	120.0	N11—C10—N9	122.7 (13)
C7—N5—C5	109.4 (14)	C9—C10—N9	106.4 (12)
C7—N5—H5	125.3	N10—C11—N9	109.5 (12)
C5—N5—H5	125.3	N10—C11—H11	125.3
C7—N6—C6	109.3 (13)	N9—C11—H11	125.3
C7—N6—H6	125.3	O3—C12—N12	121.6 (13)
C6—N6—H6	125.3	O3—C12—C9	116.4 (13)
C6—N7—H7A	120.0	N12—C12—C9	121.9 (13)
O1—Bi1—C14—Bi2	-92.7 (3)	C2—C1—C4—O1	5(2)
C11—Bi1—C14—Bi2	-176.40 (12)	N2—C1—C4—O1	-174.4 (13)
C13—Bi1—C14—Bi2	91.54 (12)	C2—C1—C4—N4	-173.0 (13)
C15—Bi1—C14—Bi2	-3.06 (9)	N2—C1—C4—N4	7(2)
C18—Bi2—C14—Bi1	-176.47 (11)	C7—N5—C5—C6	-1.8 (16)
C16—Bi2—C14—Bi1	-88.62 (12)	C7—N5—C5—C8	-178.5 (13)
C19—Bi2—C14—Bi1	91.89 (12)	C7—N6—C6—N7	178.3 (15)
C15—Bi2—C14—Bi1	3.12 (10)	C7—N6—C6—C5	-1.2 (15)
C17—Bi2—C15—Bi1	178.20 (12)	N5—C5—C6—N7	-177.7 (16)
C16—Bi2—C15—Bi1	91.18 (12)	C8—C5—C6—N7	-1(2)
C19—Bi2—C15—Bi1	-93.77 (12)	N5—C5—C6—N6	1.8 (14)
C14—Bi2—C15—Bi1	-3.07 (10)	C8—C5—C6—N6	178.7 (11)
O1—Bi1—C15—Bi2	94.8 (3)	C5—N5—C7—N6	1.0 (17)
C11—Bi1—C15—Bi2	32.2 (6)	C6—N6—C7—N5	0.2 (17)
C12—Bi1—C15—Bi2	-172.67 (11)	N5—C5—C8—O2	177.0 (13)

supplementary materials

C13—Bi1—C15—Bi2	-81.91 (13)	C6—C5—C8—O2	0.9 (19)
C14—Bi1—C15—Bi2	3.13 (10)	N5—C5—C8—N8	-5(2)
C11—Bi1—O1—C4	-170 (2)	C6—C5—C8—N8	178.5 (12)
C12—Bi1—O1—C4	-75.7 (19)	C11—N10—C9—C10	1.7 (15)
C14—Bi1—O1—C4	105.4 (19)	C11—N10—C9—C12	-178.5 (12)
C15—Bi1—O1—C4	22.4 (19)	N10—C9—C10—N11	176.9 (15)
C3—N2—C1—C2	0.2 (15)	C12—C9—C10—N11	-3(2)
C3—N2—C1—C4	179.9 (13)	N10—C9—C10—N9	-1.4 (14)
N2—C1—C2—N3	-179.8 (14)	C12—C9—C10—N9	178.8 (12)
C4—C1—C2—N3	1(2)	C11—N9—C10—N11	-177.8 (13)
N2—C1—C2—N1	-0.8 (13)	C11—N9—C10—C9	0.7 (14)
C4—C1—C2—N1	179.5 (12)	C9—N10—C11—N9	-1.3 (15)
C3—N1—C2—N3	-179.8 (13)	C10—N9—C11—N10	0.4 (15)
C3—N1—C2—C1	1.2 (15)	C10—C9—C12—O3	-2(2)
C1—N2—C3—N1	0.5 (16)	N10—C9—C12—O3	178.1 (13)
C2—N1—C3—N2	-1.0 (17)	C10—C9—C12—N12	175.8 (14)
Bi1—O1—C4—N4	-22 (3)	N10—C9—C12—N12	-4(2)
Bi1—O1—C4—C1	160.0 (14)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O4—H4C...C18 ⁱ	0.82 (12)	2.44 (14)	3.215 (11)	158 (16)
O4—H4D...C11	0.83 (12)	2.38 (13)	3.190 (12)	168 (17)
N1—H1...C16 ⁱⁱ	0.88	2.36	3.226 (12)	169
N2—H2...C19 ⁱⁱⁱ	0.88	2.30	3.166 (11)	170
N3—H3A...O1	0.88	2.33	2.869 (17)	120
N3—H3A...C11	0.88	2.82	3.649 (15)	157
N3—H3B...C18 ^{iv}	0.88	2.71	3.451 (14)	142
N5—H5...O4 ^v	0.88	1.87	2.725 (16)	163
N6—H6...C13 ^{vi}	0.88	2.40	3.230 (12)	158
N7—H7A...C15 ^{vi}	0.88	2.53	3.358 (16)	156
N7—H7B...O2	0.88	2.24	2.802 (18)	121
N8—H8A...O2 ^v	0.88	1.96	2.821 (15)	166
N8—H8B...O4 ^v	0.88	2.04	2.905 (18)	168
N9—H9...C12	0.88	2.63	3.348 (13)	140
N10—H10...C14 ^{vii}	0.88	2.37	3.249 (12)	175
N11—H11A...O3	0.88	2.30	2.850 (18)	120
N11—H11A...C15 ^{vi}	0.88	2.83	3.426 (14)	127
N11—H11B...C12	0.88	2.70	3.447 (15)	143
N12—H12A...C19 ^{viii}	0.88	2.45	3.315 (13)	168
N12—H12B...C14 ^{vii}	0.88	2.65	3.529 (15)	177

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

Fig. 1

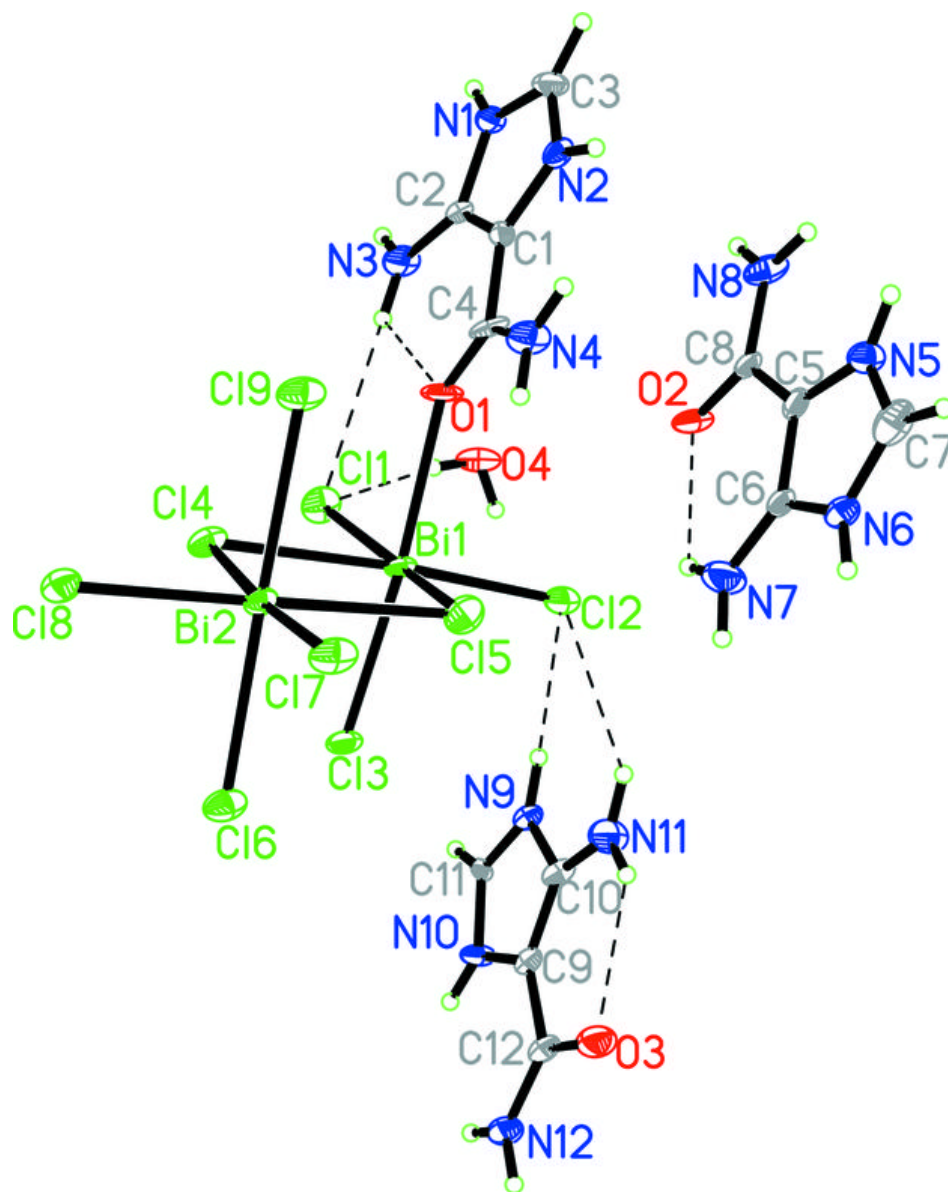


Fig. 2

